Abstracts
of the
Fifth International Conference on
Sensitivity Analysis of Model Output

SAMO 2007

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Eötvös University (ELTE), Budapest, Hungary

Program

Monday, 18 June	Tuesday, 19 June	Wednesday, 20 June	Thursday, 21 June	Friday, 22 June
	8:50 Opening			
	9:00 Andres	9:00 Young	9:00 Saltelli	9:00 Crestaux
	9:45 Cacuci	9:45 Kucherenko	9:45 Ratto	9:30 Borgonovo
			10:15 Liu	10:00 Pujol
	10:30 Coffee Break	10:30 Coffee Break	10:45 Coffee Break	10:30 Coffee Break
	11:00 Marrel	11:00 Ratto	11:15 Xu	11:00 Iooss
	11:30 Liu	11:30 Gauchi	11:45 Shahsavani	11:30 Lüdtke
	12:00 Tarantola	12:00 Bolado	12:15 Busby	12:00 Closing
	12:30 Lunch	12:30 Lunch	12:45 Lunch	12:10 End of the conference
	14:00 Frenklach	14:00 Rabitz	14:00 Briand	
	14:45 Kell	14:45 Tomlin	14:30 Wilkins	
			15:00 Yue	
	15:30 Coffee Break	15:30 Poster session	15:30 Coffee Break	
	16:00 Turányi	16:30 Koda	16:00 Zsély	
	16:30 Carrasco	17:00 Hall	16:30 Ziehn	
	17:00 Benson	17:30 Hermans	17:00 End of the session	
18:00 Registration & Welcome	17:30 End of the session	18:00 End of the session	Conference dinner	

Web site: **http://samo2007.chem.elte.hu/**

Invited lectures

(in alphabetical order of the first author)

Terry Andres (University of Manitoba, Canada)
Syllabus for a graduate course in sensitivity analysis

Dan Gabriel Cacuci (Nuclear Energy Division, Commissariat a l'Energie Atomique, France and Institute for Nuclear Technology and Reactor Safety, University of Karlsruhe, Germany)
Data assimilation and best-estimate model validation activities in Euratom-fission programs

M. Frenklach, T. Russi, R. Feeley, A. Packard (University of California, Berkeley, USA)
System Analysis and Sensitivity using Data Collaboration

Douglas B. Kell (Manchester Interdisciplinary Biocentre, UK)
Sensitivity and information theoretic analyses of biochemical networks

Sergei Kucherenko (Imperial College London, UK)
Application of global sensitivity indices for measuring the effectiveness of Quasi-Monte Carlo Methods and parameter estimation.

Herschel Rabitz (Princeton University, USA)
Controlling and understanding chemical-physical phenomena with sensitivity analysis

Alison S. Tomlin (The University of Leeds, UK)
The use of global methods in the evaluation of non linear chemical kinetic models

Peter C. Young (Centre for Research on Environmental Systems and Statistics, Lancaster, UK), M. Ratto
From dominant mode analysis to dynamical meta-modeling

Oral presentations

(in alphabetical order of the first author)

J. Benson, N. Dixon, T. Ziehn and A.S. Tomlin THE SENSITIVITY OF A 3D STREET CANYON CFD MODEL TO UNCERTAINTIES IN INPUT PARAMETERS.

E. Borgonovo, S. Tarantola MOMENT-INDEPENDENT GLOBAL SENSITIVITY ANALYSIS WITH CORRELATED INPUT FACTORS: AN APPLICATION TO A CHEMICAL REACTOR

B. Briand, C. Mercat-Rommens, G. Ducharme USING CLASSIFICATION TREES TECHNIQUES LIKE SENSITIVITY ANALYSIS IN THE FIELD OF RADIOECOLOGY

D. Busby, M. Feraille SEQUENTIAL EXPERIMENTAL DESIGN FOR STATISTICAL ANALYSIS OF NONLINEAR OUTPUTS OF COMPUTER MODELS

N. Carrasco, E. Hébrard, M. Dobrijevic, P. Pernot UNCERTAINTY ANALYSIS IN A TITAN IONOSPHERIC CHEMISTRY MODEL

W. Castaings, S. Tarantola, R. Bolado, A. Pagano, M. Ratto ESTIMATION OF THE CONTRIBUTION TO THE MEAN AND VARIANCE USING RANDOM SAMPLES

Th. Crestaux, J.M. Martinez, O. Le Maître POLYNOMIAL CHAOS EXPANSIONS FOR UNCERTAINTIES QUANTIFICATION AND SENSITIVITY ANALYSIS

D. Gatelli, S. Kucherenko, A. Pagano, M. Ratto, S. Tarantola CALCULATING FIRST ORDER SENSITIVITY MEASURES: A BENCHMARK OF SOME RECENT METHODOLOGIES

J.-P. Gauchi A NEW APPROACH TO SENSITIVITY ANALYSIS BASED ON PLS REGRESSION

J.W.Hall, R.K.S. Hankin, P. Bates BAYESIAN CALIBRATION OF A FLOOD INUNDATION MODEL

E. Hermans, F. Van den Bossche, G. Wets IMPACT OF METHODOLOGICAL CHOICES ON ROAD SAFETY RANKING

B. Iooss, M. Ribatet GLOBAL SENSITIVITY ANALYSIS OF COMPUTER MODELS WITH FUNCTIONAL INPUTS

M. Koda, T. Takabatake, T. Akana SENSITIVITY EXPERIMENTS ON ONE-CLASS SUPPORT VECTOR MACHINE

Q. Liu, T. Homma A ROBUST IMPORTANCE MEASURE FOR SENSITIVITY ANALYSIS

Q. Liu, T. Homma THE INDICATION OF THE MOMENT INDEPENDENT MEASURE AND ITS NEW CALCULATIONAL METHOD

N. Lüdtke, S. Panzeri, M. Brown, D.S. Broomhead, J. Knowles, M.A. Montemurro, D.B. Kell AN INFORMATION-THEORETIC FRAMEWORK FOR GLOBAL SENSITIVITY ANALYSIS

A. Marrel, B. Iooss, O. Roustant ANALYTICAL CALCULATIONS OF SOBOL INDICES FOR THE GAUSSIAN PROCESS METAMODEL

A. Pagano, M. Ratto AN EXTENDED USE OF THE SOBOL ESTIMATOR

G. Pujol, B. Corre SIMPLEX SCREENING

M. Ratto, A. Pagano, P.C. Young ESTIMATION OF CONDITIONAL EXPECTATIONS AND CONDITIONAL VARIANCES WITH STATE-DEPENDENT PARAMETER META-MODELS

A. Saltelli, F. Campolongo, J. Cariboni ACCELERATING FACTORS SCREENING

D. Shahsavani, A. Grimvall EXTRACTING COMPLEX NONLINEAR RESPONSE SURFACES FROM DETERMINISTIC MODELS WITH MULTIPLE INPUTS

T. Turányi, A. Lovrics, A. Csikász-Nagy, I. Gy. Zsély, J. Zádor, B Novák ANALYSIS OF A BUDDING YEAST CELL CYCLE MODEL USING THE SHAPES OF LOCAL SENSITIVITY FUNCTIONS

A. K. Wilkins, B. Tidor, J. White, P. I. Barton PHASE SENSITIVITY ANALYSIS OF LIMIT CYCLE OSCILLATORS

H. Yue, M. Brown, J. Jia, D.B. Kell SENSITIVITY ANALYSIS AND EXPERIMENTAL DESIGN OF A STIFF SIGNAL TRANSDUCTION PATHWAY

C. Xu, G.Z. Gertner A GENERAL FIRST-ORDER GLOBAL SENSITIVITY ANALYSIS METHOD

T. Ziehn, A. S.Tomlin A GLOBAL SENSITIVITY STUDY OF SULPHUR CHEMISTRY IN A PREMIXED METHANE FLAME MODEL USING HDMR

I. Gy. Zsély, J. Zádor, T. Turányi UNCERTAINTY ANALYSIS OF NITROGEN OXIDE FORMATION IN METHANE COMBUSTION

Posters

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I.A. Bashkirtseva, L. B. Ryashko, P.V. Stikhin SCALAR AND GEOMETRICAL DESCRIPTION OF 3D-CYCLE STOCHASTIC SENSITIVITY

V. Bertsch, M. Treitz, J. Geldermann, O. Rentz MULTIDIMENSIONAL SENSITIVITY ANALYSIS FOR MULTI-ATTRIBUTE DECISION MAKING UNDER PREFERENTIAL UNCERTAINTY

N. Bilal, D. E. Adams OPTIMIZATION OF COMPRESSOR VALVE DESIGN FOR MINIZIMATION OF GAS PULSATIONS USING UNCERTAINTY ANALYSIS

N. Carrasco, E. Hébrard, M. Dobrijevic, R. Thissen, O. Dutuit, M. Banaszkiewicz, P. Pernot EFFECTS OF INPUT CORRELATIONS IN A COMPLEX CHEMISTRY MODEL

N. Carrasco, P. Pernot TOWARDS A REDUCTION OF A TITAN IONOSPHERIC CHEMISTRY MODEL

W. Castaings, S. Tarantola PARTIAL DERIVATIVES AND SINGULAR VALUE DECOMPOSITION FOR THE ANALYSIS AND CONTROL OF TIME-DEPENDENT SPATIALLY DISTRIBUTED SYSTEMS

E. Chojnacki, J. Baccou, S. Destercke NUMERICAL SENSITIVITY AND EFFICIENCY IN THE TREATMENT OF EPISTEMIC AND ALEATORY UNCERTAINTY

S. Da-Veiga, F. Gamboa EFFICIENT ESTIMATION OF FIRST-ORDER SENSITIVITY INDICES

D. Delgado, C.M. Rocco S. A SENSITIVITY BASED APPROACH FOR DETERMINING THE EXTREME PROFITS AND LOSS CONTRIBUTION INDEX

E. D. Diaz, C. M. Rocco S. MERGING IMPORTANCE MEASURES USING AN ORDERED WEIGHTED AVERAGING BASED FRAMEWORK

O. Eriksson VARIANCE-BASED SENSITIVITY ANALYSIS IN UNBALANCED FACTORIAL DESIGNS

M. Flechsig, U. Böhm, T. Nocke, C. Rachimow SIMENV - A FLEXIBLE FRAMEWORK FOR SENSITIVITY AND UNCERTAINTY ANALYSES OF LARGE-VOLUME MODEL OUTPUT

I. Ghergut, H. Behrens, T. Licha, M. Sauter TRACER BTC SENSITIVITY W. R. TO FRACTURE - MATRIX PARAMETERS IN SINGLE-WELL PUSH-PULL TESTS WITH CHANGING HYDRAULIC REGIME

G. Giuliani, F. Pintaldi USE OF SENSITIVITY ANALYSIS TO IMPUTE DATA ON WAGE AND SALARY

M.A. Gómez-Villegas, P. Maín, R. Susi SOME ASPECTS OF SENSITIVITY IN GAUSSIAN BAYESIAN NETWORKS

E. Hagel THE ARPEGE/ALADIN LIMITED AREA ENSEMBLE PREDICTION SYSTEM: SENSITIVITY EXPERIMENTS USING GLOBAL SINGULAR VECTORS

S. Han, K. Wolf, O. Munz DESIGN OPTIMIZATION AND RELIABILITY ASSESSMENT OF PASSIVE AND ACTIVE STRUCTURAL SYSTEMS VIA SENSITIVITY ANALYSIS

D. Hou, Z. Toth A STOCHASTIC PERTURBATION SCHEME TO REPRESENT MODEL RELATED ERRORS IN NUMERICAL ATMOSPHERIC FORECASTS

H. Jarar Oulidi, L. Benaabidate THE USE OF G.I.S. AND P.C.A. FOR MAPPING PRECIPITATIONS IN ARID AREA: CASE OF ZIZ ET RHERIS WATERSHEDS, MOROCCO

Z. Kala SENSITIVITY ANALYSIS OF STEEL STRUCTURES WITH IMPERFECTIONS

Z. Kala, A. Omishore SENSITIVITY ANALYSIS OF FATIGUE CRACK PROPAGATION

Á. Kramarics, I. Gy. Zsély, T. Turányi REDUCTION OF A GAS-PHASE REACTION MECHANISM DEVELOPED FOR THE ANODE CHANNELS OF SOLID-OXIDE FUEL CELLS

B. Krzykacz-Hausmann The principal variance-based sensitivity indices can be estimated without assuming independence between the input variables

M. Lamboni , H. Monod, D. Makowski GLOBAL SENSITIVITY ANALYSIS FOR SIMULATION MODELS WITH MULTIPLE OUTPUTS: AN APPLICATION TO A DYNAMIC CROP MODEL

R. Landri, G. Ducharme, R. Bonnard ENTROPY-BASED SENSITIVITY ANALYSIS IN HEALTH RISK ASSESSMENT

A. Lovrics, H.M. Byrne, O.E. Jensen, L. Buttery, J.R. King MATHEMATICAL MODELLING OF MESENCHYMAL STEM CELL PROLIFERATION AND DIFFERENTIATION

P. Main, H. Navarro ANALYZING THE EFFECT OF INTRODUCING A KURTOSIS PARAMETER IN GAUSSIAN BAYESIAN NETWORKS

E. Marchand, F. Clément, J. Roberts DETERMINISTIC SENSITIVITY ANALYSIS FOR A MODEL FOR FLOW AND TRANSPORT IN POROUS MEDIA

K.Marimuthu, N.Murugan APPLICATION OF SENSITIVITY ANALYSIS IN OPTIMIZATION OF BEAD GEOMETRY OF PTA HARDFACED VALVE SEAT RINGS

E.C. Meuter CONSTRUCT: A FRAMEWORK FOR CONCEPTUALLY STRUCTURING A MODEL

C. L. Müller, G. Paul, I. F. Sbalzarini SENSITIVITIES FOR FREE: CMA-ES BASED SENSITIVITY ANALYSIS

A. Nemes, W.J. Rawls, Ya.A. Pachepsky, M.Th. van Genuchten SENSITIVITY ANALYSIS OF THE K-NEAREST NEIGHBOR TECHNIQUE TO ESTIMATE SOIL WATER RETENTION

R. Neslo, S. Tarantola, R. Cooke Stakeholder Preference with Probabilistic Inversion: Application to Competitiveness Indices

I. Pál, A. Csikász-Nagy, I. Gy. Zsély, J. Zádor, T. Turányi, B. Novák MONTE CARLO ANALYSIS OF A GENERIC CELL CYCLE MODEL

M. Petelet, O. Asserin, B. Iooss THE USE OF GLOBAL SENSITIVITY ANALYSIS METHOD IN WELDING SIMULATION

S. Pütz, J.M. Paruelo, G.E. Weber, F Jeltsch, V. Grimm, T. Wiegand COPING WITH ECOLOGICAL COMPLEXITY: HIERARCHICAL MULT-CRITERIAL, INDIRECT PATTERN ORIENTED MODEL PARAMETERIZATION

J.K. Ravalico, H.R. Maier, G.C. Dandy A NEW METHOD OF SENSITIVITY ANALYSIS FOR INTEGRATED ASSESSMENT MODELLING

G.M. Richter, M. Acutis, P. Trevisiol, K. Latiri, R. Confalonieri SENSITIVITY ANALYSIS APPLIED TO A COMPLEX CROP MODEL FOR DURUM WHEAT IN THE MEDITERRANEAN

M.F. Rivera, C. Fallico, S. Troisi UNCERTAINTY AND SENSITIVITY ANALYSIS FOR PEDOTRANSFER FUNCTIONS

M.J. Rufo, C.J. Pérez, J. Martín LOCAL SENSITIVITY ANALYSIS FOR BAYESIAN MIXTURE MODELS

C. J. Sallaberry, J.C. Helton, S. C. Hora EXTENSION OF LATIN HYPERCUBE SAMPLES WITH CORRELATED VARIABLES

H. Sulieman, P.J. McLellan PARAMETRIC SENSITIVITY ANALYSIS OF NONLINEAR MULTIPARMETER REGRESSION MODEL SYSTEMS

J. Tóth SENSITIVITY RATIOS: EXACT RESULTS

Cs. Vincze, I. Gy. Zsély, D. Szinyei, R. Mészáros, I. Lagzi UNCERTAINTY ANALYSIS OF AN OZONE DEPOSITION MODEL

Y. Wang, R. Zou, A. Ghosh A SENSITIVITY ANALYSIS BASED HYBRID ALGORITHM FOR PARAMETER DETERMINATION IN STIFF BIOCHEMICAL PATHWAYS

ORAL PRESENTATIONS

SYLLABUS FOR A GRADUATE COURSE IN SENSITIVITY ANALYSIS

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Sensitivity analysis (SA) is the scientific development of a simple empirical model for the output variation of a complex system. It uses experimentation and statistical analysis of results to generate simple models (e.g., sensitivity coefficients, regression equations or response surfaces).

Unlike undergraduates, grad students encounter complex systems. SA is the tool they need to understand them. A graduate course in SA can have a wide appeal to students in science, engineering, and business. The professor should be able to accommodate students with diverse backgrounds.

Typically "complex system" means a simulation model with many input parameters. To set up an analysis, the student must learn to assess parameter uncertainties/ranges, design sets of experiments, compute parameter sets from experimental designs, and record inputs and outputs to be analyzed. A student needs to know how to use several statistical procedures.

Practitioners may combine several of these steps in a package like SimLab [1], and so such tools should be demonstrated. Pedagogically, it is more effective to teach students how to use a spreadsheet package (e.g., Microsoft Excel [2]) for SA, so that the student can examine and modify each step in the SA procedure, without knowing a particular programming language.

The scope of the course beyond the preliminaries should include discussion of:
- sampling designs (random, one-at-a-time, fractional factorial, latin hypercube, quasirandom …);
- regression analysis (correlations, linear regression, interpretation of standard results);
- analysis of variance (in fractional factorial results, using Sobol' and total sensitivities);
- transformations (log, power, rank);
- plotting results (scatterplots, contour plots, histograms and frequency polygons).

Student activities for credit should include:
- reading about a published SA technique, and presenting it in class (research, presentation skills);
- implementing a published SA technique (technical proficiency, application of theory to practice);
- carrying out a case study (mastery of skill set).

A good reference book has been [3], and a new textbook is under development.

The overall goal of the course should be that the graduate student knows when and how to apply basic SA techniques, and where to find additional resources for more challenging projects.

References

[1] SIMLAB Documentation, Version 3.0.8. http://simlab.jrc.it/docs/html/index.html.
[2] Microsoft Office Excel 2007 product guide. http://office.microsoft.com/search/redir.aspx?AssetID=XT101662581033&CTT=5&Origin=HA101680001033.
[3] Saltelli A, Chan K, Scott ME: Sensitivity Analysis. John Wiley & Sons Ltd., Toronto, 2000.

DATA ASSIMILATION AND BEST-ESTIMATE MODEL VALIDATION ACTIVITIES IN EURATOM-FISSION PROGRAMS

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As is well known, a physical system and/or the result of an indirect experimental measurement are characterized by independent variables, dependent variables, and relationships between these quantities. Such relationships can be modelled mathematically in terms of: (a) linear and/or nonlinear equations that relate the system's independent variables and parameters to the system's state (i.e., dependent) variables; (b) inequality and/or equality constraints that delimit the ranges of the system's parameters; and (c) one or several quantities, customarily referred to as system responses (or objective functions, or indices of performance, or results of indirect measurements), which are to be analyzed as the parameters vary over their respective ranges. Mathematical models also include parameters whose actual values are not known precisely, but may vary within some ranges that reflect our incomplete knowledge or uncertainty regarding them. Furthermore, the methods needed to solve various equations numerically introduce themselves (numerical) errors. The effects of such errors and/or parameter variations must be quantified in order to assess the respective model's range of validity. Moreover, the effects of uncertainties in the model's parameters on the uncertainty in the computed results must also be quantified. Generally speaking, the objective of sensitivity analysis is to quantify the effects of parameter variations on computed results. Terms such as influence, ranking by importance and dominance, are all related to sensitivity analysis. On the other hand, the objective of uncertainty analysis is to assess the effects of parameter uncertainties on the uncertainties in computed results. Sensitivity and uncertainty analyses can be considered as formal methods for evaluating data and models because they are associated with the computation of specific quantitative measures that allow, in particular, assessment of variability in output variables and importance of input variables (see, e.g., Refs [1] and [2], and references therein).

Models of complex physical systems usually involve two distinct sources of uncertainties, namely: (i) stochastic uncertainty, which arises because the system under investigation can behave in many different ways, and (ii) subjective or epistemic uncertainty, which arises from the inability to specify an exact value for a parameter that is assumed to have a constant value in the respective investigation. Epistemic (or subjective) uncertainties characterize a degree of belief regarding the location of the appropriate value of each parameter. In turn, these subjective uncertainties lead to subjective uncertainties for the response, thus reflecting a corresponding degree of belief regarding the location of the appropriate response values as the outcome of analyzing the model under consideration. A typical example of a complex system that involves both stochastic and epistemic uncertainties is a nuclear power reactor plant: in a typical risk analysis of a nuclear power plant, stochastic uncertainty arises due to the many hypothetical accident scenarios which are considered in the respective risk analysis, while epistemic uncertainties arise because of the many uncertain parameters that underlie the estimation of the probabilities and consequences of the respective hypothetical accident scenarios.

Sensitivity and uncertainty analysis procedures can be either local or global in scope. The objective of local analysis is to analyze the behaviour of the system response locally around a chosen point or trajectory in the combined phase space of parameters and state variables. On the other hand, the objective of global analysis is to determine all of the system's critical points (bifurcations, turning points, response maxima, minima, and/or saddle points) in the combined phase space formed by the parameters and dependent (state) variables, and subsequently analyze these critical points by local sensitivity and uncertainty analysis. The methods for sensitivity and uncertainty analysis are based on either deterministic or statistical procedures. In principle, both types of procedures can be used for either local or for global sensitivity and uncertainty analysis, although, in practice, deterministic methods are used mostly for local analysis while statistical methods are used for both local and global analysis.

Most of methods currently used in the nuclear industry and technical safety organizations can be roughly decomposed in four sequential steps. The end-status of each step determines if the next step is performed or not. The first step is devoted to analyzing the code's applicability and identifying uncertain parameters and important phenomena of the transient scenario under consideration. On this basis, the code's predictive capability is verified against the model's inventory, the model's origin and background. Finally, one identifies the output variables (i.e., results) of interest for post-processing. The second step is devoted to reviewing the correlations that involve the uncertain parameters, and identifying the parameter that are potentially significant for the physical phenomena observed during the transient scenario under consideration. This (second) step thus corresponds to a "sensitivity analysis". In the third step, experimental uncertainties of the initial and boundary conditions and expert judgment (supported, when available by the "code qualification test-experiment matrix")

are employed to obtain uncertainty bands and subjective probability density functions for the uncertain parameters. In the fourth step, the various uncertainties are combined probabilistically via "response surface methods" in order to derive "uncertainties" for the results of interest. Examining carefully all of these steps clearly reveals that a significant amount of conservatism remains embedded even in the "best-estimate" codes, and that the "code validation and qualification" processes are not yet entirely objective. In particular, it seems necessary to incorporate concepts of data adjustment and assimilation [3] into the construction, validation and qualification of best-estimate simulation tools.

The development of software modules for validation and verification of simulation programs, including global sensitivity and uncertainty analysis, is a generic issue of fundamental importance for the safe operation of all types of reactors, while allowing reductions in design margins. Numerical simulations comprise transversal activities common to all types of reactors, and also include specific issues concerning specific types of reactor systems. Besides performing specific experiments and developing specific simulation models, essential activities are "code verification" ("is the code solving the mathematical model correctly?"), "code validation" ("does the model represent reality?"), and "code qualification" (certifying that a proposed simulation/design methodology/system satisfies all performance and safety specifications). Code validation and qualification (V&Q) can be attained only by selected benchmarking, taking into account systematically (i.e., using sensitivities) all sources of uncertainties (computational, experimental, etc.). The validation and qualification of numerical simulations against experiments requires the inclusion of methods of sensitivity and uncertainty analysis together with data assimilation in the presence of both computational and experimental uncertainties.

The development of standardized validated and qualified tools for numerical simulations is a key activity within the EURATOM-Fission Programs. This paper will highlight the activities and methods regarding sensitivity and uncertainty analysis, and best-estimate validated simulation code systems planned within the FP-6 EURATOM Coordination Action "Sustainable Nuclear Fission Technology Platform" (SNF-TP). The SNF-TP [4] proposes research structures and programs for developing a coherent European strategy for: (i) improving the performance of currently operating (Generation II) and future near-term (Generation III and III+) Light Water Reactors (LWR) while maintaining a high degree of safety, performing studies regarding the feasibility of novel designs, and establishing a unified approach of LWR life time extension; (ii) establishing a sustainable, closed fuel cycle for electricity production using innovative (Generation IV) fast neutron reactor systems in conjunction with partitioning and transmutation (P&T) technologies; (iii) establishing a commercially viable High Temperature Reactor (V/HTR) for process heat and hydrogen production; (iv) assuring adequate training to preserve and enhance the human competence in the nuclear field, and maintaining/renewing the infrastructure necessary for achieving sustainability of nuclear energy; and (v) implementing a Strategic Research Agenda for conceiving and coordinating the European research and development in nuclear science and technology.

References

[1] D.G. Cacuci, *Sensitivity and Uncertainty Analysis: Theory*, **Volume 1**, Chapman & Hall/CRC, Boca Raton, 2003.
[2] D.G. Cacuci, M. Ionescu-Bujor, and M.I. Navon, *Sensitivity and Uncertainty Analysis: Applications to Large Scale Systems*, **Volume 2**, Chapman & Hall/CRC, Boca Raton, 2005.
[3] D.G. Cacuci, M.I. Navon, and M. Ionescu-Bujor, *Computational Methods for Data Analysis and Assimilation*, Chapman & Hall/CRC, Boca Raton, 2007.
[4] "Sustainable Nuclear Fission Technology Platform (SNF-TP)", EURATOM Contract Nr. FP6-036410, July 2006, European Commission, Brussels.

ANALYTICAL CALCULATIONS OF SOBOL INDICES FOR THE GAUSSIAN PROCESS METAMODEL

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Introduction

This paper deals with the analytical formulations for the Gaussian process model of the first order Sobol indices $S_i = \mathrm{Var}[\mathrm{E}(Y|X_i)]/\mathrm{Var}(Y)$ (1) where X=(X_1,…, X_d) and Y is the model input and output variables. The Gaussian process model (Sacks et al. [3]), also called kriging, is often used as a metamodel to approximate complex and expensive computer codes. Because of their lower computational cost, metamodels are useful in uncertainty, sensitivity and optimisation studies, which require a large number of function evaluations. The estimation of one Sobol index is usually done by sampling adequately the input parameters space via Monte Carlo or other algorithms, which can require thousands model evaluations (Saltelli et al. [4]). In these algorithms, the full model (computer code) can be directly replaced by a metamodel. Some recent works have addressed the possibility to take advantage of the known analytical formula of some metamodels to derive analytical expressions of Sobol indices: Chen et al. [1] which use tensor-product formulation and Oakley and O'Hagan [2] which consider the Bayesian formalism of Gaussian processes. Our work proposes to develop the analytical formulation of Sobol indices for the Gaussian process model viewed as a global stochastic model and not as a simple predictor (as in Chen et al. [1]). On a simple example, comparisons are made between the Sobol indices based on the predictor and those based on the global model, in terms of the metamodel predictivity.

The Gaussian process model (Gp model)

Gp modeling considers the deterministic computer code output $y_{code}(x)$ as the realization of a random function $Y(x,\omega)$ defined on Ω x R^d, including a regression part and a Gaussian stochastic process $Z(x,\omega)$:

$$Y(x,\omega) = F(x)\beta + Z(x,\omega) \qquad (2)$$

with β a regression parameter vector and $F(x)=[f_0(x),\ldots, f_k(x)]$ a vector of elementary functions. We take $Z(x,\omega)$ centred, second order stationary with variance σ^2 and a generalized exponential correlation function: $\mathrm{Cov}_\Omega(Y(x,\omega),Y(u,\omega)) = \sigma^2 R_{\theta,p}(x,u) = \sigma^2 \prod_{i=1}^{d} \exp\left(-\theta_i |x_i - u_i|^{p_i}\right)$ with $\theta_i>0$ and $0<p_i\leq 2$. Gp model parameters (β, σ^2, θ, p) are estimated by maximum likelihood on a learning sample (X_s, Y_s) made by n simulations of computer code: $X_s=(x^{(1)},\ldots,x^{(n)})$, $Y_s=y_{code}(X_s)$. Conditioning the joint probability distribution by the observed data (X_s, Y_s), the conditional Gaussian process $Y_{Gp/(Xs,\,Ys)}$ is defined on Ω x R^d and characterized by:

$$\begin{aligned} &\mathrm{E}_\Omega\left[Y_{Gp/(Xs,Ys)}(x,\omega)\right] = F(x)\beta + {}^t r_{\theta,p}(x) R_S^{-1}\left[{}^t Y_s - {}^t F_S \beta\right] \\ &\mathrm{Cov}_\Omega\left[Y_{Gp/(Xs,Ys)}(u,\omega), Y_{Gp/(Xs,Ys)}(v,\omega)\right] = \sigma^2\left\{R_{\theta,p}(u,v) + {}^t r_{\theta,p}(u) R_S^{-1} r_{\theta,p}(v)\right\} \end{aligned} \qquad (3)$$

where $r_{\theta,p}(x) = \left[R_{\theta,p}(x^{(1)},x),\ldots,R_{\theta,p}(x^{(n)},x)\right]$, $F_s=F(X_s)$ and R_S is the covariance matrix of X_s. The expression of conditional Gp model mean is used as a predictor and often denoted $\hat{Y}(x)$. The variance expression corresponds to the mean square error of the predictor and gives a local indicator of prediction accuracy. These analytical expressions are important advantages in uncertainty propagation, optimization and sensitivity analysis studies, contrary to other metamodels which give only the predictor. To validate the predictor, we use a test sample, made by new computer code simulations, to estimate the predictive residual sum of squares (PRESS) and its associated predictivity coefficient Q_2 (corresponding to R^2 for prediction points).

Sensitivity analysis

From the expression of conditional Gp model, two approaches to compute Sobol indices are possible:

- only the predictor expression $\hat{Y}(x)$ is used, in other words the mean of Gp process;
- the whole global conditional Gp process $Y_{Gp/(Xs,\,Ys)}$ is used.

The second approach takes into account not only the mean of conditional Gp model but also its covariance structure. In this case, following the Sobol approach (1), we define a new sensitivity measure $\tilde{S}_i$ which is a random variable. Its expectation can be considered as a sensitivity indice (denoted $\mu_{\tilde{S}_i}$) and its variance

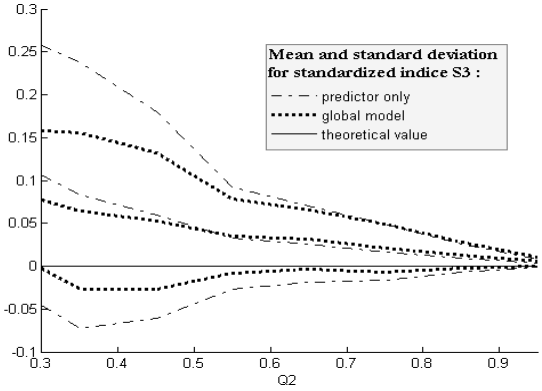
(denoted $\sigma^2_{\tilde{S}_i}$) as an indicator of sensitivity indice accuracy. The two approaches can be defined as follows:

$$\underline{\text{Approach 1}}: \mathrm{S_i} = \mathrm{Var}_{X_i}\mathrm{E}_{X_1,\ldots X_{i-1},X_{i+1},\ldots,X_d}\mathrm{E}_{\Omega}\left[\mathrm{Y}_{\mathrm{Gp/(Xs,Ys)}} / X_i\right] / \mathrm{Var}_{X_1,\ldots,X_d}\ \mathrm{E}_{\Omega}\left[\mathrm{Y}_{\mathrm{Gp/(Xs,Ys)}}\right]$$

$$\underline{\text{Approach 2}}: \begin{cases} \mu_{\tilde{S}_i} = \mathrm{E}_{\Omega}\mathrm{Var}_{X_i}\mathrm{E}_{X_1,\ldots X_{i-1},X_{i+1},\ldots,X_d}\left[\mathrm{Y}_{\mathrm{Gp/(Xs,Ys)}} / X_i\right] / \mathrm{E}_{\Omega}\mathrm{Var}_{X_1,\ldots,X_d}\left[\mathrm{Y}_{\mathrm{Gp/(Xs,Ys)}}\right] \\ \sigma^2_{\tilde{S}_i} = \mathrm{Var}_{\Omega}\mathrm{Var}_{X_i}\mathrm{E}_{X_1,\ldots X_{i-1},X_{i+1},\ldots,X_d}\left[\mathrm{Y}_{\mathrm{Gp/(Xs,Ys)}} / X_i\right] / \mathrm{E}_{\Omega}\mathrm{Var}_{X_1,\ldots,X_d}\left[\mathrm{Y}_{\mathrm{Gp/(Xs,Ys)}}\right] \end{cases} \quad (4)$$

For the two approaches, the analytical formulas above lead to numerical integrals, and more precisely to one-dimensional integrals in the case of independent inputs, which is another advantage of Gp metamodel.

To compare and study the two indices, we consider a simple example based on the Ishigami function $f(X_1, X_2, X_3) = \sin(X_1) + 7\sin^2(X_2) + 0.1X_3^4\sin(X_1)$ where $X_i \sim \mathcal{U}[-\pi\ ;\ \pi\ ]$. The theoretical values of Sobol indices are known: $S_1 = 0.42$, $S_2 = 0.58$ and $S_3 = 0$. To study the convergence of S_i and $\mu_{\tilde{S}_i}$ relatively to the accuracy of Gp modeling represented by the coefficient Q_2, we simulate different learning samples with varying size *n*. For each size *n*, a Latin Hypercube sample is simulated, the Ishigami function is evaluated on the n data points, the conditional Gp model is built on this learning sample and the predictivity coefficient Q_2 is estimated on a new test sample of size 10000. The Sobol indices are computed for the two approaches (4). To observe the results, empirical mean and standard deviation of each indice are computed for same values of Q_2 (or same classes of Q_2). Figure (1) illustrates the convergence of S_3 and $\mu_{\tilde{S}_3}$ and figure (2) shows the convergence of the ratio of S_1 and S_2. Sobol indices computed with the whole model $\mu_{\tilde{S}_i}$ is more robust and less dispersed, particularly for low accuracy values of Gp model ($Q^2 < 0.8$). The convergence to the true value is faster with the whole Gp model. However, for high values of accuracy of Gp model ($Q^2 > 0.9$), the two approaches give the same values and the first one (with only the predictor) remains easier to compute. In all cases, the second approach taking into account the covariance structure is more robust and allows to estimate the uncertainty of the sensitivity coefficient with $\sigma_{\tilde{S}_i}$. It justifies the use of conditional Gp model as metamodel.



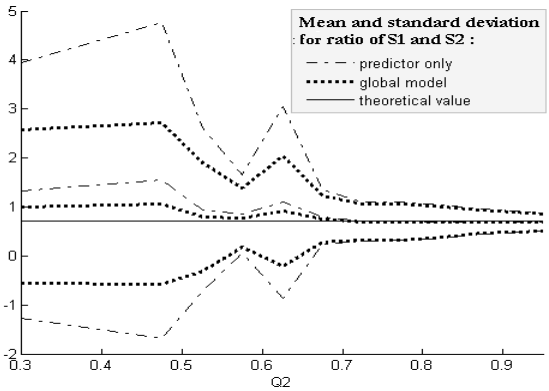


Figure 1: Convergence of Sobol indice S_3 **Figure 2: Convergence of the Sobol indice ratio S_1/S_2**

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A ROBUST IMPORTANCE MEASURE FOR SENSITIVITY ANALYSIS

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1. Introduction

One issue that can not be ignored in risk assessment is the existence of uncertainties of input parameters. Generally the study of the output uncertainty of a model due to the uncertainties of the model input parameters is called uncertainty analysis (UA), while the determination of the input parameter that most influence the model output is the job of sensitivity analysis (SA).

Given a model $Y=g(X)$, where Y is the model output of interest, $X=\{X_1, X_2, \ldots X_n\}$ is the set of input parameters, the traditional way to measure the influence of a input parameter on the output is $S_{xi}=\partial Y/\partial X_i$, which only looks at the importance of a parameter in the neighbourhood of its nominal value.

It shows poor performance when a model is nonlinear and non-monotonic. To take the full range of an input distribution into consideration, Hora & Iman [1] proposed a variance-based measure $Var_{xi}[E(Y|X_i)]$, which represents the expected reduction of output variance due to the ascertaining of parameter X_i. Homma & Saltelli [2] improved Hora & Iman's measure further by proposing two sensitivity indicators $S^1_{xi}=Var_{xi}[E(Y|X_i)]/Var(Y)$, and $S^T_{xi}=E_{x-i}[Var(Y|X_{-i})]/Var(Y)$.

Variance-based measure might not be robust when, for example, dealing with a highly-skewed or fat-tailed distribution [3]. Iman & Hora [3] proposed a bivariate measure $(R_\alpha, R_{1-\alpha})$ to calculate the importance of input parameters, $R_\alpha=Y^*_\alpha/Y_\alpha$, and $R_{1-\alpha}= Y^*_{1-\alpha}/Y_{1-\alpha}$, where Y_α, $Y_{1-\alpha}$ represent the α and $1-\alpha$ quantiles of the unconditional distribution of a model output, Y^*_α and $Y^*_{1-\alpha}$ represent the conditional distribution of this output. Though the pair $(R_\alpha, R_{1-\alpha})$ provides a wider range of information about the change in output distribution due to a change of input variation, it does not sufficiently reflect the characteristics of the whole output distribution [4].

Based on information theory [5], Park & Ahn[4] adopted the discriminator $I(i:o)=\int f_i(x)Ln[f_i(x)/f_o(x)]dx$ to describe the relative impact on the change of the output distribution induced by various distributional changes in the inputs. One criticism of this measure was that the use of data fitting procedures to get the PDFs(Possibility Density Function) $f_i(x)$ and $f_o(x)$might bring about additional uncertainty [6].

In addition, Chun, Han and Pak[6] adopted Minkowski distance, which was originally used to measure the distance between two points, to estimate the difference between two CDFs (Cumulative Distribution Function) of the model output. The 2-norm Minkowski distance normalized with the mean of output distribution for the base case is proposed, which is written as $MD(i:o)=(\int_0^1 [y_p^i - y_p^o]^2)^{1/2} \Big/ E(Y^o)$.

To calculate $I(i:o)$ and $MD(i:o)$, one needs to assume a change of input distribution, such as uncertainty is completely eliminated and so on. Therefore, the importance ranking based on $I(i:o)$ and $MD(i:o)$ are sensitive to the assumed input distributional change.

Suppose no change of the distributions of input parameters, Borgonovo [7] proposed a moment independent measure, $\delta_i = \frac{1}{2} E_{Xi}[s(X_i)]$, which evaluates the influence of the entire input distribution on the entire output distribution. The parameter $s(X_i)=\int|f_Y(y)-f_{Y|Xi}(y)|dy$, measures the difference between the unconditional and conditional PDFs. Further explanation of δ_i can be referred to Liu & Homma(this issue).

Given the current distribution of each input parameter, in this work the authors proposed a new measure, which is different from δ_i, to estimate the influence of input parameters on the model output of interest.

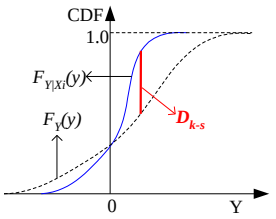

Fig. 1 Difference of $F_1(y)$ and $F_2(y)$ is measured by D_{k-s}.

2. A new sensitivity analysis measure

Let $F_Y(y)$ be the unconditional CDF of the model output Y, and $F_{Y|Xi}(y)$ be the CDF of the output Y when an input parameter X_i is fixed at a value, e.g., x_i^*. In statistical testing, e.g., the Kolmogorov-Smirnov test, we know the difference of two distributions can be measured by the greatest vertical distance of the two curves, $D_{k-s}=sup|F_Y(y)- F_{Y|Xi}(y)|$, as shown in Fig. 1. It has been pointed out that two-sided Kolmogorov-Smirnov test based on D_{k-s} are consistent against all types of differences(e.g. differences between means(or medians), difference in variances) that may exist between two distributions [8]. Intuitively it comes into mind that if the area surrounded by the two curves is adopted to measure the deviation of $F_{Y|Xi}(y)$ from $F_Y(y)$(see Fig. 2), it will be more meaningful than D_{K-S}. This is the origin of this new measure.

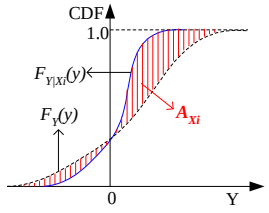

Fig. 2 Deviationg of $F_{Y|Xi}(y)$ from $F_Y(y)$ is measured by A_{Xi}.

The surrounded area A_{Xi} can be calculated as:

$$A_{X_i} = \int |F_Y(y) - F_{Y|X_i}(y)|\, dy \tag{1}$$

Or

$$A_{X_i} = \int_0^1 |Y(\alpha) - Y_{X_i}(\alpha)|\, d\alpha \tag{2}$$

Where $Y(\alpha)$ and $Y_{Xi}(\alpha)$ is the inverse function of $F_Y(y)$ and $F_{Y|Xi}(y)$, respectively.

If there is no interaction between the two curves, i.e., the difference $Y_{Xi}(\alpha)$-$Y(\alpha)$(or $F_Y(y)$-$F_{Y|Xi}(y)$)does not change its sign over the entire range of Y, it is known from Eq.(2) that A_{Xi} measures the absolute value of the difference of the output expectations in the two different conditions, i.e., $A_{Xi}=|E(Y|Xi)-E(Y)|$, this is the indication of A_{Xi} in this case.

One can easily see that the expected deviation of $F_{Y|Xi}(y)$ from $F_Y(y)$ can be calculated with

$$E_{X_i}(A_{X_i}) = \int f_{X_i}(x_i) A_{X_i}(x_i) dx_i = \int f_{X_i}(x_i) [\int_0^1 |Y(\alpha) - Y_{X_i}(\alpha)|\, d\alpha]\, dx_i \tag{3}$$

$E_{Xi}(A_{Xi})$ can therefore be used to measure the influence of the parameter X_i on the output Y. The normalized expression S_{Xi} is employed formally as the sensitivity indicator of X_i.

$$S_{X_i} = \frac{E_{X_i}(A_{X_i})}{E(Y)} \tag{4}$$

Where $E(Y)$ is the expectation of the model output Y given the current distributions of input parameters.

3. Computational method for this measure

For most risk analysis problems, the output distribution can not be preliminarily known. Monte Carlo method is popularly used to obtain the distribution of a model output. To calculate the sensitivity indicator of a given parameter X_i (Suppose the number of samples is

n.), one first generates the output distribution $F_Y(y)$. It can be approximated by the empirical CDF $S_Y^n(y)$, which is easily obtained from Monte Carlo simulation [6].

$$S_Y^n(y) = \sum_{k=1}^{n} T(y > y_k) / n \tag{5}$$

$$T(y > y_k) = \begin{cases} 1, & if \ y > y_k \\ 0, & if \ y \le y_k \end{cases} \tag{6}$$

Where n is the sample size and k is the sample index. The quantiles $Y(\alpha)(\alpha=k/n, k=1,2,\ldots n)$ can easily be obtained from the inverse function of $S_Y^n(y)$.

The expectation of the output Y is then calculated from

$$E(Y) = \sum_{k=1}^{n} y_k / n \tag{7}$$

Now we generate a value $x_i^{(1)}$ for X_i from its distribution. With other input parameters randomly sampled from their distributions, we can get $F_{Y|Xi=xi^{(1)}}(y)$(approximated by $S^n_{Y|Xi=xi^{(1)}}(y)$). Based on Eq.(10), $A_{Xi}(x_i^{(1)})$can be obtained. We then generate another value $x_i^{(2)}$ for X_i, get $F_{Y|Xi=xi^{(2)}}(y)$, and calculate $A_{Xi}(x_i^{(2)})$. Repeating the above procedures for n times in total, finally we can estimate S_{Xi}

$$S_{X_i} = E_{X_i}(A_{X_i}) / E(Y) = [\sum_{k=1}^{n} A_{X_i}(x_i^k) / n] / E(Y) \tag{8}$$

4. Concluding remarks

In this work a new sensitivity measure, S_{Xi}, which considers not only the entire range of input variation, but also the entire range of output distribution, is proposed. Its geometrical meaning is intuitive and physical indication is clear. A Monte Carlo-based computational method is presented to estimate S_{Xi}. It is expected that this measure is robust. Further refinement of the computational method for S_{Xi} and the comparison of S_{Xi} with others measures are in progress.

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CALCULATING FIRST ORDER SENSITIVITY MEASURES: A BENCHMARK OF SOME RECENT METHODOLOGIES

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This work compares some recent techniques to execute sensitivity analysis of model output. We highlight strengths and weaknesses of each technique in terms of efficiency and computational cost, thus enabling the user to choose the more suitable method depending on the computational model analysed.
The paper focuses on three recently developed techniques, which are not yet commonly known in the literature: the State Dependent Parameter modeling (SDP) [1], the Random Balance Designs (RBD) [2], and the formula for estimating small sensitivity indices proposed by Kucherenko and Mauntz [3].

The SDP technique is a full meta-modelling approach, which is based on recursive filtering and smoothing estimation, to estimate the truncated high-dimensional model representation (HDMR) expansion up to the third order. The method is theoretically simple and all measures of interest are computed by means of a single set of model runs. As it can be applied using any kind of Monte Carlo sampling technique (or even using a sample coming from an experiment), the technique is very flexible. As other meta-modelling approaches in the literature ([4, 5] or the Gaussian emulator by Oakley and O'Hagan [6]; see also [7], for a review of smoothing approaches to sensitivity analysis), it is very efficient and allows for a significant reduction in the cost of the analysis. When coupled with low discrepancy sampling methods (e.g. quasi-random sequences), the efficiency of SDP estimates can be optimally exploited.

The RBD procedure combines Satterthwaite's random balance designs [8] with the Fourier Amplitude Sensitivity Test (FAST) (see [9]). Contrarily to FAST, in RBD the input space is explored by using one single frequency: this has the advantage to make the computational cost independent from the number of input factors. Therefore RBD remains significantly cheap even for models with several parameters. Furthermore, the method is easy to implement and handy to use.

The approach of Kucherenko and Mauntz is a variant of the method of Sobol'. The approach yields more accurate estimation formulas with a lower computational cost. Improved formulas are based on the extended version of Sobol' presented in [10]. All comparison studies show a significant improvement in the accuracy for improved formulas especially in the case of small sensitivity indices.

The benchmark will be carried out on two test models. The first one is the Oakley and O'Hagan analytic function; it is composed of 15 input factors, of which five are very influential on the output variance, five are relatively influential and the remaining five are almost non influential [6].

The second test case is the Level E model. The model predicts the radiological dose to humans over geological time scales due to the underground migration of radionuclides from a nuclear waste disposal site through a system of natural and engineered barriers. We consider 12 independent uncertain parameters that can influence the radiological dose predictions. The core of the model is a set of partial differential equations which describe the nuclide migration in the geosphere. The model is time dependent: the simulated time frame ranges from $2 \cdot 10^4$ to $9 \cdot 10^6$ years. Of the 12 parameters, we concentrate on the two most influential ones and on a non influential one, so that to highlight different behaviours of the methods with respect to the parameters' importance.

For both test models we will execute the three sensitivity methods at similar number of model evaluations, and at increasing number of model evaluations, in order to investigate their relative accuracy. The relative merits of the methods are also discussed depending on the degree of importance of the input factors. Graphs with confidence bounds for the sensitivity indices are provided to assess the robustness of the sensitivity estimates.

Acknowledgement:

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SYSTEM ANALYSIS AND SENSITIVITY USING DATA COLLABORATION

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Predictive ability of chemical kinetics models, as of models in general, is one of the most sought-after characteristics that underlie scientific activity in reaction chemistry. Reliable model predictions are needed for both establishment of poorly-understood reaction mechanisms and quantitative application of established mechanisms. The current level of predictiveness in most cases is far from satisfactory, and one is interested in identifying possible actions that could measurably improve it: What causes/skews the model predictiveness? Are there new experiments to be performed, old repeated, and/or theoretical studies to be carried out? What impact could a planned experimental work have? What would it take to bring a given chemical kinetics model to a desired level of accuracy? et cetera.

The mathematical quest for the model predictiveness typically takes the form of propagation of errors [1-4], sensitivity analysis [5-8], and straight-forward optimization [9-14]. All such venues follow the two-state approach: estimation of model parameters and their uncertainties (generally, from experimental data) followed by the analysis of the influence of the estimated parameter values and uncertainties on model prediction. So doing presumes model parameters to be "unique", predetermined values and often with individual, uncorrelated uncertainties.

An alternative approach, which we termed Data Collaboration, allows one to transfer uncertainties of the experimental data into model prediction directly. It is a framework designed to make inferences from experimental observations in the context of an underlying model. In the previous studies, we addressed collaborative features of this approach [15], mutual consistency of a set of experiments [15,16], and discrimination among competing reaction models [17]. In the present study, we return to our initial objective [18]: model prediction. We show that Data Collaboration allows one to assess the propagation of uncertainty more deeply— determining which experiment/parameter contributes the most to the current uncertainty in model prediction, ranking such effects, and considering new or even hypothetical experiments— thereby providing guidance in selecting additional experiments to perform.

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SENSITIVITY AND INFORMATION THEORETIC ANALYSES OF BIOCHEMICAL NETWORKS

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A major part of the systems biology agenda involves the modelling and analysis of biochemical networks [1-5], including their sensitivity analysis [6]. This is typically done as ODE models in environments (such as Gepasi [7-9] and Copasi [10], with the networks encoded and annotated in the Systems Biology Markup Language (www.sbml.org/ and see [11; 12]). Biochemical networks tend to come in two flavours – metabolic (in which there is mass transfer involving chemical change) and informational or signalling (in which there is essentially not). Sensitivity analysis has been popularised in a local form when applied to the former kinds of (metabolic) network as Metabolic Control Analysis [13-15], but has been comparatively little applied to signalling networks.

NF-κB is a transcription factor that affects the production of many proteins, and has been implicated in cancer, apoptosis, rheumatoid arthritis and other disease syndromes, and NF-κB is therefore part of an important signalling network. We analysed a model of the NF-κB system [16; 17] containing some 64 reactions and 23 variables, in which the nuclear concentration of NF-κB exhibited damped oscillations and found using local sensitivity analysis that only some 8-9 of these reactions contributed significantly to the oscillations [18]. This enormous decrease in the number of possible pairwise interactions to consider between them (from 64^2 to 8^2) allowed us to determine that the sensitivity of appropriate output features to individual reactions could depend even qualitatively (in sign) on the value of other parameters [19], giving weight to the view that biochemical networks must be analysed not just at the level of the individual reaction [20; 21]. As with the positive feedforward loop [2], it seems that downstream events respond not to amplitude but to frequency in this system, thereby solving the problem of crosstalk [4; 17; 22; 23].

Local sensitivity analyses are essentially linear for small amplitude changes in parameters, but clearly these oscillating systems are highly nonlinear. Nevertheless similar conclusions can be drawn from global sensitivity analyses [24; 25].

Any biochemical network can be treated as a 'communication channel', and these are usually analysed using the methods of information theory [26; 27]. We have recently shown that the associations between inputs and outputs of such networks can be quantified via a decomposition of their mutual information into different components characterizing the main effect of individual inputs and their interactions [28]. Unlike variance-based approaches to sensitivity analysis (as typically used in both local and global sensitivity analysis), our novel methodology can easily accommodate correlated inputs.

Overall, sensitivity analysis is a major component of the systems biology modelling of biochemical networks, and it is important to develop and apply suites of new tools with which to carry it out. Making these tools available as Web Services [29; 30] will allow one to exploit environments such as Taverna [31-33] for incorporating them into biochemical workflows [4; 5],

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ANALYSIS OF A BUDDING YEAST CELL CYCLE MODEL USING THE SHAPES OF LOCAL SENSITIVITY FUNCTIONS

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The cell cycle is the sequence of events by which a growing cell replicates all of its components and divides them into two sister cells. The eukaryotic cell division cycle is driven by an underlying molecular network, which is centred around complexes of cyclin-dependent kinases and cyclins. Chen *et al.* [1] have created a detailed model to describe the cell cycle of budding yeast. This model is a system of algebraic-differential equations having 13 variables and 73 parameters.

A dynamical system, such as the cell cycle can be characterized by the following initial value problem

$$\mathrm{d}\mathbf{Y}/\mathrm{d}t = \mathbf{f}(\mathbf{Y},\mathbf{p}), \qquad \mathbf{Y}(0) = \mathbf{Y}^0$$

where t is time, $\mathbf{Y}$ is the n-vector of variables, $\mathbf{p}$ is the m-vector of parameters, $\mathbf{Y}_0$ is the vector of the initial values of the variables, and $\mathbf{f}$ is the right-hand-side of the differential equations. Due to the presence of very different time-scales in most models, the dynamical dimension can be less than n. If the dynamical dimension is n_1 in a period, this means that the same results could be obtained by using an ODE having n_1 variables, while the values of other variables are kept constant or calculated by algebraic equations.

By calculating the eigenvalues of the Jacobian, we have determined [2] the stability of the cell cycle trajectories. Based on the sign of the real part of the eigenvalues, the cell cycle can be divided into excitation and relaxation periods. During an excitation period, the cell cycle control system leaves a formerly stable steady state. During relaxation periods, the control system asymptotically approaches the new steady state. In the Figure, the excitation periods are denoted by grey shading. The dynamical dimension of the model changed [2] accordingly: it reached 7 in the excitation periods and decreased to 1 in each relaxation period.

The local sensitivity function $s_{ik}(t)$ can be calculated (see *e.g.* [3]) by solving the following initial value problem:

$$\dot{\mathbf{S}} = \mathbf{J}\mathbf{S} + \mathbf{F} \qquad \mathbf{S}(0) = \mathbf{0}$$

where $\mathbf{S}(t)=\{s_{ik}(t)\}=\{\partial Y_i/\partial p_k\}$ is the time dependent local sensitivity matrix, $\mathbf{J}$ is the Jacobian ($\mathbf{J}=\{\partial f_i/\partial Y_j\}$) and matrix $\mathbf{F}$ contains the derivatives of the right-hand-side of the ODE with respect to the parameters ($\mathbf{F}=\{\partial f_i/\partial p_k\}$). The $s_{ik}(t)$ local sensitivity functions show the effect of a small perturbation of parameter k on variable i.

Local sensitivity functions were calculated for all variables and all parameters. The sensitivity functions of enzyme concentration Cln2 are plotted in the Figure. The sensitivity functions rise in some excitation periods and fall in all relaxation periods. The reason is that an effective parameter change soon causes deviations in the values of variables. These small deviations are amplified in the autocatalytic excitation regimes and the deviations are diminished in the relaxation regimes.

It is also apparent from the Figure that several sensitivity functions have similar shape. The fact that some local sensitivity functions may have similar shape was first observed in flame models by Rabitz *et al.* (see *e.g.* [4]). We detected this phenomenon also in other combustion systems [5], [6] and called it the global similarity of sensitivity functions. We have proved analytically [5], that global similarity emerges if the dynamic dimension of the model is low at least in some periods and if excitation periods are present. Both requirements were found numerically in combustion models showing global similarity [5], [6]. Low dynamical dimension in some periods and presence of excitation periods are also characteristic for the budding yeast model.

A closer inspection of the local sensitivity functions of the budding yeast model suggested that for each variable (*i.e.* protein concentration) the shape of the sensitivity functions could be grouped. Such a feature was not found in combustion models, because in high temperature combustion models the excitation is caused by a single group of strongly coupled reactions. In the case of the budding yeast cell cycle, several loosely connected excitation centres are present, which are firing one after the other according to a strict order. This causes the multiple similarities of the sensitivity functions.

A semi-automatic classification of the shapes of the $s_{ik}(t)$ functions in time interval $[t_1, t_2]$ was carried out in the following way. First, the functions were normalized to unit peak value: $\hat{s}_{ik}(t) = |s_{ik}(t)| / \max |s_{ik}(t)|$. Then, the integrated difference of the two normalized sensitivity functions was put into distance matrix $\mathbf{C}$:

$$C_i(k,l) = \int_{t_2}^{t_1} \left(\hat{s}_{ik}(t) - \hat{s}_{il}(t)\right)^2 \mathrm{d}t$$

This distance matrix was used as an input of a clustering code. The clustering calculations revealed that for each variable, 2 or 3 main similarity groups were detected. Note, that several sensitivity functions did not show similarity with the functions belonging to any of these groups.

If two sensitivity functions of variable *i* have similar shape, it means that the perturbation of the corresponding parameters have similar effect, which is an important structural information. Global similarity of the sensitivity functions of two parameters means that the change of one parameter can be fully compensated by an appropriate change of the other parameter. This is important information at the validation of complex dynamic models. For the budding yeast model, each parameter was changed by 10% and all other parameters were tuned one-by-one to check the presence of compensation effects. The results were in good accordance with the outcome of clustering calculations.

The joint application of local sensitivity and time scale analyses is a very powerful set of tools for the investigation of complex dynamic models. It reveals the excitation periods, the change of dynamic dimension and the effect of parameter perturbation. Similarities of local sensitivity functions carry important information on the role of parameters in the model. Our calculations revealed substantial new information on a frequently studied biochemical system, the cell cycle of the budding yeast.

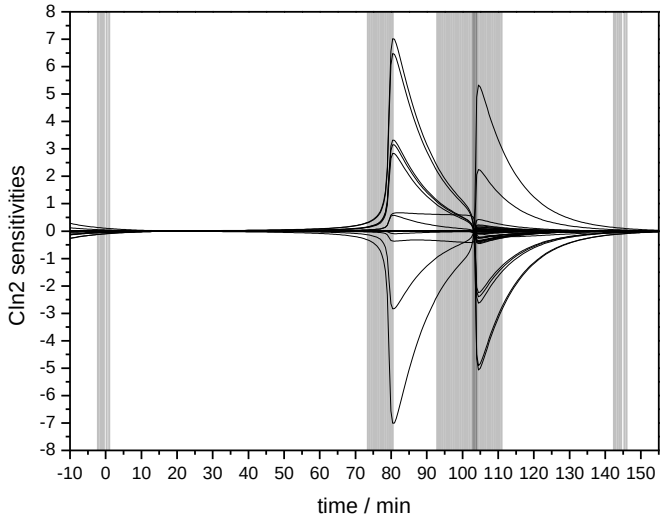

Figure: The local sensitivity functions of the enzyme concentration Cln2 for a whole cell cycle. Time zero marks the division of the cell. The length of a cell cycle is 144.92 minute. Grey shadings and white areas mark excitation and relaxation periods, respectively. The dark grey stripe near 104 minute indicates a strong excitation period.

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UNCERTAINTY ANALYSIS IN A TITAN IONOSPHERIC CHEMISTRY MODEL

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The Ion Neutral Mass Spectrometer (INMS) of the Cassini spacecraft revealed a surprisingly rich ion-neutral chemistry in the ionosphere of Titan [1]. The modelling of such a complex chemistry, producing heavy hydrocarbons and nitriles ions, is challenging. It involves hundreds of ion-molecule reactions, in addition to an even more complex photochemical-transport model for the neutral atmosphere. The reactions are parametrized by rate constants and branching ratios of products, which have been measured in the laboratory, with often sizeable uncertainties. Validation of the ionospheric chemistry model presently relies on the comparison of simulated ion mass spectra (MS) with INMS data, and thus on the estimation of prediction uncertainty on the concentrations of ions.

An error budget has been undertaken for the pertinent sources of uncertainty (chemical parameters, neutral densities...) [2]. Considering the large uncertainties and non-linear correlations associated to input parameters, and the non-linearities in the chemistry model, uncertainty propagation was done by Monte Carlo sampling. It pointed out neutral densities as a major source of uncertainty, in comparison to the chemical parameters [3]. Large uncertainties (about one order of magnitude) actually characterize the simulated mass spectra, in particular at the higher masses (m/z > 50 amu) (Fig. 1).

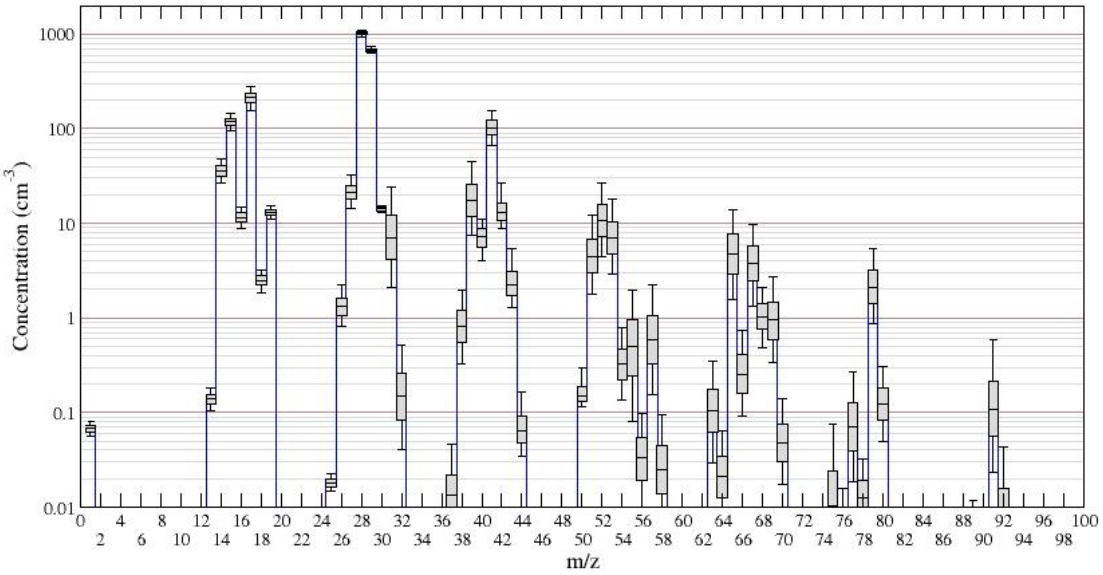

Figure 1: Simulated Ion Mass Spectrum of Titan ionosphere, with uncertainties resulting from ion-molecule reaction parameters and neutral species concentrations. Altitude 1200 km, daytime conditions.

In order to identify the individual parameters responsible for these large uncertainties, we started a global sensitivity analysis, based on input/output correlations. Our aim is to select key reactions in need of more accurate (and costly) laboratory measurements. For the ionospheric chemistry model, we identified a small set of ion-molecule reactions and also a set of neutral species, responsible for the large uncertainties on the concentrations of ions.

We then analysed the 1D photochemical model for neutral species and pointed out the major reactions responsible for the uncertainties in the key neutral species. A spectacular result is the hypersensitivity of the prediction uncertainties to the eddy profile used to model turbulent transport of neutral species. This work pinpoints the needs for tight constraints on the eddy diffusion coefficient (Fig. 2).

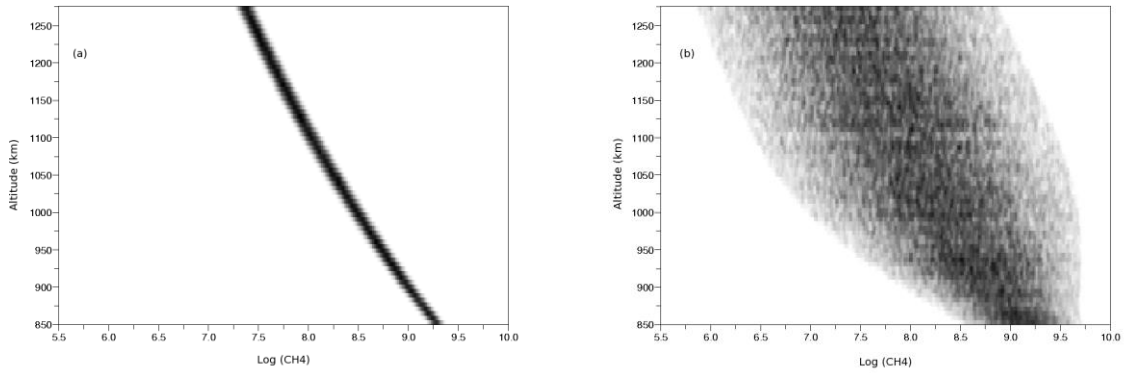

Figure 2: Hypersensitivity of the photochemical model with regard to the eddy diffusion coefficient : probability densities of CH_4 concentration profiles obtained with (a) a high homopause level (1040 km), (b) a low homopause level (68O km).

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THE SENSITIVITY OF A 3D STREET CANYON CFD MODEL TO UNCERTAINTIES IN INPUT PARAMETERS.

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Accurate models of air flows in urban streets are an essential prerequisite to predicting the dispersion of traffic related pollutants. They are therefore an important component of the modelling tools available to assist in managing air quality in urban areas. Although much progress has been made in the development of three dimensional computational fluid dynamic (CFD) models of turbulent flows in urban streets, their evaluation with respect to relevant field and laboratory data is less common. Since the models usually include parameterisations of some important features, their evaluation benefits from the inclusion of sensitivity studies that highlight the impact of uncertain input parameters on predicted flow fields. For example, a description of the velocity profile at the inlet boundary usually depends on the parametrisation of the overall surface "roughness" of the upwind domain. Defining this roughness parameter in variable urban street geometries is highly uncertain. The background wind direction is another parameter that affects predicted flow fields, and yet it is often measured at a significant distance from the area of interest and is therefore uncertain. As such parameters are often used to adapt the model to different scenarios, sensitivity analysis can be used to predict the effects of adjusting a particular parameter.

In this work, global sensitivity studies using both High Dimensional Model Representations (HDMR) and Monte-Carlo sampling have been carried out on the k-ε closure urban CFD model MISKAM [1]. The scenario studied is that of a complex street canyon in the City of York, UK, with all geometric features of importance within 100m of the section of interest included in the model description [2]. The outputs of interest are the mean wind flow and turbulent kinetic energy (TKE), both of which affect the potential dispersion of pollutants and are the inputs to a coupled Lagrangian dispersion model [2]. The sensitivity of both the TKE and the mean flow fields to the input parameters is detailed, both within a canyon cross section, and at specific measurement points to aid comparison with field data. This analysis gives insight into how model parameters can influence the predicted outputs, as well as the relative strength of their influence. The use of these techniques for identifying problems in the model structure is also shown.

A comparison of the Monte-Carlo sampling [3] and HDMR methods [4] was also undertaken. This shows that in terms of computational expense and quantity of sensitivity information, HDMR methods outperform Monte-Carlo based techniques. Ten thousand model runs were performed using random sampling for three particular background wind directions to allow for accurate comparison of the two methods. Both Pearson and Spearman rank correlation coefficients were calculated in relation to each of the input parameters, as well as sensitivity indices using HDMR, thus allowing the ranking of parameters in terms of importance. The advantages of the HDMR method include that it can highlight the specific form of the first order response to each parameter and that it can quantify interactions between parameters i.e. their second order effects. It is also shown to be computationally less expensive for this case study, although for some examples this may be offset by the extra development time. Monte-Carlo sampling coupled with standard regression techniques, although simpler to implement, can account only for linear effects. This can however be extended to monotonically varying effects if a rank correlation method is used [3].

Four main input parameters are addressed in this study, three of which are surface roughness lengths, determining the flow over a surface. The inflow roughness length is used to determine one-dimensional wind and turbulence profiles at the inlet boundary. The surface roughness length describes the flow over the model's ground level, while the wall roughness describes flow over the building surfaces, including roofs. The wind direction is varied over 20 degree ranges, which is designed to simulate the uncertainties in wind direction that may occur in a full scale experiment. The value ranges (Table 1) chosen for each parameter are based on both the limitations of the model and information from previous field studies.

The analysis shows that the sensitivity of the flow structures in and above the canyon to each parameter is very location dependant. In order to present these spatial effects, first order sensitivity indices as represented by the correlations shown in Table 1, are produced at every cross-sectional grid point. Thus, the influence of each parameter can be shown in terms of location as demonstrated for inflow roughness in Figure 1. It is also found that different model outputs are sensitive to different input parameters. The structure of the model can often directly explain these differences. Only small second order effects are found using the HDMR analysis. Hence,

the first order sensitivity coefficients are similar to the correlation coefficients calculated from the Monte-Carlo random sampling as shown in Table 1.

Input parameter	Pearson R^2	Spearman Ranked R^2	HDMR first order
surface roughness(0.5-50cm)	0.0002	0.0007	0.0007
wall roughness(0.5-10cm)	0.4420	0.4582	0.4507
inflow roughness(5-50cm)	0.2808	0.3008	0.2845
background wind direction (90±10°)	0.2059	0.2006	0.2113

Table 1. Example of sensitivity indices for normalised TKE at an in-canyon measurement point for 90±10° background wind direction

Potential problems in the model assumptions/parametrisations were revealed by the sensitivity analysis, since the source of unexpected model responses could be identified. In this particular case, initial sensitivity tests revealed that the above roof roughness length was miss-specified in the model code. For the corrected model, the surface roughness was found to have the lowest overall influence on flow patterns and turbulence within the canyon. In the case of cross canyon flow (background wind of 90° - from the right in Figure 1) the wall and inflow roughness were found to be the most important parameters influencing TKE in the canyon. For along canyon background flow, uncertainties in the wind direction were the most important influence on in canyon flow features. This is not surprising since small deviations in wind direction determine whether the flow is directly channelled down the canyon, or is impeded by local building structures. This high sensitivity has implications for the specification of appropriate reference wind measurements in practical situations. The analysis also tests assumptions made in the model setup. For example, ideally the model domain should be large enough that the inflow conditions have minimal influence on the in-canyon flow. However, the sensitivity studies show a significant partial variance for inflow roughness for several wind angles, indicating that the model domain could ideally be larger. Increasing the model domain would have implications for the computational expense of the calculations.

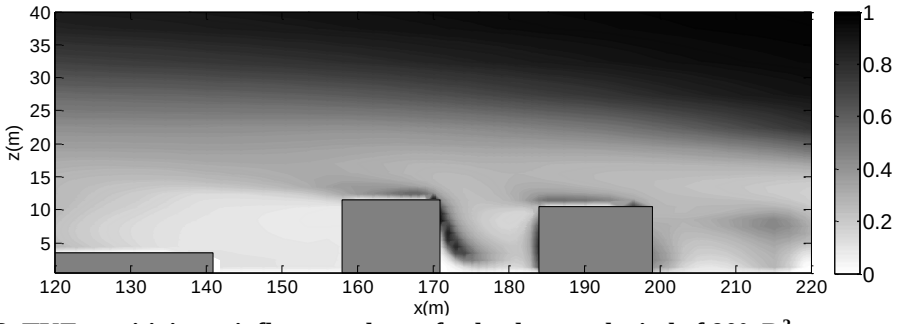

Figure 2. TKE sensitivity to inflow roughness for background wind of 90°, R^2 cross-section.

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FROM DOMINANT MODE ANALYSIS TO DYNAMICAL META-MODELLING

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The simplest *Transfer Function* (TF) model is a linear regression in which the dependent output variable is computed as an additive sum of several 'input' variables. The statistical identification and estimation of such models is straightforward and can be accomplished by ordinary multiple regression analysis. However, transfer functions are normally used for the modelling of linear, constant parameter, discrete or continuous-time dynamic systems. Such models, which are simply an alternative form of the equivalent ordinary difference and differential equations, can be obtained from measured input-output data using statistical methods of identification and estimation for TF models, such as those available in the CAPTAIN Toolbox[1] for Matlab™. Furthermore, TF models can be generalized in two major ways to include *Time Variable Parameter* (TVP) and *State Dependent Parameter* (SDP) transfer function relationships. The TVP model represents non-stationary systems, where the parameters can vary over time in an unknown, stochastic manner (see e.g. [1]); while the parameters in the SDP model are dependent on other time variable states and so can represent a wide class of nonlinear, stochastic systems (see e.g. [2]). Once again, identification and estimation of such models can be accomplished with the help of algorithms in the CAPTAIN Toolbox.

The present paper will show how this generalized class of TF model can also be utilized to improve the computational and statistical efficiency of sensitivity analysis and facilitate the 'emulation' [3] of large system models. It will first outline the nature of SDP models for stochastic static and dynamic systems and introduce methods for the non-parametric identification and parametric estimation of such models. It will then show how such an approach can be used to efficiently process the *Monte Carlo Simulation* (MCS) results obtained from sensitivity analysis. The paper will also show how generalized TF modelling can be used in *Dominant Mode Analysis* (DMA), a useful form of model reduction [4], and it will demonstrate how this can provide a basis for the synthesis of computationally efficient emulation versions of large simulation models. These various methodological procedures will be illustrated by two main examples. The first example will show how SDP estimation is able to identify and estimate an SDP model for a simulated Lorenz Strange Attractor system based on noisy measurements of its three state variables. The second example will show how the generalized TF modelling can be used to obtain an emulation version of a large macro-economic simulation model.

SDP estimation is a special form of time variable parameter estimation for models formulated as a regression relation, in which the dependent variable is normally the output y_k of a system which is computed as an additive sum of the 'input' variables x_i, $i = 1,\ldots,n$, i.e.,

$$y_k = a_1(v_{1,k})x_1 + a_2(v_{2,k})x_2 + \ldots + a_n(v_{p,k})x_p + e_k \qquad e_k = N(0,\sigma^2) \tag{1}$$

Here a_i are state dependent parameters that vary over time because they are a function of the associated (normally measured) variable $v_{i,k}$; while e_k is assumed to be a zero mean, serially uncorrelated and normally distributed random noise sequence (white noise) with variance σ^2. As shown in [5,6] Equation (1) forms the basis for the use of SDP estimation in sensitivity analysis. Here, the mathematical or computational model usually takes the static form:

$$y = f(x_1,\ldots,x_p) \tag{2}$$

where the model parameters (input factors) x_i have a domain of variability U, linked to the uncertainty about their precise value. The SDP equation (1) is used to approximate (1), with the input variables representing the input factors and the product of the SDPs and their associated input variables providing estimates of the first order sensitivity functions. The advantage of using the SDP model in this manner is that the number of MCS realizations required to estimate the sensitivity functions is considerable reduced in relation to conventional methods. This static' concept of meta-modelling to sensitivity analysis is also the basis of the Gaussian emulator [2] and of the Random Sample – High Dimensional Model Representation based on polynomial regression [6].

In the case of dynamic systems, the 'input variables' to the system will normally contain past sampled values of the dependent variable, as well as present and past sampled values of input variables that affect the output

[1] See http://www.es.lancs.ac.uk/cres/captain/.

variable. In this form, the model is a nonlinear SDP version of the well known linear *AutoRegressive eXogenous variable* (ARX) model. This SDARX model is used in the initial non-parametric identification stage of SDP modelling. In the single input, single output case, the more general SDP Transfer Function (SDTF) model takes the form:

$$y_k = \frac{b_0(v_{n+1,k}) + b_1(v_{n+2,k})z^{-1} + \ldots + b_m(v_{n+m+1,k})z^{-m}}{1 + a_1(v_{1,k})z^{-1} + a_2(v_{2,k})z^{-2} + \ldots + a_n(v_{n,k})z^{-n}} u_{k-\delta} + e(t) \quad (3)$$

where z^{-r} is the backward shift operator, i.e. $z^{-r}y_k = y_{k-r}$ and δ is introduced as a delay on the input variable in order to allow for any pure time delay in the system. Equation (3) can be extended straightforwardly to include multiple input variables and, as such, provides the basis for final parametric estimation of the SDP model and for the dominant mode analysis used in the full *dynamical* meta-modelling approach discussed here and exemplified in the second example. In the *dynamical* case, the computational model under analysis takes the modified form:

$$y_k = f(y_{k-1},\ldots,y_{k-n},u_{k-\delta},\ldots,u_{k-m-\delta} \mid x_1,\ldots,x_p) \quad (4)$$

The typical approach for meta-modelling and sensitivity analysis in the case of dynamical models is to repeat a series of static analyses on a set of grid points along the time co-ordinate. Our meta-modelling procedure, on the other hand, first identifies, based on DMA, a SDTF model that best approximates the features of the original complex dynamical model for a 'nominal' set of parameters values x_i. Second, a MC set of realizations of the model (4) is generated sampling x_i from their domain *U*, and a corresponding MC set of SDTF approximations is estimated. Third, the relationship between the x_i parameters of the original model and the coefficients $[a_1,\ldots,a_n,b_0,\ldots,b_m]$ of the SDTF approximation is mapped by applying the usual 'static' form techniques [2,5-7], e.g. estimating HDMR component functions of the links

$$[a_1 = g_1(x_i),\ldots a_n = g_n(x_i), b_0 = g_{n+1}(x_i),\ldots, b_m = g_{n+m+1}(x_i)] \quad (5)$$

The second step of our procedure also includes validation checks, whereby the structure of the SDTF model identified on the 'nominal' set of parameters of (4), is checked to hold also for all the MC realizations. Such a validation step might include an iterative DMA and identification procedure in order to select the SDTF structure that best fits the original model in the entire domain *U* (or at least in its largest part). In the case of *stochastic* models (i.e. u_k are stochastic processes), validation also checks the effectiveness of the identified SDTF to fit random realisation of the stochastic dynamical system.

This three-step procedure defines a full *dynamic* meta-model, whereby for every parameter set of the original model a corresponding set of coefficients for the SDTF is derived, that produce a computationally efficient and operationally equivalent dynamic simulation model that can replace the original large simulation model. This approach has the advantage that it is not based on a series of static analyses on grid points: rather, the SDTF meta-model mimics the relevant dynamical features of the original model, allowing for a full *dynamic* approximation.

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APPLICATION OF GLOBAL SENSITIVITY INDICES FOR MEASURING THE EFFECTIVENESS OF QUASI-MONTE CARLO METHODS AND PARAMETER ESTIMATION

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Many problems in physics and numerical analysis are concerned with high dimensional integrals. While the classical grid methods are very efficient for low dimensional integrands, they become computationally impractical when the number of dimensions n increases as the number of required integrand evaluations grows exponentially. This effect is known as "the curse of dimensionality". In contrast, the convergence rate of Monte Carlo (MC) integration methods dos not depend on the number of dimensions n. However, the rate of convergence $O(1/N^{-1/2})$, where N is the number of sampled points, attained by MC is rather low. A higher rate of convergence can be obtained by using deterministic uniformly distributed sequences also known as low-discrepancy sequences (LDS) instead of pseudo-random numbers. Methods based on the usage of such sequences are known as Quasi Monte Carlo (QMC) methods. Asymptotically, QMC can provide the rate of convergence $O(1/N)$. For sufficiently large N, QMC should always outperform MC. However, in practice such sample sizes quite often are infeasible, especially when high dimensional problems are concerned. Some numerical experiments demonstrated that the advantages of QMC can disappear for high-dimensional problems. There were claims that the degradation in performance of QMC occurs at $n > 12$ [1]. At the same time there are known high-dimensional problems for which QMC significantly outperforms MC.

Global sensitivity analysis (SA) offers a general practical way to predict the efficiency of QMC algorithms. Using the Sobol' method of global sensitivity indices the classification of some important classes of integrable functions is developed [2]. Functions with respect to their dependence on the input variables can be divided into three categories: functions with not equally important variables (type A), functions with equally important variables and with dominant low order terms (type B) and functions with equally important variables and with dominant interaction terms (type C). For functions of type A and B, QMC is even in the high dimensional case superior to MC while for functions of type C, QMC looses its advantage over MC because of the importance of higher-order terms in the corresponding ANOVA decomposition. The results of numerical tests verify the prediction of the suggested classification.

The technique for prediction the efficiency of QMC methods was extended for the case of Wiener path integrals. In [2] it was applied for analysis the differences in performances of two well-known approximations of a test path integral. The standard and the Brownian discretization schemes used in MC option pricing were compared in [3]. Global SA reveals that the variance of the samples generated for the Brownian path slowly decreases with time step index for the standard discretisation for the case of Asian call options. The higher order interactions in the ANOVA decomposition of payoff functions are very important. Therefore, the effective dimensions for standard discretization is close to the real dimension. Although the standard discretisation with QMC sampling is superior to MC, the convergence rate of the QMC method is much lower than that of the Brownian bridge discretisation and it decreases as dimensionality grows.

The Brownian bridge discretisation of the Brownian path results in significant improvement of the accuracy of QMC especially when the number of time steps n is large. For the Brownian bridge discretisation the sensitivity indices of the first few variables are much larger than those of the subsequent variables. Application of the Brownian bridge discretization greatly reduces the effective dimension and consequently increases the efficiency of QMC. Its efficiency practically does not depend on the problem dimensionality.

A new approach for parameter estimation within the framework of optimal experimental design (OED) is developed. OED allows the identification of a set of experiments with conditions that deliver measurement data the most sensitive to the unknown parameters. One of the common ways to design experiments is to use scalar functions of the Fisher information matrix (FIM) evaluated at the nominal values of the parameters. This information matrix is based on the linear sensitivity coefficients of the response variables. The results of a FIM based OED depend on the nominal values used for the parameters. Moreover, preliminary experiments and model calibration tests need to be carried out in order to obtain a first guess for the parameter values and a slowly converging iterative scheme is required [4]. These linear methods are not sufficient for dealing with complex OED problems, especially those in which nonlinear interactions between parameters are present.

These limitations can be overcome by the application of global sensitivity indices and defining the Global Fisher Information Matrix (GFIM) as

$$FIM(\hat{p}, x) = \sum_{r=1}^{N} \sum_{s=1}^{N} {Q^G}_r^T Q_s^G \ ,$$

where matrix Q_r^G has a form

$$Q_r^G = \begin{bmatrix} S^r_{\hat{p}_1}(t_1)\ S^r_{\hat{p}_2}(t_1) \cdots S^r_{\hat{p}_L}(t_1) \\ S^r_{\hat{p}_1}(t_2)\ S^r_{\hat{p}_2}(t_2) \cdots S^r_{\hat{p}_L}(t_2) \\ \vdots \\ S^r_{\hat{p}_1}(t_N)\ S^r_{\hat{p}_2}(t_N) \cdots S^r_{\hat{p}_L}(t_N) \end{bmatrix}.$$

Here $S^r_{\hat{p}_l}(t_n)$ is the Sobol' sensitivity index for parameter p_l of the *r*-th response variable at t_n -th moment of time. Once GFIM is defined the maximization of the determinant

$$J_{OED} = \det(GSIM).$$

leads to an optimal vector of input variables. This approach was applied to some cases studies in [5]. The results demonstrated methods ability to significantly reduce the required experimental work and illustrated the effectiveness of the global SA techniques for the design of reliable dynamic experiments.

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AN EXTENDED USE OF THE SOBOL' ESTIMATOR

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In this paper we show an extended use of the Sobol' estimator to be used with Monte Carlo (MC) samples that do not follow the standard Sobol' design for computing sensitivity indices [1]. Sobol' offered a Monte Carlo strategy to compute variance-based indices of any order that is based on a Monte Carlo exploration of the input space. To make an example, to estimate $V_i = V[E(Y \mid X_i)]$, the following algorithm is used

$$\tilde{V}_i = \sum_{j=1}^{N} f\left(x_{j1}^a, x_{j2}^a, \cdots x_{ji}^a, \cdots x_{jk}^a\right) f\left(x_{j1}^b, x_{j2}^b, \cdots x_{ji}^a, \cdots x_{jk}^b\right) \quad (1)$$

where N is the sample size of a MC simulation, k the number of independent factors, and the superscript a,b stand to indicate that different independent input MC matrices have been used:

$$\mathbf{A} = \begin{pmatrix} x_{11}^a & \cdots & x_{1k}^a \\ \cdots & \cdots & \cdots \\ x_{N1}^a & \cdots & x_{Nk}^a \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} x_{11}^b & \cdots & x_{1k}^b \\ \cdots & \cdots & \cdots \\ x_{N1}^b & \cdots & x_{Nk}^b \end{pmatrix} \quad (2)$$

This applies also for sets of factors

$$\tilde{V}_{\mathbf{I}} = V[E(Y \mid \mathbf{X}_{\mathbf{I}})] = \sum_{j=1}^{N} f\left(x_{j1}^a, x_{j2}^a, \cdots \mathbf{X}_{j\mathbf{I}}^a, \cdots x_{jk}^a\right) f\left(x_{j1}^b, x_{j2}^b, \cdots \mathbf{X}_{j\mathbf{I}}^a, \cdots x_{jk}^b\right)$$

where $\mathbf{X}_{\mathbf{I}}$ denotes a group of factors indexed by $\mathbf{I} = (i_1, .. i_g)_{1 \le g \le k}$. Using the standard Sobol' procedure, estimating all first order effect requires $N(k+1)$ model evaluations, while it takes $N(2^k - 1)$ runs to estimate the full variance decomposition. When a replicated Latin-hypercube design (rLHS) is used, only two replicas are sufficient for the entire set of first order effects, thus reducing the cost from $N(k+1)$ to $2N$ model evaluations, whatever the number input factors.

Here we propose to extend the idea of rLHS in two directions. The first is to exploit low discrepancy sampling techniques, like Sobol' quasi-random sequences [2]. The second proposes the following simplified form of the estimators (1-2):

$$\tilde{V}_{\mathbf{I}} = V[E(Y \mid \mathbf{X}_{\mathbf{I}})] = \sum_{j=1}^{N} f\left(x_{j1}^a, x_{j2}^a, \cdots \mathbf{X}_{j\mathbf{I}}^a, \cdots x_{jk}^a\right) f\left(x_{j(a,b)1}^b, x_{j(a,b)2}^b, \cdots \mathbf{X}_{j(a,b)\mathbf{I}}^b, \cdots x_{j(a,b)k}^b\right) \quad (3)$$

where $j(a,b) = \arg\min_{l=1,\ldots,N}(|| \mathbf{X}_{l\mathbf{I}}^b - \mathbf{X}_{j\mathbf{I}}^a ||)$ is the row-index of the re-sample matrix $\mathbf{B}$, where the $\mathbf{X}_{\mathbf{I}}$ co-ordinates have the smallest Euclidean distance w.r.t. the $\mathbf{X}_{\mathbf{I}}$ co-ordinates in the j-th row of the sample matrix $\mathbf{A}$. In this way, one can think of applying a generic sample design of dimension $2N$ and estimate main effects as well as higher order interaction effects with the approximated estimator (3). In the case of Sobol' sequences, this is done by generating a sample of dimension N and $2k$ columns and use the first k columns for the matrix $\mathbf{A}$ and the remaining ones for matrix $\mathbf{B}$. It is worthwhile to note that, using the approximated estimator (3) one has to implicitly rely on a smoothness assumption of the mapping $Y = f(\mathbf{X})$, whereby the original Sobol' procedure does not, i.e. the latter provides a robust and unbiased estimates of sensitivity indices regardless to any hypothesis on f, but square-integrability.

Convergence properties of the proposed estimator are shown by means of Monte Carlo experiments. Comparisons with other classical approaches are also considered.

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A NEW APPROACH TO SENSITIVITY ANALYSIS BASED ON PLS REGRESSION

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In this presentation, we propose the use of the Partial Least Squares (PLS) regression in order to more effectively carry out the Sensitivity Analysis (SA). This regression method is very well-known for data analysis in many different scientific fields (chemometrics, biometrics, etc). It was proposed by [1] and is explained in detail in [2] and [3]. Two advantages are particularly relevant for conducting a SA of a model ouput. These two advantages are: *i*) the very efficient way to manage the stochastic and structural dependences – because the partial covariances are taken into account – between the inputs; *ii*) the possibility of having a smaller number of simulations (because no matrix inversion is needed for estimating the SA indexes) than the number of inputs, which is extremely useful if simulations are very time-consuming. More information on the principle and properties of PLS regression will be given in the lecture and in a subsequent paper. We only provide the main steps of our methodology below.

The general methodology we propose is composed of four steps:

(a) N Monte Carlo simulations of the output are generated via a computer model, which leads to a simulation matrix S of N rows and p columns (the p inputs). It should be observed that the correlation structure between the p inputs is obtained by application of the method given in [4].

(b) A full quadratic polynomial model (p linear effects, p quadratic effects, $p(p\text{-}1)/2$ first-order interactions between inputs, and one intercept) is built from the p inputs, leading to a matrix M of N rows and k columns.

(c) A particular method of stepwise PLS regression – the BQ method described in [5] – is used for selecting the significant and significant expanded inputs. Even if the value of k is very large (2000, for example), the procedure works well and quite rapidly.

(d) A final PLS regression model is estimated (by means of SIMCA software Version 9.0, Umetrics AB, Sweden) with the inputs selected in step (c). If its R^2 is large enough (typically > 80%), we can consider that this final model is valid and hence provides estimated centred and scaled PLS coefficients, which can be seen as SA indexes (see Fig. 1 of the following example). Eventually, the adequate normalisation can be applied to these indexes for obtaining percentages.

Following are some results about a successful application to a real SA problem. This application is concerned with the exposure to the mycotoxin Ochratoxin-A (OTA) in food, for the population of French children. An elementary exposure to OTA is defined by the product of a food consumption (normalised by the individual weight) by the contamination level of this food. A global exposure is the sum of several (eight here) elementary exposures. The exposure distribution was estimated in [6], as well as its 95^{th} quantile for estimating risk assessment exposure to OTA in food. A first SA was reported in [7] and at the SAMO 2001 Conference. The second SA we propose here is easier to achieve thanks to the PLS regression, and especially, to the fact that the whole variation domain of the 32 inputs can be taken into account, to the contrary of the study in [7] where Fig. 6 clearly shows the ellipsoidal domain of an input couple. The output we are interested in is thus the 95^{th} quantile relative to the parameters of the probability density functions (*pdf*, the inputs of the SA) of the consumption and contamination distributions of the eight types of food. Indeed, these parameters are not certain and their potential ranges were estimated in [7] from real consumption and contamination data. Therefore, it is crucial to quantify the sensitivity of this high quantile to the variation of these inputs. In this case, we have p = 32 and k = 561. One trial was achieved with N = 318 (note that $N < k$), and the second with N = 12,698. The SA indexes are very similar for these values of N. However, we only show the significant SA indexes for N = 12,698 ($100 \times R^2$ = 96%) in Fig.1.

Some brief comments can be made here. First of all, only six SA indexes are significantly different from zero among the 560 indexes; the word "significantly" has a particular meaning in the PLS that will be explained in the lecture and the subsequent paper. Secondly, we observe that the type of food "CEREALS" (see a detailed definition of this word in [6]) is the only type of food that is involved in the SA and, moreover, the SA indexes relative to the parameters of the contamination distributions are preponderant. Thus, it is of particular importance to have accurate values for these parameters and, consequently, we need to improve the collecting process of contamination data for "CEREALS".

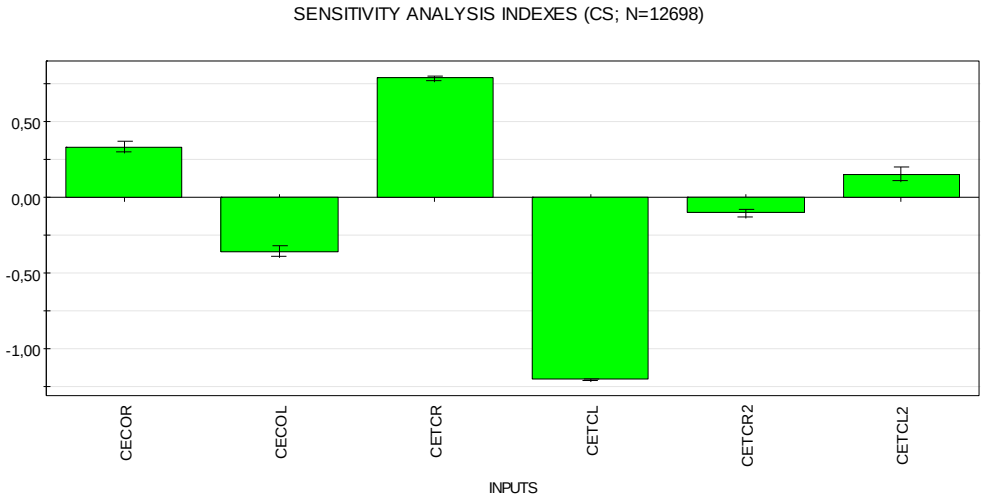

Fig. 1: SA indexes for the 95th quantile with their bootstrap type confidence intervals; inputs (all relative to "CEREALS") are: cecor = the shape parameter of the consumption Gamma *pdf*, cecol = the scale parameter of the consumption Gamma *pdf*, cetcr = the shape parameter of the contamination Gamma *pdf*, cetcl = the scale parameter of the contamination Gamma *pdf*, and quadratic CETCR and CETCL terms.

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ESTIMATION OF THE CONTRIBUTION TO THE SAMPLE MEAN AND SAMPLE VARIANCE USING RANDOM SAMPLES

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A considerable amount of information is lost when the mean and variance of a dependent variable is calculated from a random sample. Considering a general model *f* with k independent input factors $\boldsymbol{Y} = f(\boldsymbol{X_1},\boldsymbol{X_2},\cdots\boldsymbol{X_k})$, when the appropriate sampling strategy is adopted, the sophisticated variance-based methods are very efficient in inferring how the variance of the output ***Y*** can be quantitatively apportioned to the different independent variables. However, the multidimensional averaging characterizing global sensitivity analysis methods provide only part of the information available from the mapping between the input factors and the response of interest. In fact, for a given input factor $\boldsymbol{X_j}$, it is not possible to assess how a specific quantile of this variable contributes or fails to contribute to the mean and variance of the ***Y***. In this paper the contribution of $\boldsymbol{X_j}$ is also decomposed across its range and provides useful information for a number of settings related to Global Sensitivity Analysis (factor mapping, factor prioritization and factor fixing).

In the radioactive waste management framework, Sinclair [1] investigated the way infinitesimal changes to the probability density function (*PDF*) of an input factor $\boldsymbol{X_j}$ can alter overall features of performance (mean and variance of ***Y***). The marginal dependence of $E(\boldsymbol{Y})$ on the various input factors was employed and portrayed graphically. Nevertheless, Sinclair considered his 'sensitivity plot', as he called it, as a useful graphic tool for estimating sensitivity 'by eye' [1]. This study has three objectives: The first one is to extend the idea behind the contribution to the sample mean plot to the variance, developing also the contribution to the sample variance plot, the second one is to develop statistical tests for both plots, the third one is to extend Sinclair's qualitative assessment of parameter sensitivities to quantitative sensitivity measures for the mean and variance of the model response ***Y***.

Let us consider that a Monte Carlo sample **S** of size *N* is generated for the inputs and that the corresponding model response ***Y*** is also estimated. Let us also consider that the sampling technique used doesn't introduce any bias, as for example random sampling or proportional stratified sampling. In order to build both plots for a given input variable, let us say $\boldsymbol{X}_1$, and the response ***Y***, firstly we sort the realisations of $\boldsymbol{X_1}$, generating the series of values $\{x_1^{(1)},x_1^{(2)},\ldots,x_1^{(N)}\}$, and the corresponding series of values $\{y^{(1)},y^{(2)},\ldots,y^{(N)}\}$. Auxiliary variables ***M*** and ***V*** are defined, whose sampled values are obtained from the sampled values of ***Y*** in the order defined by $\boldsymbol{X}_1$ as

$$m_i = \frac{1}{N}\sum_{j=1}^{i} y^{(j)} \qquad v_i = \frac{1}{N}\sum_{j=1}^{i}(y^{(j)} - \bar{y})^2 \quad , \tag{1}$$

which are further normalised being divided by the sample mean and the sample variance respectively. Then, they are plotted versus the cumulative distribution function of $\boldsymbol{X_1}$. So, the contribution to the sample mean plot is the plot of the normalised values m_i versus $F_{X1}(x_1)$ and the contribution to the variance plot is the plot of the normalised values v_i versus $F_{X1}(x_1)$.

Plotting $F_{X1}(x_1)$ in the x axis means that equal lengths represent approximately regions of equal probability of the input variable. The more the plot deviates from the diagonal in a given region, the more that region of the input variable contributes to the sample mean or the sample variance. In fact, non-important input variables produce plots close to the diagonal, since large and small output values can be equally found in any of their regions.

These plots provide a qualitative view of the importance of the input variable considered, nevertheless, it is important to be able to measure how important, how statistically significant, is its departure from the diagonal. This task needs the help of a statistical test.

In order to set up a test we need to define a null hypothesis and a measure of discrepancy with the null hypothesis. The null hypotheis is the 'non-importance' of the input variable considered, and we will interpret 'non-importance' in statistical terms as a random assignation of output values to the inputs. So, if the output values seem to be randomly assigned to the values of a given input variable, we will consider that the different parts of that input variable contribute approximately equally to the output variable sample mean, so that it will be considered as a non-important effect on the output variable.

As a measure of discrepancy with the null hypothesis we consider the maximum distance between the contribution to the sample mean plot and the diagonal (same for the contribution to the sample variance). This measure of discrepancy with the null hypothesis is a reasonable one since lack of random association between inputs and outputs will produce departures from the diagonal.

The next step is the computation of the distribution of the measure of discrepancy under the null hypothesis and the design of the corresponding decision rule. With this purpose, a permutation test [2] has been set up. This test is specific for each output variable given that the distribution under the null hypothesis depends on its values. So, we proceed as follows: we generate a large number of permutations of the set of sampled output variable values, say 10^4, then we produce a plot for each random permutation, so that we get a 'cloud' of plots that could be obtained under random conditions. For each plot the maximum distance (absolute value) between the curve and the diagonal is computed. Using order statistics, we estimate the different quantiles of the random variable 'maximum distance between the curve and the diagonal'. In order to perform a test, we choose a test significance level and select the appropriate value of the maximum distances above which we reject the null hypothesis. Figure 1 shows an example of contribution to the mean plots. The red lines provide the 99% band. Under random conditions only 1% of the curves generated have at least one point outside the band contained within the two red lines. W and V^1 are quite relevant parameters while T and K are not. While this conclusion cannot be inferred from the classic scatter plots visualization, the proposed representation gives an added value with respect to the sensitivity assessment. The value of the statistics 'maximum distance between the curve and the diagonal' can approximately be considered as a measure of importance of a given parameter.

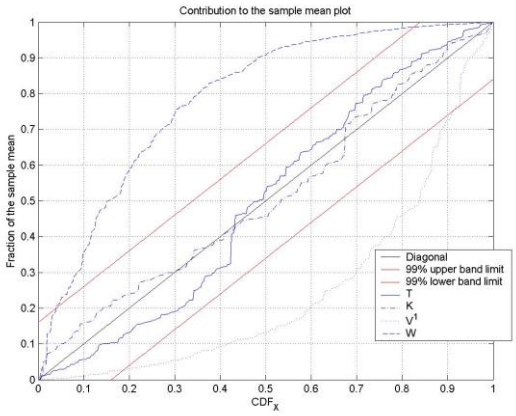

Figure 1.- Contribution to the mean plot for four input variables in a radioactive waste management model. The null hypothesis is rejected for parameters whose curves lie out of the 99% band, identifying them as important parameters.

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CONTROLLING AND UNDERSTANDING CHEMICAL-PHYSICAL PHENOMENA WITH SENSITIVITY ANALYSIS

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Random Sampling-High Dimensional Model Representation (RS-HDMR) is a practical approach to HDMR that can provide efficient global sensitivity analysis of complex nonlinear systems with independent or correlated probability density functions of inputs. HDMR expresses the model output $f(x)$ as a finite hierarchical correlated function expansion in terms of the input variables ($x_1, x_2, \ldots, x_n$): $f(x) = f_0 + \sum_i f_i(x_i) + \sum_{ij} f_{ij}(x_i, x_j) + \ldots$. The HDMR component functions are *optimally* constructed from a set of generated/measured data for each specific function f(x). The individual RS-HDMR component functions also have a direct statistical correlation interpretation, which permits the model output variance, σ^2, in a desired input domain to be decomposed into its input contributions ($\sigma^2 = \sum_i \sigma_i^2 + \sum_{i,j} \sigma_{ij}^2 + \ldots$), due to the independent variable action σ_i^2, the pair correlation action σ_{ij}^2, etc., where σ_i^2, σ_{ij}^2, … are defined as the covariances of $f_i(x_i)$, $f_{ij}(x_i; x_j)$, … with $f(\mathbf{x})$, respectively. The global sensitivity indexes, S_i, S_{ij}, … are defined as σ_i^2/σ^2, σ_{ij}^2/σ^2, ….The magnitudes of S_i, S_{ij}, … may be used to quantitatively identify the important inputs and input pairs, triples, etc. After deducing the component functions, the HDMR expansion can be used to explore the input $\rightarrow$ output relationships of the particular systems. To reduce sampling effort, the RS-HDMR component functions are approximately represented by weighted optimal orthonormal polynomial expansions. The orthonormal polynomial expansion coefficients of RS-HDMR are sequentially determined by least-squares regression. The probability density function of inputs is involved only implicitly through sampling, and the inputs can have an arbitrary independent or correlated probability density function. This feature is especially beneficial for real systems whose input probability density functions are often correlated and unknown. RS-HDMR technique will be illustrated with several examples.

THE USE OF GLOBAL METHODS IN THE EVALUATION OF NON LINEAR CHEMICAL KINETIC MODELS

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The use of computational modelling as a design or strategic planning tool is increasing within engineering and environmental applications. Examples include the design of efficient combustion devices, the optimisation of chemical process plant and the prediction of the response of pollution levels to changes in emissions. For such applications, models often require the coupling of a range of complex processes including chemical kinetic interactions, turbulent fluid flow and molecular diffusion. The evaluation of such models is crucial to understanding the confidence that can be placed in their predictions, as well as providing vital information for model improvement. A key model subcomponent in many applications is the chemical mechanism employed. The rapid improvement in computational power in the preceding decades has facilitated the use of substantially more detailed kinetics than the single step approximations used in early reactive flow applications. Furthermore, it has become apparent that the inclusion of detailed kinetic processes is critical to the successful prediction of a range of important phenomena. In addition, the development of automatic procedures for chemical mechanism generation [1,2], means that kinetic mechanisms are becoming available in ever increasing detail. Examples include the Master Chemical Mechanism (MCM) used for the prediction of tropospheric gas phase chemistry and containing up to 4500 species and over 12,000 reactions [1], and mechanisms describing the oxidation of a range of fuels as generated by the EXGAS code [2].

Despite the detail available, the use of such comprehensive schemes in complex reactive flow models is not without problems. The sheer size of such schemes often prohibits their use in models describing complex flow phenomena such as 3 dimensional simulations of turbulent reactive flow, even using the massively parallel computers available today. However, the schemes are usually developed for general use and therefore may contain a significant number of species and reaction steps that are not required to model particular sets of conditions. In addition, many of the reaction steps and thermochemical parameters in such schemes have not been directly measured or modelled using *ab initio* techniques, but have been estimated using structural additivity relationships, making the data highly uncertain in some cases. The evaluation of the predictive uncertainty that results is therefore crucial. Making use of such comprehensive schemes for solving practical problems therefore requires developments in two areas: i) methods for the identification of redundant processes that can be removed from the scheme without substantially affecting the predictions of the outputs of interest ii) identifying those of the remaining parameter that drive the output uncertainty of the model and therefore require improved categorisation. Both steps fall within the realm of sensitivity and uncertainty analysis.

The identification of redundant species and reactions can be addressed by the use of local sensitivity coefficients. Often, the numbers of species can be significantly reduced for a given application, with only limited numbers of full model runs required to evaluate the sensitivity coefficients. The use of sensitivity analysis for model reduction has been the subject of several reviews [3,4]. The reduction of the model is a useful preliminary step for the assessment of model uncertainty, since the global methods required to achieve this usually necessitate a substantial number of model runs. Following the removal of redundant steps from the mechanism, the predictive uncertainty from the reduced scheme can be assessed in a more computationally efficient way. Even so, reduced chemical mechanisms remain a challenge for global methods, since the uncertain input data can include both reaction rate coefficients for each reaction, as well as thermochemical data for each species. The number of input parameters can therefore be large, even following model reduction. For automatically generated mechanisms, the uncertainty ranges for many parameters can also be large, leading to the requirement for global rather than local methods. This complexity can be dealt with in a number of ways. Screening methods such as the Morris method [5] and its variations can be employed to first identify unimportant parameters. A subsequent full global analysis can then be performed using a range of sampling methods for a reduced number of parameters. Alternatively, the use of High Dimensional Model Representation (HDMR) based methods [6,7] can be used without the need for prior screening, since they can be coupled with optimisation techniques that automatically exclude unimportant component functions (see paper by Ziehn and Tomlin). The application of these approaches to a range of case studies in chemical kinetics will be discussed.

Case Study Examples

Isolation of chemical kinetics from other aspects of the fluid flow assists in the evaluation of chemical mechanisms. This usually means the design of experiments which use simple geometries where the reactor is well mixed or exhibits simple flow characteristics such as laminar flow. In atmospheric studies, the well mixed smog chamber is often used for isolating kinetic processes. In combustion, similar well stirred reactor studies

are available as well as one dimensional laminar flames. More recently, the use of experiments performed in micro-gravity conditions has enhanced the pool of data available, since under such conditions the complex mixing caused by convection is removed from the problem. Such experiments mean that the physical part of the problem is substantially simplified so that sufficient chemical detail can be included in the computational model for the evaluation of detailed mechanisms. The number of parameters related to physical processes such as diffusion is also reduced. Examples are chosen here to highlight particular issues of relevance to nonlinear kinetics. These include i) the prediction of auto-ignition delay for the low temperature oxidation of propane in a well stirred reactor. The implications of the highlighted uncertainties for predictions of ignition delays obtained under microgravity will be discussed. ii) the prediction of auto-ignition delay for the combustion of CO + H_2 mixtures at high pressures, iii) the prediction of NO emissions from a premixed laminar methane air flame with trace sulphur and nitrogen compounds.

For each example, it is demonstrated that only a few parameters contribute substantially to the output variance of the kinetic model, despite the large numbers of species and reactions present in the schemes studied and the large uncertainty ranges adopted in many cases. Screening methods are shown to successfully identify the main parameters of importance which can be further studied using sampling based methods. On the other hand, HDMR methods are shown to provide an automatic way of identifying unimportant parameters within the analysis, thus removing the necessity to employ screening methods, even for problems with a high dimensional input space. HDMR also provides an automatic way of producing an importance ranking for the parameters, including both first and higher order effects. Substantial nonlinearities are found in the output response of the models, which can be highlighted by the HDMR component functions.

It is shown that identification of the parameters driving uncertainties from the kinetic models can inform the need for new theoretical studies of specific reaction rate or thermochemical data. For the example of CO + H_2 auto-ignition delays, the rate constant assigned to the HO_2+CO reaction was found to be particularly significant and was subsequently reassessed using *ab initio* techniques [8] as a result of the uncertainty analysis. The adoption of the new rate is shown to improve the agreement with the high pressure ignition delay studies. For the propane study, the original reaction scheme appeared to exhibit too high a reactivity when compared to experimental results. Uncertainties in thermochemical data (heats of formation) were seen to have a significant effect on the prediction of ignition delays. Tests suggest that the adjustment of a few key parameters within their uncertainty ranges would be enough to substantially improve the agreement of the model with both terrestrial and micro-gravity experiments. Optimisation is problematic however, since a large number of parameter combinations are capable of giving overlap with the experimental values. This suggests the requirement for further theoretical studies of the key species identified. For the laminar flame, under conditions of low fuel to oxygen ratio, no overlap exists with the experimental data, despite large uncertainty ranges in input data. Suggestions for structural improvements to the model are therefore required in this case.

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SENSITIVITY EXPERIMENTS ON ONE-CLASS SUPPORT VECTOR MACHINE

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One-Class Support Vector Machine (OC-SVM) is a most popular method in outlier detection or anomaly detection. It is based on the kernel trick and standard SVM procedures, and, in a quadratic programming formulation, uses a trade-off parameter that defines the ratio between number of samples in data class and that of outlier class, i.e., class of support vectors. The sensitivity of the trade-off parameter involved in the OC-SVM is investigated with respect to noisy mislabelled data, and some original modification of the method is proposed.

1. Introduction

In binary classification (e.g., operating or failed), support vector machines (SVMs) have attracted much attention recently because of their excellent quality in various real-world applications [1]. Utilizing the kernel trick that is a method of converting a linear classification algorithm into a non-linear one by replacing a dot product in high dimensional feature space with kernels, SVM can find the maximum-margin hyperplane that separates two clouds of data points at equally located distance. SVM is reputed to achieve high performance, not suffering from the curse of dimensionality even when the number of training samples is small compared to the feature vector dimensionality. The great advantage of SVM is that the algorithm often does not suffer from overfitting and enhance a generalization capability. In order to use kernels as dot product, note that the kernel function must be symmetric and positive semi-definite.

A powerful extension of SVM to one-class problems is referred to as One-Class SVM (OC-SVM) [2]. Using an appropriate kernel function, OC-SVM first maps the data points into a high dimensional feature space, and then finds the hyperplane that separates, with maximum margin, the feature vectors from the origin of the transformed space. The kernel most commonly used in SVM and OC-SVM is the Gaussian radial basis function. The OC-SVM interprets the origin of the transformed feature space as the second class and feature vectors that are classified as belonging to the second class are regarded as outliers or anomalies. In the risk management applications, OC-SVM is typically used for classification of anomalies and malfunctions occurring in nuclear components and systems from measured operational data [3].

In the quadratic programming formulation of OC-SVM, there is a parameter that controls a trade-off between maximizing the distance of the hyperplane from the origin, and containing most of the training samples in the domain created by the hyperplane. The paper explores sensitivity investigations of this trade-off parameter involved in the OC-SVM against noisy mislabelled data since the parameter significantly influences the quality of classification. In addition, we propose some original modification of the method based on the sensitivity experiments.

2. Sensitivity Analysis in OC-SVM

Let $x \in \mathbf{R}^m$ be a measurement vector. Using the Gaussian radial basis function as kernel

$$k(x_i, x_j) = \exp(-\left\|x_i - x_j\right\|^2 / 2\sigma^2), \qquad i, j = 1, \cdots, n$$

where σ denotes the standard deviation, OC-SVM can be formulated as the following quadratic programming problem:

$$\min_{w,\rho,\xi} \quad \frac{1}{2}\|w\|^2 + \frac{1}{\nu n}\sum_{i=1}^{n}\xi_i - \rho$$

$$\text{s.t.} \quad \langle w \cdot \phi(x) \rangle \geq \rho - \xi_i, \quad \xi_i \geq 0$$

where ϕ is the appropriate mapping function, w and ρ denote the weight vector and threshold level, respectively, $\nu \in (0,1)$ is the trade-off parameter, and ξ_i are slack variables that penalize the objective function with allowing some of the feature vectors to be located in between the origin and desired hyperplane. Recall that the parameter ν theoretically defines the ratio between number of samples in data class and that of outlier class, i.e., class of support vectors.

In order to perform the anomaly detection, a dataset of known anomalies is used to train OC-SVM with the proper label, say, +1. When all the training data are correctly labelled, the resulting model can recognize

whether the test data belongs to the known or unknown anomaly class. However, if the class label is noisy, i.e., some data are mislabelled, it often becomes crucial to discriminate true (failed states) and false anomalies since there is a number of possible situations with false-positive and false-negative cases. For system reliability evaluation, the correctly classified failed states provide most valuable information. In the present study, the sensitivity is defined by the percentage of correctly classified anomalous events belonging to the known and/or unknown anomaly class with varying a value of the trade-off parameter ν.

3. Sensitivity Experiments

For experimental investigations, we take Spam E-mail Database from UCI Repository of machine learning databases [4]. Only preliminary results are presented here with appropriate pre-processing of Spam E-mail Database, where OC-SVM is used to eliminate possible mislabelled data. In Fig. 1, we plot the classification accuracy against the level of mislabel with varying a value of ν involved in the OC-SVM used as a pre-processor.

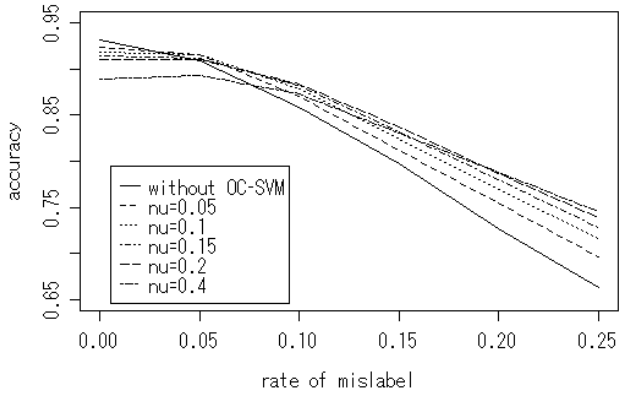

Fig. 1 depicts that there may be some optimal value of ν against the level of anomaly or percentage of mislabelled data. Although it is too early to draw any definite conclusions, OC-SVM may be useful for the one class anomaly recognition tasks. But, at the same time, preliminary results warn us against its uncritical use. In addition, some original modification of the method is proposed based on conceptual and experimental investigation details of which will be presented at the conference.

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BAYESIAN CALIBRATION OF A FLOOD INUNDATION MODEL

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The need to estimate and communicate uncertainty in predictions of flood extent and estimates of flood risk is now widely appreciated [1]. Decision-makers can legitimately expect technical specialists to provide and justify uncertainty estimates so that they can make risk-based decisions that account for uncertainty. In this paper we are concerned with the problem of uncertainty analysis in the use of (usually quite complex) numerical models to predict flooding. Current practice in flood modelling is typically based upon rather *ad hoc* procedures for model calibration based around *tuning* of model parameters until the model predictions give reasonable correspondence to some observed dataset, whilst also remaining within 'plausible' ranges of the parameter values, which are not directly measurable in nature. Data with which to compare model predictions are usually scarce and may be of questionable accuracy. A less deterministic approach has been proposed by Beven [2], which makes use of 'informal' likelihood functions in order to generate uncertainty estimates for model predictions, an approach that has been criticised for being incoherent in a formal sense [3].

Kennedy and O'Hagan [4] (hereafter KOH2001) have proposed a Bayesian approach, based upon the following characterisation of the calibration problem:

$$z_i = \rho\eta(\mathbf{x}_i, \theta) + \delta(\mathbf{x}_i) + e_i$$

A computer model enacts a deterministic function of input variables **x** and a vector of calibration parameters θ. However, the computer model will tend to be computationally expensive, so it will only be feasible to do a limited number of model runs. It is therefore replaced by a Gaussian process $\eta(\mathbf{x}_i, \theta)$, scaled as necessary by ρ, that can emulate the computer model response on the basis of a set of training runs. It is acknowledged that even with the best possible values of the calibration parameters θ the computer model is not a perfect representation of reality. It is separated from reality by a model inadequacy function $\delta(\mathbf{x}_i)$, which is also taken to be a Gaussian process. The 'true' process of interest is not observable. Instead we observe z_i which is the true process contaminated by some observation error e_i. Full details of the KOH2001 are described in [4] and [5]. The methodology has now been implemented in the R programming language in a package called BACCO. The R routines are described by Hankin [6], can be freely downloaded from http://cran.r-project.org/ and have already been successfully applied in other applications [7].

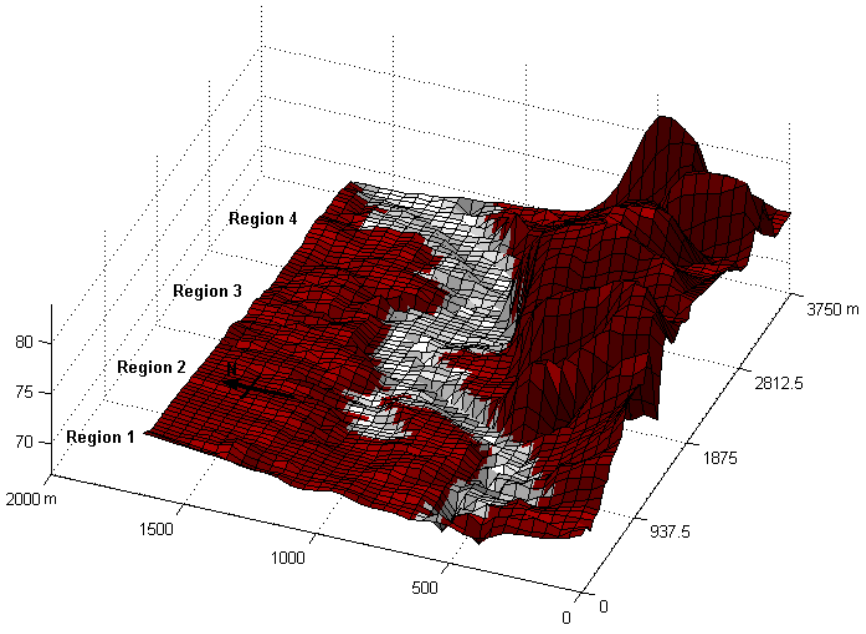

Figure 1 DEM of the Thames case study site with the SAR image of the flood outline super-imposed

In this paper we apply BACCO to the calibration of a computer simulation of flooding on a reach of the River

Thames (UK) for which a Synthetic Aperture Radar image of the extent of flooding was available for model calibration [8] (Figure 1). The flood model is LISFLOOD-FP, a raster-based inundation model specifically developed to take advantage of high resolution digital elevation models (DEM) [9]. Channel flow is handled using a one-dimensional approach that is capable of capturing the downstream propagation of a flood wave and the response of flow to free surface slope. Floodplain flows are similarly described in terms of continuity and momentum equations, discretized over a grid of square cells, which allows the model to represent 2-D dynamic flow fields on the floodplain. The model calibration parameters are the Manning friction coefficients for the river channel and floodplain, but previous research has shown rather small sensitivity to the floodplain friction coefficient [10], so here we deal with just one calibration parameter, the river channel friction coefficient n_c.

Recent attempts have been made to undertake Bayesian calibration with pixelated spatial data using a likelihood function for binary data [11]. In this paper we re-project the spatial flood outline data onto the DEM in order to generate observations of flood elevations at either side of the floodplain. The procedure introduces, and to some extent amplifies, errors due to inaccuracies in the satellite observation and DEM, but results in the calibration process being based upon water surface elevation, which is a more primitive variable in flood modelling than flood outline. The errors can be accounted for within the framework of KOH2001.

The analysis takes place in two steps:

1. calibration, in which the observations are used to generate posterior distributions for n_c, the model inadequacy $\delta(\mathbf{x}_i)$ and the observation error e_i.
2. calibrated prediction, in which the posterior distributions for n_c, the model inadequacy $\delta(\mathbf{x}_i)$ and the observation error e_i are combined with a distribution for the discharge Q in the river to generate a probabilistic prediction of flood depth at points in the floodplain, which incorporates all sources of uncertainty.

As well as providing a sound approach to calibrated prediction, the process provides new insights into the sensitivity of the model simulations to the distribution of the calibration parameters and the extent to which model inadequacy can be successfully identified from a single spatial observation.

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IMPACT OF METHODOLOGICAL CHOICES ON ROAD SAFETY RANKING

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In recent years, the interest in and the use of indicators and indexes are rapidly increasing. Their usefulness for policymakers and communication purposes is a key advantage. Trends can be identified, problems predicted, policy targets and priorities set, the impact of measures assessed, attention achieved, … [1,2]. In domains like economy (the human development index), technology (the technology achievement index) and sustainability (the environmental sustainability index) the aggregation of indicators in one index is common [3].

In this research we focus on the road safety domain which is currently showing much interest in the use of indicators. For the most influencing road safety risk factors, indicators are presently being developed and data collected on the European level [4,5]. Although countries are often compared on their level of road safety by means of the number of traffic deaths per million inhabitants, the development of a road safety performance index will provide valuable insights. There are a number of disadvantages linked to accident data, like for example the lack of uniformity in definitions and the problem of under-registration [6]. However, the most important drawback is that knowledge of the number of accidents and casualties in a country is insufficient to understand the processes that lead to these accidents. If one wants to enhance the road safety level in a country, a set of measures has to be identified, able to tackle the real problem.

Road safety indicators can help in this respect. Based on a set of carefully selected indicators, the safety conditions can be reflected, the impact of safety interventions can be measured and the safety performance of different countries can be compared [5]. Not only will an insight be gained into the domains that need additional efforts from policymakers, the aggregation of useful information into one road safety index will be a valuable tool for the road safety domain. A sound methodology for constructing a road safety performance index is however prerequisite for its use. To this end, a composite indicator methodology has to be elaborated.

In the past, limited attention has been paid to the construction of a road safety index, and we believe that a methodologically valid composite indicator approach is a new, challenging and necessary matter in road safety. In order to develop an acceptable index, the subjective choices involved in the process of developing a road safety index need to be justified and their impact on the end result quantified. As there is no agreement or a priori knowledge on the best or ideal method to be used in the steps defined in [1], several possible methods need to be tested. Sensitivity and uncertainty analysis is a requirement for composite indicators. The end result – for example the ranking of countries based on their road safety index score – can be heavily influenced by the choices made in the index construction process. As stated in [7] the iterative use of uncertainty and sensitivity analysis contributes to the well-structuring of the composite indicators, provides information concerning the robustness of the countries' ranking and identifies ways to reduce the uncertainty in the ranking for a better monitoring and policy.

In the study at hand, various methodological aspects used in other composite indicator studies [1,3] are investigated and adapted to the specific context of road safety. We will illustrate some methodological topics on a dataset consisting of 7 road safety indicators (related to the domain of alcohol, speed, protective systems, visibility, vehicle, infrastructure and trauma management) and 18 countries. In the literature [8], these 7 domains are generally agreed to be very important road safety risk factors. For now, for each domain only one indicator was defined based on policy relevance, clarity and data availability [2].

As part of the development of a road safety index, we will study the impact of the weighting method, expert selection and indicator selection on the average shift in rank of the 18 countries in our dataset. More specifically, we will test two commonly used weighting methods [3] both based on expert opinions, namely the Analytic Hierarchy Process (AHP) and Budget Allocation (BA). The results of comparisons in pairs of the road safety indicators as well as the allocation of a budget over the indicator set were obtained from 9 road safety experts from different European countries. The average indicator weights over the experts are often used. However, we will assess the impact of selecting the weights from one particular expert. In addition, the change in rank will be studied in case one of the seven indicators is no longer included in the road safety index. The result of the analysis will indicate how robust the ranking is, which of these methodological choices has the largest impact on average rank shift and which input factor needs special effort in order to reduce the output variance. It can also be shown which countries are favoured under a particular set of assumptions.

The output variable of interest is the average change in the country rankings for all possible scenarios. Due to the specific nature of this composite indicator we will compare the road safety ranking against the reference ranking based on the number of traffic deaths per million inhabitants.

First, a probability distribution function is assigned to each input factor from which values are drawn for each sample. Multiple evaluations of the model with randomly selected input factors will be performed, considering simultaneously all sources of uncertainty. For non-linear models (which is the case here) variance-based techniques for sensitivity analysis are the most appropriate [9]. These techniques are model independent (thus suitable for non-linear and non-additive models), they capture interaction effects apart from the fractional contribution of input factor x_i to the variance of the model output y, and they explore the whole range of variation of each factor.

The largest shift in country ranking occurs when the weights of expert 6 from the budget allocation method are used and the infrastructure indicator is no longer part of the dataset. In addition, the first-order indexes S_i – which capture the fractional contribution to the model output variance due to the uncertainty in x_i – and the total effect indices S_{ti} – which concentrate all the interactions involving factor x_i in one single term – are calculated for each input factor. These indices give us insight in the amount of output variance that is explained by the input factors singularly, indicate which factors are mostly involved in interactions with other factors, which factors can be fixed without a significant impact on the output and which factor could reduce the output variance most if more information was found. This information needs to be considered in the building process of a composite road safety indicator.

To conclude, the development of a road safety index is a challenging and necessary task. Uncertainty and sensitivity analyses are a prerequisite to develop a methodologically sound index with a large acceptance. In this study, a first attempt was described in which the impact of three aspects on the country ranking was the focus: the selection of the weighting scheme, the expert and the indicators. In the future, the impact of several aggregation methods, normalisation techniques and imputation practices for missing data will be incorporated. Finally, the development process of a road safety index needs more elaboration and the analysis of uncertainty and sensitivity is indispensable for obtaining a robust road safety index in the end.

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ACCELERATING FACTORS SCREENING

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We introduce a new method for screening factors in mathematical or computational models with large numbers of factors. In factors screening one tries to identify active factors in a factors rich model with a minimum number of computer simulations. The method proposed here represents an improvement over the best available practice for this setting, the method of elementary effects (Morris 1991 [1], Campolongo et al. 1999 [2], Campolongo et al. 2000 [3], Saltelli et al. 2004 [4], Campolongo et al. 2007 [5]). Reviews of screening methods for computer experiments are in [3-6].
The proposed new method can offer both estimates of the first order and of the total order sensitivity indices.

Acknowledgement:

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ESTIMATION OF CONDITIONAL EXPECTATIONS AND CONDITIONAL VARIANCES WITH STATE-DEPENDENT PARAMETER META-MODELS

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In this paper we deal with the joint estimation of conditional expectations and conditional variances using the state-dependent parameter (SDP) meta-modeling approach, useful for applications in global sensitivity analysis (GSA) and in the more general meta-modeling framework. In GSA, the mapping $Y = f(\mathbf{X})$ between an output Y of a computational model and a set of uncertain input factors $\mathbf{X} = (X_1,...,X_k)$ is analyzed in order to quantify the relative contribution of each input factor to the uncertainty of Y. In meta-modeling exercises, the goal is to build a statistical approximation $\hat{f}(\mathbf{X})$ to the computational model $f(\mathbf{X})$ that is sufficiently accurate to be used in place of the original one (operationally equivalent) and that, at the same time, can be computed in a much faster way. Variance-based analysis is the most popular method in GSA. Variance based sensitivity indices of single factors or of groups of them are defined as [1]:

$$S_{\mathbf{I}} = \frac{V[E(Y \mid \mathbf{X}_{\mathbf{I}})]}{V(Y)}, \qquad (1)$$

where $\mathbf{X}_{\mathbf{I}}$ denotes a group of factors indexed by $\mathbf{I} = (i_1,..i_g)_{1 \le g \le k}$, and they tell the portion of variance of Y that is explained by $\mathbf{X}_{\mathbf{I}}$. There is a clear link between GSA and meta-modeling. First, the approximation $\hat{f}(\mathbf{X})$ can be used to compute sensitivity indices in place of the original computational mapping $f(\mathbf{X})$. Second, the variance based sensitivity measures can be interpreted as the non-parametric R^2 or correlation ratio, used in statistics to measure of the explanatory power of covariates in regression [2,3]. In fact, it is well known that the inner argument $E(Y \mid \mathbf{X}_{\mathbf{I}})$ of (1) is the function of the subset of input factors $\mathbf{X}_{\mathbf{I}}$ that approximates $f(\mathbf{X})$, by minimizing a quadratic loss (i.e. maximizing the R^2). This leads to the second link between GSA and meta-modeling, whereby estimating functions $E(Y \mid \mathbf{X}_{\mathbf{I}})$ provides a route for both a model approximation and sensitivity estimation. Smoothing methods that provide more or less accurate and efficient estimations of $E(Y \mid \mathbf{X}_{\mathbf{I}})$ are becoming a popular approach to sensitivity analysis [4,5,6,7]. SDP modeling is one class of non-parametric smoothing approach first suggested by Young [8]. The estimation is performed with the help of the `classical' recursive (non-numerical) Kalman filter and associated fixed interval smoothing algorithms and has been applied for sensitivity analysis in [9,10]. In great summary a state dependent model approximating $E(Y \mid \mathbf{X}_{\mathbf{I}})$ based on a Monte Carlo sample of dimension N can be written as:

$$Y_t = E(Y \mid \mathbf{X}_{\mathbf{I},t}) + e_t = p_{\mathbf{I},t}(s_{\mathbf{I}}) + e_t \qquad (2)$$

where e_t is the 'observation noise' (i.e. what is not explained by $\mathbf{X}_{\mathbf{I}}$) and $p_{\mathbf{I},t}(s_{\mathbf{I}})$ is a state dependent parameter, depending on a state variable $s_{\mathbf{I}}$ that moves according to a generalised sorting strategy $t = 1,...,N$ along the co-ordinates of the single factor or group of factors indexed by **I**. According to this generalised sorting strategy, the group of input factors of interest **I** is characterised by a low frequency spectrum (e.g. by some quasi-periodic pattern) while the remaining ones present a white spectrum. In this way, the estimation of $E(Y \mid \mathbf{X}_{\mathbf{I}})$ reduces to the extraction of the low frequency component of the sorted output Y. To do so, the SDP's are modelled by one member of generalised random walk (GRW) class of non-stationary processes. For instance, the integrated random walk (IRW) process turns out to provide good results, since it ensures that the estimated SDP relationship has the smooth properties of a cubic spline. Given the IRW characterisation, the model (2) can be put into state space form as:

$$\begin{aligned} Y_t &= p_{\mathbf{I},t} + e_t \\ p_{\mathbf{I},t} &= p_{\mathbf{I},t-1} + d_{\mathbf{I},t-1} \\ d_{\mathbf{I},t} &= d_{\mathbf{I},t-1} + \eta_{\mathbf{I},t} \end{aligned} \qquad (3)$$

where e_t (observation noise) and $\eta_{\mathbf{I},t}$ (system disturbances) are zero mean white noise inputs with variance σ^2 and $\sigma^2_{\eta_{\mathbf{I},t}}$ respectively. Given this formulation, SDP's are estimated using the recursive Kalman Filter (KF) and associated recursive Fixed Interval Smoothing (FIS) algorithm. The hyper-parameters associated with (3), i.e. the noise variances σ^2 and $\sigma^2_{\eta_{\mathbf{I},t}}$, are optimised by maximum likelihood (ML), using prediction error

decomposition. In this way, the SDP approach is couched with optimal ML estimation and seems more elegant and flexible than the scatter plot smoothing used by Hastie, Tibshirani and others [4,5,7,11]. For example, Random Walk (RW) or Smoothed Random Walk (SRW) might be preferable in certain circumstances because they yield less smooth estimates. Indeed, if any sharp changes or jumps seem possible, then these can be handled using `variance intervention' (see [12]). In particular, all effects that cannot attributed to shifts in the mean, are not accounted for by $E(Y \mid X_i)$ and the related variance-based sensitivity indices. For example, if we consider Figure 1, in panel (a) we show the estimate of $E(Y \mid X_i)$, in (b) we show that the 'observation noise' $e_i = Y - E(Y \mid X_i)$ has a clear heteroschedastic nature, which is not taken into account by any shift in the mean, but that can be modelled by assuming that the variance of e_i is modulated by X_i in some state-dependent manner. This is done by the state-dependent decomposition

$$\log(e_{i,t}^2) = m_{i,t}(s_i) + n_t$$

where now the state dependent parameter $m_{i,t}(s_i)$ accounts for the modulation effect, shown in panel (c). Moreover, remembering the conditional variance expression

$$V(Y \mid X_i) = E(Y^2 \mid X_i) - (E(Y \mid X_i))^2 = E((Y - E(Y \mid X_i))^2 \mid X_i) = E(e_i^2 \mid X_i)$$

we get the estimate $V(Y \mid X_i) = \exp(m_i)E(\exp(n_t))$ shown with the black line in panel (d), compared with the horizontal grey line showing the variance of e_i, given by $\sigma^2 = E[V(Y \mid X_i)]$. Moreover, feeding back the estimated state-dependency of σ^2 with variance intervention [12] in the recursive estimation of $E(Y \mid X_i)$, one will get a much more accurate and efficient estimation of the whole pattern and in particular of the sharp change at $X_i = 0.5$.

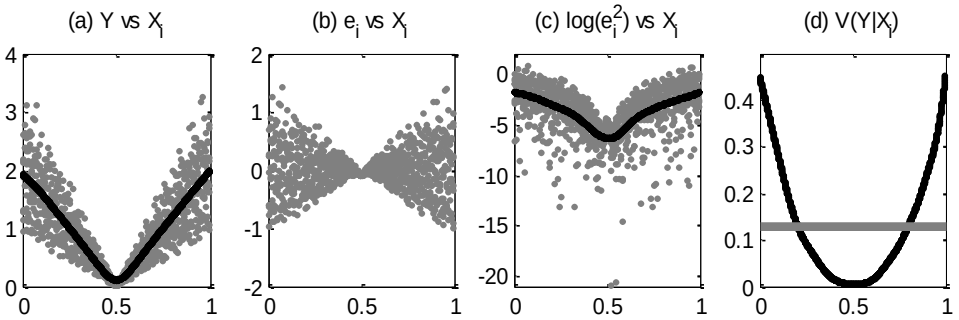

Figure 3

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THE INDICATION OF THE MOMENT INDEPENDENTMEASURE δ AND ITS NEW CALCULATIONAL METHOD

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5. Introduction

In risk assessment problems, the uncertainties of input parameters are transferred through the model to the output, and bring about the issue of output uncertainty. The goal of sensitivity analysis (SA) is to quantify the relative importance of each input parameter [1]. Iman and Hora [2] proposed that an ideal SA measure should be easy to interpret, easy to compute, and robust. Saltelli[3] pointed out that a SA technique should be global, quantitative and model free. Borgonovo [4] further extended Saltelli's requirements for a SA measure by adding the fourth feature, moment independence.

In [4] Borgonovo proposed a SA indicator δ_i, which estimates the influence of the entire input distribution on the entire output distribution. It does not refer to any particular moment of the output. For the readers' convenience, the derivation of δ_i is briefly described here. Let $f_Y(y)$ be the unconditional probability density function (PDF) of the model output Y, and $f_{Y|Xi}(Y)$ be the conditional PDF of Y, given a value (e.g., $x_i^{(1)}$) of an input parameter X_i. The shift between $f_Y(y)$and $f_{Y|Xi}(y)$ is measured by the total area $s(X_i)$, which is surrounded by these two curves (Fig. 1). It is given by

$$s(X_i) = \int | f_Y(y) - f_{Y|X_i}(y) | dy \qquad (1)$$

Let the value of X_i changes over its distribution, the expected shift is

$$E_{X_i}[s(X_i)] = \int f_{X_i}(x_i)\ s(X_i) dx_i \qquad (2)$$

The SA indicator δ_i is defined as

$$\delta_i = \tfrac{1}{2} E_{Xi}[s(X_i)] \qquad (3)$$

δ_i has the property of $0 \le \delta_i \le 1$ [4].

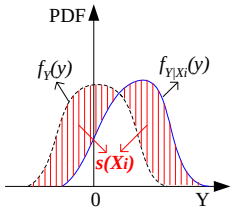

Fig. 1 Shift of $f_{Y|Xi}(y)$ from $f_Y(y)$ is measured by s_{Xi}.

From Fig. 1, it is known that the essence of δ_i (more precisely, $s(X_i)$) is to measure the difference of two PDFs by estimating the area surrounded by them. Obviously it is neither the difference of the means (medians), nor the difference of the variance between the two distributions. Then what is it? Is there any relationship with other statistics? Let us come to probe this issue.

6. Indication of δ_i

Let $F(y)$ and $f(y)$ be the CDF (Cumulative Distribution Function) and PDF of an output of interest Y, respectively. It is known from statistic textbooks that

$$F(y) = \int_{-\infty}^{y} f(u) du \qquad (4)$$

$F(y)$ is non-negative and monotonically increasing ($0 \le F(y) \le 1$).

Let $f_1(y)$ and $f_2(y)$ be two density distributions and suppose they are intersected, as shown in Fig. 2(a). The area surrounded by the two curves is given by the integral

$$s = \int | f_2(y) - f_1(y) | dx = s_1 + s_2 + s_3 + s_4 \qquad (5)$$

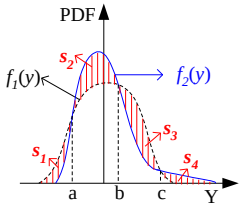

Fig. 2(a) $f_1(y)$ and $f_2(y)$.

Where s_1, s_2, s_3 and s_4 are the surrounded areas for $y \in (-\infty, a]$, $y \in (a, b]$, $y \in (b, c]$ and $y \in (c, +\infty]$, respectively.

For $y \in (-\infty, a]$, because $f_1(y) - f_2(y) \ge 0$, we have

$$s_1 = \int_{-\infty}^{a} [f_1(y) - f_2(y)]\ dy = F_1(a) - F_2(a) \qquad (6)$$

Correspondingly, we have

$$s_2 = [F_1(a) - F_2(a)] + [F_2(b) - F_1(b)] \qquad (7)$$

$$s_3 = [F_1(c) - F_2(c)] + [F_2(b) - F_1(b)] \qquad (8)$$

$$s_4 = F_1(c) - F_2(c) \qquad (9)$$

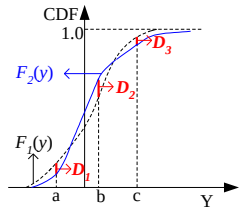

Fig. 2(b) $F_1(y)$ and $F_2(y)$.

Finally, we obtain $s = 2 \times \{[F_1(a) - F_2(a)] + [F_2(b) - F_1(b)] + [F_1(c) - F_2(c)]\}$ (10)

From Fig. 2(b) we know $D_1 = F_1(a) - F_2(a)$, $D_2 = F_2(b) - F_1(b)$ and $D_3 = F_1(c) - F_2(c)$. Therefore, the surrounded area s between two PDFs can be converted to the distance between their CDFS, and it is equal to two times of $D_1 + D_2 + D_3$. Since $0 \le F(y) \le 1$, we have $0 \le D_1 + D_2 + D_3 \le 1$. This relationship holds for any kinds of intersection

between two PDFs. Hence we derive the property of the area s: $s \in [0, 2]$.

From the above discussion, we know that the area surrounded by two PDFs can be converted to the distance between their CDFs. This remains us of the Kolmogorov-Smirnov test, in which the difference of two CDFs is measured by the statistic, the greatest vertical distance between them. It has been pointed out that the two-sided Kolmogorov-Smirnov is consistent against all types of differences (e.g., differences in means, medians, variance) that may exist between two distributions [5]. When there is only one intersection between two PDFs (i.e., no intersection between their CDFs), the surrounded area s between two PDFs is just two times of the greatest vertical distance between two distributions. In this case, the area s is equivalent to two times of the statistic used in Kolmogorov-Smirnov test. For other cases, the area s surrounded between two PDFs can be regarded as the refinement of the statistic used in Kolmogorov-Smirnov test. This can be the indication of δ_i.

Now let us prove the property of δ_i. For the surrounded area $s(X_i)$(in Eq. (1)), since $0 \le s(X_i) \le 2$ holds for any give value of X_i, we get $0 \le E_{Xi}(s(X_i)) \le 2$. Because δ_i is equal to one half of $E_{Xi}(s(X_i))$, we have $0 \le \delta_i \le 1$. So far, the property of δ_i is proved in a way different from that in [4].

7. A new calculational method for δ_i

Based on the discussion in Section 2(refer to Fig. 2), it is known that the area surrounded by two PDFs (assume n points of intersection between them) is equivalent to two times of the sum of the vertical distances between their CDFs when the values of Y are the same as those of all the n intersection points. Therefore, different from Borgonovo's approach [4], a new calculational method for δ_i was proposed.

Suppose that the unconditional PDF $f_Y(y)$ and the conditional PDF $f_{Y|Xi=xi^{(1)}}(y)$(given a random value $x_i^{(1)}$ of the input parameter X_i) can be analytically derived. Based on Eq. (4), we get their CDFs $F_Y(y)$ and $F_{Y|Xi=xi^{(1)}}(y)$, respectively. Since the relationship $f_Y(y)-f_{Y|Xi=xi^{(1)}}(y)=0$ happens at the points of intersection, we can obtain the values of Y at these points of intersection, assume them to be $a_1, a_2, ..., a_m$. Thus the area surrounded by the two PDFs is equal to

$$s(x_i^{(1)}) = 2\times[(|F_Y(a_1)- F_{Y|Xi=xi^{(1)}}(a_1)|+|F_Y(a_2)-F_{Y|Xi=xi^{(1)}}(a_2)|)+\ldots+|F_Y(a_m)-F_{Y|Xi=xi^{(1)}}(a_m)|] \quad (11)$$

We then generate a second value $x_i^{(2)}$for X_i, derive $f_{Y|Xi=xi^{(2)}}(y)$ and $F_{Y|Xi=xi^{(2)}}(y)$, and get $s(x_i^{(2)})$. Repeating the above steps for the total sampling size, we can finally estimate

$$\delta_i = \frac{1}{2}E_{Xi}[s(X_i)] = \frac{1}{2}[\sum_{k=1}^{n} s(x_i^{(k)})/n] \quad (12)$$

If $f_Y(y)$ and $f_{Y|Xi)}(y)$ can only be obtained empirically, Monte Carlo method will be suitable to get them. Firstly, the empirical CDF $F_Y(y)$ is obtained [6]:

$$F_Y(y) = \sum_{k=1}^{n} T(y > y_k)/n \quad (13)$$

$$T(y > y_k) = \begin{cases} 1, & if\ y > y_k \\ 0, & if\ y \le y_k \end{cases} \quad (14)$$

Where n is the sample size and k is the sample index.

According to statistics textbooks, we get the PDF

$$f_Y(y) = \frac{dF(y)}{dy} = \lim_{\Delta y \to 0}\frac{\Delta F(y)}{\Delta y} \approx \frac{\Delta F(y)}{\Delta y} \quad (15)$$

In the same way, we can get the empirical $F_{Y|Xi}(y)$ and $f_{Y|Xi}(y)$. Then we can repeat the above procedures to find the points of intersection of $f_Y(y)$ and $f_{Y|Xi}(y)$, calculate $s(x_i^{(1)})$(then $s(x_i^{(2)})$, …). Finally we can estimate δ_i.

8. Concluding remarks

In this work, the moment-independent SA measure δ_i is analyzed. It is demonstrated that the area surrounded by two PDFs is equivalent to two times of the sum of the vertical distances between their corresponding CDFs when the values of output of interest are the same as those of all the intersection points of the two PDFs. It can be regarded as the refinement of the Kolmogorov-Smirnov test statistic. Further, a new calculational method for δ_i is proposed. Improvement of this method is under way.

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A GENERAL FIRST-ORDER GLOBAL SENSITIVITY ANALYSIS METHOD

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One of the most popular sensitivity analysis techniques is Fourier Amplitude Sensitivity Test (FAST). The main mechanism of FAST is to assign each parameter with a distinct integer frequency (characteristic frequency) through a periodic sampling function. Then, for a specific parameter, the variance contribution can be singled out of the model output by the characteristic frequency based on a Fourier transformation. One limitation of FAST is that it can only be applied for models with independent parameters. However, in many cases, the parameters are correlated with one another. In this study, we propose to extend FAST to models with correlated parameters. The extension is based on the reordering of the independent sample in the traditional FAST. Another limitation of FAST is that, due to the aliasing effect between parameters by using integer characteristic frequencies, we need very large sample size models with many parameters. In this study, we adopted the improvement to overcome the aliasing effect limitation proposed by Tarantola et al. [1]. In this way, FAST can be a general first-order global sensitivity analysis method for linear/nonlinear models with as many correlated/uncorrelated parameters as the user specifies. We apply the improved FAST to linear, nonlinear, non-monotonic and real application models. The results show that the sensitivity indices derived by our proposed FAST are in a good agreement with that from the correlation ratio sensitivity method, which is a nonparametric method for models with correlated parameters.

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EXTRACTING COMPLEX NONLINEAR RESPONSE SURFACES FROM DETERMINISTIC MODELS WITH MULTIPLE INPUTS

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Applications of computer code models can become computationally very expensive if they require model runs for many different sets of inputs. Accordingly, it is often of great interest to derive computationally cheaper surrogate models that can mimic the output of the original model. The currently used techniques for estimating response surfaces for deterministic models with multiple inputs are usually based on design criteria that tend to favour regular fractional factorial designs or an almost uniform coverage of the experimental region (Bursztyn and Steinberg [1]). Moreover, it is common that a global parametric or nonparametric model is fitted to the computed responses for all design points (Iooss *et al.* [2]). Here, we develop a local approximation technique that is particularly appropriate for single-output deterministic models for which the curvature or roughness of the response surface varies markedly over the experimental region. In addition, we illustrate the performance of our method by deriving surrogate models of the INCA-N model (Whitehead *et al*. [3]), which is a hydro-geochemical model of the flows of water and nitrogen through a river basin.

A suitable experimental design for deriving surrogate models should be space-filling and have a particularly good coverage of regions where the response surface is so rough or nonlinear that it is difficult to extrapolate observed model outputs to outputs for previously untried inputs. We propose a sequential design in which a p-dimensional experimental region $D = \{\boldsymbol{x};\ a_i \le x_i \le b_i,\ i = 1, \ldots, p\}$ is partitioned into cuboid-shaped sub-regions, and the corners and centre of D are taken as an initial set of design points (figure 1-(*i*)). New sub-regions are formed by estimating the roughness of the response surface in each of the existing sub-regions and then splitting the one having the maximum roughness into two halves. New design points are formed by taking the centre and corners of the new sub-regions (figure 1- (*ii*) and (*iii*)).

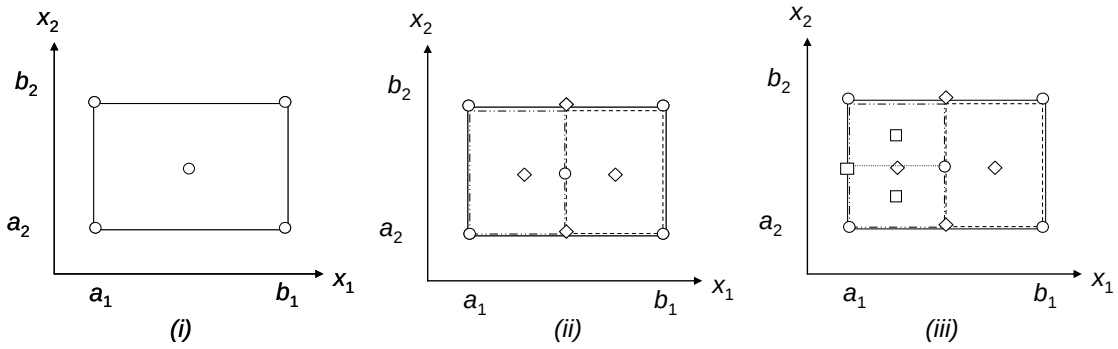

Figure 1. Design points selected in the first three steps of our sequential algorithm.

The roughness of the response surface in a given sub-region D_i is estimated by employing a simple local regression technique. First, a second-order polynomial

$$P_{D_i} = a_0 + \sum_{j=1}^{p} a_j x_j + \sum_{j=1}^{p} b_j x_j^2 + \sum_{j<k} c_j x_j x_k$$

is fitted to the model outputs for all design points in a minimal neighborhood of D_i. Then, we compute

$$R(D_i) = V(D_i)(4\sum_j \hat{b}_j^2 + 2\sum_{j<k} \hat{c}_{jk}^2)$$

where V(D_i) denotes the volume of D_i. Finally, the sub-region having the maximum R-value is split into two halves along the axis for which $|\hat{b}_j|$ achieves its maximum value.

The behaviour of the proposed design algorithm can be illustrated by the results obtained when the INCA-N model was used to examine how the average annual loss of nitrogen from an agricultural soil is related to the denitrification rate and the maximum nitrate uptake rate by the crop grown on that soil. The left diagram in figure 2 shows a response surface obtained by running the INCA-N model for a dense grid of design points. The right diagram shows the design points that were selected when a surrogate model was derived. In particular, it can be seen that the design points are concentrated to sub-regions where the response is non-linear.

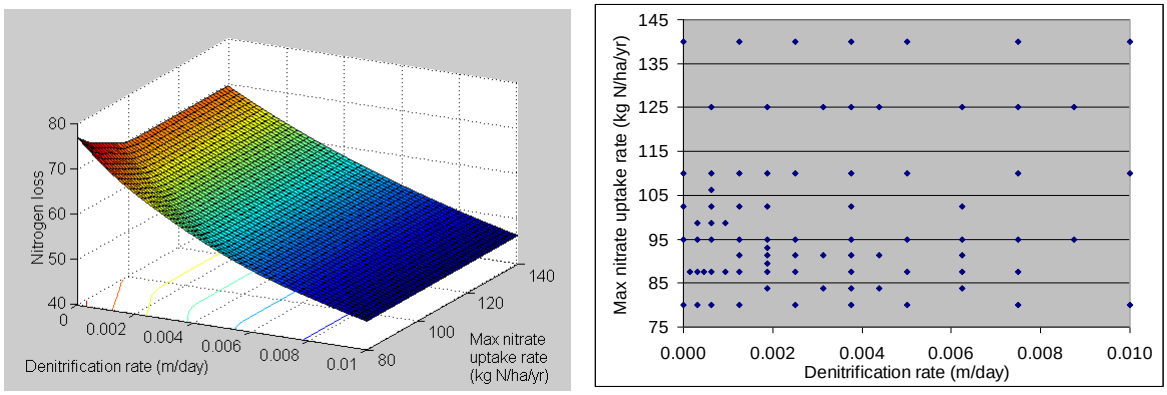

Figure 2. Response surface for nitrogen losses computed with the INCA-N model (left). Design points selected by our sequential design algorithm (right).

Further computer experiments involving the INCA-N model showed that high efficiency surrogate models could be derived for the relationship between the average annual loss of nitrogen and various subsets of model parameters controlling the turnover of nitrogen. This makes such surrogate models attractive for sensitivity and uncertainty analyses that can require thousands of model runs. Figure 3 shows the efficiency achieved for models with five and seven parameters, respectively. In particular, it can be seen that, even though the model under consideration was moderately nonlinear, our design was superior to grid designs with the same number of design points.

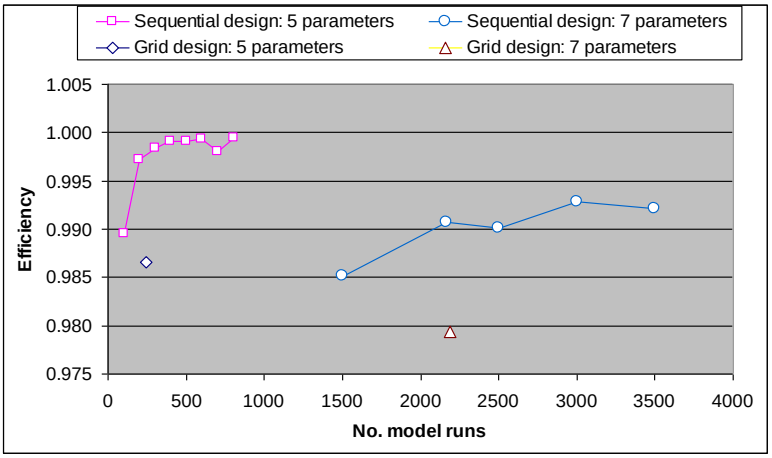

Figure 3. Efficiency of surrogate models derived from INCA-N simulations using our sequential design and regular grid designs. Model output: average annual nitrogen loss from an agricultural soil. Model inputs: parameters controlling the turnover of nitrogen.

Acknowledgements:

The authors are grateful for financial support from the Ministry of Science, Research and Technology of I.R. Iran, and the Swedish National Research Council.

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SEQUENTIAL EXPERIMENTAL DESIGN FOR STATISTICAL ANALYSIS OF NONLINEAR OUTPUTS OF COMPUTER MODELS

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An innovative sequential experimental design technique is proposed for the statistical analysis of expensive simulators with generally nonlinear outputs. The main objective is uncertainty analysis of outputs of complex computer models, such as oil reservoir simulators [5]. Such simulators usually require several hours or days for a single run, therefore direct sampling methods for uncertainty analysis (Monte Carlo) are usually impractical.

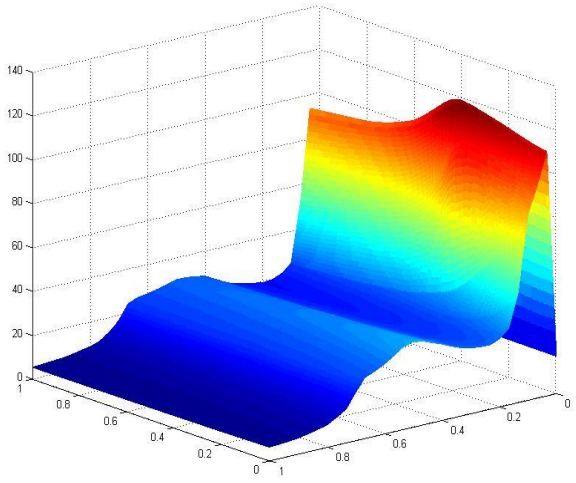
To reduce the number of necessary runs, the simulator output is approximated using different statistical regressions techniques such as low order polynomials or non-parametric regressions models based on stochastic Gaussian processes, such as kriging [3] or Bayesian approaches [2].
In this work we focus on non-parametric regression, which is more suited for nonlinear outputs than classical regression [4]. The objective is to build an accurate approximation of the model output as a function of its uncertain input using the least possible number of simulator runs.

To this end, we combine non-parametric regression with a new sequential experimental design based on the statistical information provided by the stochastic process used in the approximation.
A response $f(x)$ is modelled as a realization of a Gaussian process $Z(x)$ with a certain mean and covariance function. The mean and the covariance are generally unknown and are usually estimated by maximizing the marginal density of the data. To model the different impact of each input on the output, the covariance function $C(x, y)$ of the Gaussian process is taken as anisotropic:

$$C(x,y) = \exp\left(-\sum_{i=1}^{d} \left(\frac{x_i - y_i}{\lambda_i} \right)^2 \right)$$

where λ_i are correlation lengths corresponding to the different inputs.
At each step of the sequential design, the correlation lengths are estimated and are used to perform adaptive domain decomposition in order to split the input domain into quasi-uncorrelated input regions. Then new experimental points to be simulated are added into each region, according to customized predictivity criteria. Note that the number of points used in the sequential design will depend on the complexity of the function to approximate and on the desired accuracy of the approximation.

Several applications to standard test cases from oil reservoir simulation and also to standard analytic functions, will be presented. Comparisons are made with the well known maximin latin hypercube design showing, in all the considered test cases, a substantial improvement of the sequential design in increasing the approximation accuracy using the same number of simulations. Our customized accuracy estimation based on cross-validation, is used to find a threshold number N* after which adding simulation points do not sensibly increase the accuracy. An explanation of this behaviour, the "non-stationarity" of the response (as observed in the example shown in figure below) will be presented and discussed.



Example of non-stationary response surface: oil production rate as a function of two uncertain parameters (IC Fault Model)

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USING CLASSIFICATION TREES TECHNIQUES LIKE SENSITIVITY ANALYSIS IN THE FIELD OF RADIOECOLOGY

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This study is realized in the framework of the SENSIB project (an acronym referring to radioecological sensitivity) [1] which has been developed since 2003 by the French Institute for Radioprotection and Nuclear Safety (IRSN) and benefits from the financial support of ADEME, French Environment and Energy Management Agency. The main goal is to develop a standardised tool with a single scale of indexes in order to describe and compare the sensitivity of various environments to radioactive pollutions. Each index will represent a level of response of an environment to a pollution; for example an index of 1 refers to a low sensitive territory whereas a level of 5 refers to a high sensitive territory.
This communication focuses solely on the agricultural aspects of the SENSIB project. The objective is to determine whose factors (agronomical or radioecological) are of prime influence on the radioactive contamination of agricultural productions and will be the bases for the indexes construction. The identification of characteristics of the French territories whose stronger influence the fate of a radioactive contamination in the environment is based on radioecological models. These models are generally non–linear and utilize agronomical and radioecological input variables, often linked by linear and/or non-linear relations. That is why in order to obtain more knowledge and precision of how the models work, we decided to perform an original global sensitivity analysis by using classification trees techniques [2,3]. Contrary to the other methods of global sensitivity analysis [4], the classification trees techniques allow to determine which input variables or associations of input variables contribute mainly to the different categories (predetermined) of the model output. So, the pathways linking the input variables and the output of the model can be more precisely described and used to propose recommendations to mitigate the consequences of environmental radioactive contamination.

The method used to perform the sensitivity analysis is the CART method (Classification And Regression Trees) developed by Breiman et al [5]. The method is non-parametric and enables the construction of regression or classification trees depending on whether the output variable is quantitative or qualitative. A classification tree is constructed by successively splitting the data set into subsets called nodes. A recursive binary partitioning process is applied whereby parent nodes are always divided into two descending nodes (intermediate or terminal), and this process is repeated by considering each intermediate node as a parent node (see Figure 1).

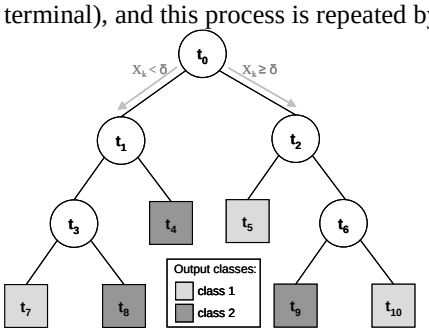

Figure 1: Example of classification tree

By performing a division δ on one of the input variables X_k, the root node t_0 (containing all of the output values) is divided into two child nodes t_1 and t_2 (two data sets): the node t_1 contains the output values for which $X_k < \delta$ and the node t_2 contains the complementary set. This process is then repeated on the descending nodes; they are also splitted into two child nodes. When the nodes are not divided, they are called terminal nodes or leaves and are assigned to a class of the output variable. Thus, each branch originating from the root node t_0 of the tree constitutes a path which, by a series of yes/no questions, arrives at a terminal node.

The building of a classification tree rests on a splitting criterion based on an impurity function (a pure node contains only values of one class of the output variable). Different splitting criterion exists, we use for the present study the entropy criterion defined by:

$$i(t) = -\sum_{k=1}^{m} P(k/t)\log(P(k/t))$$

where m is the number of classes of the output variable and P(k/t) the conditional probability of class k knowing that we are in the node t. Every splitting d at the node t leads to an impurity reduction:

$$\Delta i(d,t) = i(t) - p_g i(t_g) - p_d i(t_d)$$

where p_g et p_d are the proportion of the values in the left and the right nodes, respectively. The best splitting d* maximizes the impurity reduction: $\Delta i(d^*,t) = Max\{\Delta i(d,t); d \in D\}$.
The building of a classification tree by the CART method rests on the successive application of the three following steps:

- *Growing maximal tree*. The data set is splitting successively in order to build an extended tree. The splitting process is stopped when the node is pure or when the number of values in the node is less than a fixed size.
- *Tree pruning*. A sequence of trees is build. It consists in removing the large-sized branches of the extended tree which involve a weak increase of the misclassification rate. In order to measure this increase, a complexity parameter α is calculated and as it increases, more and more branches are pruned away leading to smaller trees.
- *Selection of the optimal tree*. Among this sequence of subtrees, the optimal tree has to be selected. The selection is based on the evaluation of the predictive error using a cross-validation or a pruning sample.

This method was applied on the concrete example of the transfer of strontium 90 to lettuce, the strontium 90 being released in an agricultural media due to an accidental emission in the atmosphere. The classification tree obtain (with the S-PLUS software) is presented on the Figure 2.

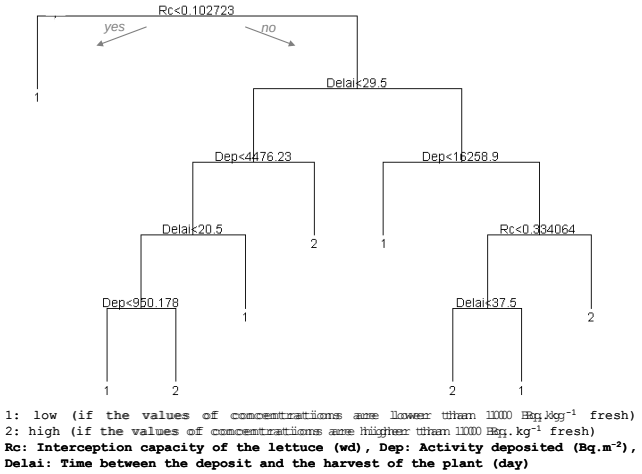

Figure 2: Classification tree obtained

The primary node is based on the input variable Rc, interception rate (range [0, 1]). From the left branch of the tree, we can deduce a first decision rule: *if* Rc < 0.1 *then* ^{90}Sr activity = low. Because the variable Rc can be correlated with the stage of growing of vegetable, such an indication of Rc can be translated directly in operational countermeasure for the farmers.
Variables or association of input variables whose characterize high values of activity are deduced from another branch of the optimal tree, for example:
if Rc ≥ 0.1 *and* Delai < 29.5 *and* Dep ≥ 4476.23 *then* ^{90}Sr activity = high.
Thereby, a complete examination of the tree structure allows determining whose combinations of factors are responsible to low and high values of radioactive contamination.

However, one of the disadvantages of classification trees is their instability [6]. A little modification in the data set (used to build the tree) can lead to a very different tree. This instability has an impact on the tree nodes (splits), on the tree size, and moreover on the prediction. To avoid this problem and to stabilize the results of predictions, methods based on model aggregation like Bagging [7] or Random Forest [8] are proposed. These methods can clearly improve the capacities of the predictors, however the tree structure is lost and so the potential decisions rules which result from it are also lost. In order to preserve the tree structure and to obtain more stable decisions rules, a node-level stabilizing procedure is proposed [9]. By using this algorithm a new extended tree is build. The new optimal tree obtained is more stable and support a more robust identification of the most sensitive variables. This method was applied on the preceding example and allows us proposing robust recommendations to mitigate the consequences of environmental radioactive contamination.

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PHASE SENSITIVITY ANALYSIS OF LIMIT CYCLE OSCILLATORS

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A comprehensive analysis is presented of the different types of phase sensitivities of limit cycle oscillators with respect to parameters. A general framework based on the solution of a boundary value problem is presented which permits exact calculation of the desired quantities. Furthermore, a decomposition of the state sensitivities into a sum of three terms each with a specific contribution to the overall sensitivity is discussed in detail. Numerical examples are used to demonstrate the techniques and validate the results. Example systems are taken from the biological literature, where limit cycle oscillators of different levels of detail are used to model the circadian clock mechanism.

The sensitivity analysis of limit cycle oscillators is, compared to the sensitivity analysis of other dynamical systems, complicated by several factors. First, from any initial condition within the region of attraction, the periodic orbit is reached only in asymptotic fashion, but it is of interest to study its exact properties. Furthermore, it is desired to analyze derived properties which are implicit in the mathematical description of the limit cycle, such as amplitude, period and phase of oscillation, and their parametric dependencies.

A boundary value formulation, similar to the one proposed by Rosenwasser and Yusupov [1], avoids dealing with transients and allows the direct computation of the period sensitivities of the limit cycle. A boundary value problem (BVP) is formulated similarly to those used in circuit analysis [2], in such a fashion that the first *n* equations ensure the periodicity of the solution, and the *(n+1)*st equation is a phase locking condition (PLC) which defines a reference for time zero. When these equations are formally differentiated with respect to the parameters, the resulting matrix equation can be solved for the period sensitivities and the sensitivities of the initial conditions on the limit cycle, as found from the solution of the BVP. Using these initial condition sensitivities, the sensitivity trajectories can be integrated along with the dynamic system, and amplitude sensitivities can be obtained from the sensitivities at the extrema of the various state variables [1].

The work presented here shows that the choice of PLC is of significance not only for the numerical well-posedness of the resulting BVP, but more importantly for the computation and interpretation of meaningful sensitivities of derived properties, in particular those of the peak-to-peak sensitivities, as described below.

As shown in [1,3-4], the state sensitivities can be separated into an unbounded, period-dependent part and a strictly periodic part,

$$\mathbf{S}(t) = -\dot{\mathbf{y}}(t)\frac{t}{T}\frac{\partial T}{\partial \mathbf{p}} + \mathbf{Z}(t), \tag{1}$$

where $\mathbf{S} \equiv \frac{\partial \mathbf{y}}{\partial \mathbf{p}}$ are the sensitivities of the state variables with respect to the parameters, $\frac{\partial T}{\partial \mathbf{p}}$ are the period sensitivities with respect to the parameters, and $\mathbf{Z}(t)$ are the T -periodic sensitivities of the state variables with respect to the parameters at a fixed period.

This work introduces an exact and unique decomposition of the periodic part $\mathbf{Z}(t)$ into a periodic, phase dependent part and a periodic, amplitude dependent part. (A similar decomposition into amplitude and phase components was used for oscillator noise analysis [5]). The full sensitivity is thus composed of three specific contributions:

$$\mathbf{S}(t) = -\dot{\mathbf{y}}(t)\frac{t}{T}\frac{\partial T}{\partial \mathbf{p}} + \mathbf{W}(t) + \dot{\mathbf{y}}(t)\boldsymbol{\delta}$$

where $\boldsymbol{\delta}$ is a constant row vector that describes the influence of the PLC on the solution of the BVP and contains information about the sensitivities in the direction tangential to the periodic orbit. $\mathbf{W}(t)$ are the state sensitivities for constant period and constant phase, in other words the $\mathbf{W}(t)$ term describes only the influence of the parameters on the amplitudes of the different state variables and therefore the shape of the limit cycle.

This new decomposition is the starting point for the definition and computation of different types of phase sensitivities. First, a sensitivity of the phase set by the PLC with respect to the parameters is discussed. This quantity is then used to define a particular type of sensitivity, which is unique to oscillatory systems, and is termed a "peak-to-peak" sensitivity. It describes how an infinitesimal change in parameters would cause a change in the time between two peaks or troughs of different state variables. The choice of PLC is obvious in this case, an extremum of a state variable of interest is chosen as the time reference. A simple equation is derived for the exact computation of these sensitivities and the results are compared to the proportional sensitivity of the peak-to-peak distance with respect to overall period change (i.e., stretching or compressing of the oscillation). In doing so, information about the flexibility of the system is gained, in the sense of whether the time span between specific events (e.g., peaks) can be varied independently of the overall period.
This quantity is of interest in the context of circadian biology; while the total length of day is constant at 24 hours, the length of the sunlit day, or the time between dawn and dusk, undergoes seasonal variation. It could be hypothesized that the clock mechanism might have the capability of adjusting to this variation by varying the peak-to-peak distances of pertinent state variables without varying the period of oscillation. This hypothesis is evaluated using peak-to-peak sensitivity analysis.

A different type of phase sensitivity analysis is the analysis of phase shifts caused by perturbing the state variables from the limit cycle. Such perturbations cause temporary deviations from the periodic orbit that decay over time, but result in permanent phase shifts that are a functions of the perturbation and the system parameters. The sensitivity of this permanent phase shift with respect to the perturbed variables and also with respect to the system parameters is derived and computed exactly and efficiently.
The sensitivity of the phase shift with respect to the perturbed states was approximated in the past using a limit finding process [4]. We show, however, that this sensitivity information is contained in the first left eigenvector of the Monodromy matrix of the limit cycle oscillator, with appropriate scaling.

The sensitivities described above were computed for two model systems. The first test system is a simple model of the circadian clock, called the Goodwin oscillator, composed of 3 state variables and 6 parameters [6]. The second test system is the most detailed ordinary differential equation model of the circadian clock currently published, which consists of 73 state variables and 231 parameters [7]. All results were compared to finite difference approximations, to demonstrate the methods are accurate yet far more efficient.

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SENSITIVITY ANALYSIS AND EXPERIMENTAL DESIGN OF A STIFF SIGNAL TRANSDUCTION PATHWAY MODEL

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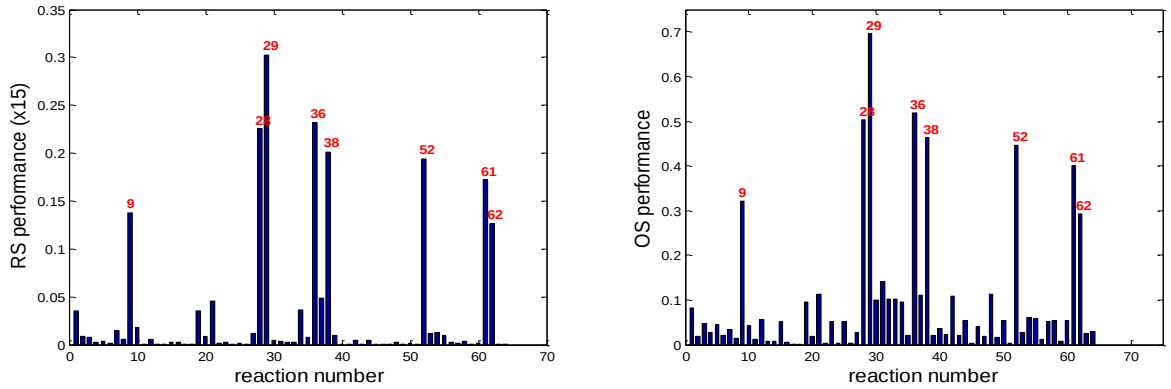
Sensitivity analysis is normally used to analyze how sensitive a system is with respect to the change of parameters or initial conditions and is perhaps best known in systems biology via the formalism of metabolic control analysis [1, 2]. The nuclear factor κB (NF-κB) signalling pathway is an important cellular signalling pathway, of which protein phosphorylation is a major factor controlling the activation of further downstream events. The NF-κB proteins regulate numerous genes that play important roles in inter- and intra-cellular signalling, cellular stress responses, cell growth, survival, and apoptosis. As such, its specificity and its role in the temporal control of gene expression are of crucial physiological interest.

The mathematical model used in this work is the TNFα-mediated NF-κB model provided by Hoffmann *et al.* [3]. In this model (and experimentally) there are significant oscillations in the concentration of NF-κB in the nucleus (NF-κB$_n$) [3-5]. The dynamics of the system is described by a set of ordinary differential equations (ODEs) with given initial conditions. As this system involves a large number of reactions and the parameters span several orders of magnitude, the ODEs turn out to be nonlinear and stiff. The direct differential method (DDM) is used to calculate the local sensitivities as a function of time. Relative sensitivity coefficients are used for parameter ranking and experimental design. In order to consider the complete dynamics of the oscillation system, two performance indices are proposed for analysis. One is to use a single variable (nuclear NF-κB) to form the L^2-norm performance, the other is to include all species concentration profiles to formulate the Euclidean-norm function. For this system, the local sensitivity analysis using nuclear NF-κB only and all species produce consistent results (see fig 1 (a) and (b)).



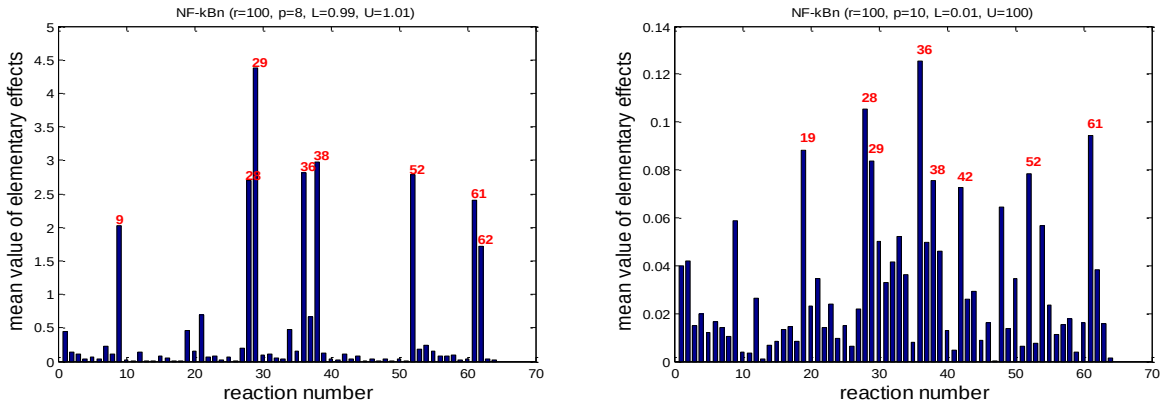
(a) single variable: NF-κB$_n$ (b) all variables included

Figure 1. Relative sensitivity indices with single variable and multiple variables

The Morris method [6] is used to investigate the global sensitivity of the system. It is supposed that a finite distribution of elementary effects associated with each input can be estimated. Two sensitivity measures were proposed for each factor: μ, an estimate of the mean of the distribution, and σ, an estimate of the standard deviation of the distribution. These two measures are used as indicators of which inputs should be considered important. Modifications to the original Morris method is proposed to deal with the case that the parameters are within wide and different intervals. Simulation results in terms of μ are given in fig.2 with both wide and narrow ranges being considered. It can be seen that when the parameter range is very small, global analysis makes similar results as that of the local analysis (see fig.1 (a) and fig2. (a)). However, when the analysis range is large, it produces a different sensitivity pattern from the local analysis (see fig.1 (a) and fig2. (b)). This is because global sensitivity analysis can provide information on interactions between parameters and also reveal the non-linear effects from simultaneous parameter variation while local sensitivity analysis can't.

Optimal experimental design on the IKK activation intensity is then performed based on sensitivity analysis. Under the assumption of uncorrelated measurement noise with zero-mean Gaussian distribution, the information content of measurements can be quantified by the Fisher information matrix (FIM) [7, 8]. In general, the smaller the joint confidence intervals for the estimated parameters are, the more information is

contained in the measurements. The FIM is formulated from the sensitivity matrix. Along with the Cramer-Rao theorem, the FIM is used to determine the optimal step input signal such that the estimated parameters have the minimum variance. Taking IKK as the step input and nuclear NF-κB as the system output, four commonly used optimal design criteria, i.e., A-optimal, D-optimal, E-optimal and the modified E-optimal design, are used for calculation. Simulation shows that the optimal initial concentration of IKK is 0.1 μM under the modified E-optimal design, and it is 0.06 μM under the other three optimal designs. The 95% confidence intervals of these two results are illustrated in fig.3 when two sensitive parameters are considered each time. It can be seen that the optimal input amplitude should be 0.06 μM because its confidence interval ellipsoid is smaller.



(a) narrow range [0.99, 1.01] θ_0 (b) wide range [0.01, 100] θ_0

Figure 2. Global sensitivity analysis results in terms of the mean value of the elementary effects in Morris method (θ_0 stands for nominal value in simulation)

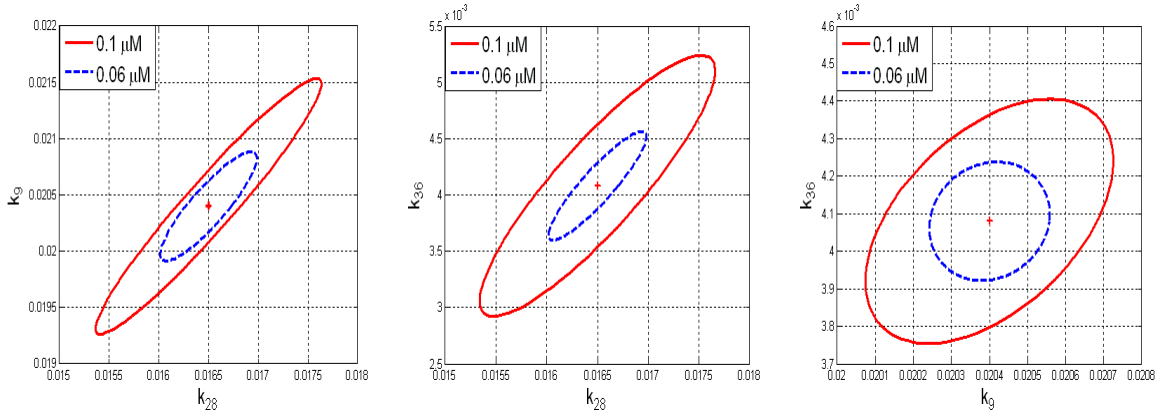


Figure 3. Confidence intervals of two different amplitudes of the step input

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UNCERTAINTY ANALYSIS OF NITROGEN OXIDE FORMATION IN METHANE COMBUSTION

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The combustion of methane is one of the most frequently modelled chemical reactions due to its high academic and industrial importance. Methane is the main component of natural gas, which is widely used for power generation and heating. NO is the major pollutant formed during natural gas combustion. Methane combustion mechanisms are widely used for the prediction of the NO production and can be used for the design of low-NOx burners. No quantitative investigation of the uncertainty of the NO production has been published. Also, the uncertainty of the ratios of the various NO formation routes is not known.

In this study, the Leeds Methane Oxidation Mechanism [1], extended with an NO-formation mechanism [2] was used. This joint mechanism is capable of simulating the formation of NO during methane combustion at a wide range of conditions. The mechanism contains 340 irreversible reactions of 56 species. The kinetic data were updated based on a literature search and the thermodynamic data were revised using Burcat's recent thermodynamic database [3].

The NO formation kinetics was investigated at the conditions of the experiments of Bartok *et al.* [4]. This set of experiments is a frequently used benchmark of NO formation during methane combustion. The experiments were carried out in a perfectly stirred reactor at atmospheric pressure. The residence time was 3 ms and the equivalence ratio was changed between 0.67 and 1.75. The simulations were carried out with the PSR code [5] of the CHEMKIN-II package. This program was modified for calculating the local enthalpy-of-formation sensitivity coefficients and carrying out sequential calculations with several different parameter sets as required by the global uncertainty analysis methods. Local uncertainties were calculated by program KINALC [3].

Combustion models include thousands of parameters, like kinetic parameters, thermodynamic data, diffusion coefficients etc. In this study, the uncertainty of rate coefficients and enthalpy-of-formation data were considered. For the rate coefficients, lognormal distribution was assumed; the variance was determined [6] from the uncertainty factor *f*, which was available from several kinetic databases. Normal distribution was assumed for the enthalpies-of-formation of each species; the expected values and the variances were determined from thermodynamic databases. The uncertainties of all kinetic and thermodynamic parameters were assumed to be independent.

Based on local sensitivity coefficients and the variance of parameters, and using the rules of error propagation [6] uncertainty of the calculated NO concentration was determined. This local uncertainty analysis allows computationally cheap investigation of the contribution of parameters to the uncertainty of results and the determination of the ratio of the kinetic and thermodynamic uncertainties.

Monte Carlo Analysis with Latin Hypercube Sampling (LHS MC) [7] was carried out; 1000 parameter sets were generated and used in the simulations in each case. Processing the results, the probability density function of the calculated NO concentration was determined. Also, this analysis shows [7], which are the possible maximum and minimum NO concentrations that can be achieved by tuning all parameters simultaneously within their physically realistic limits.

At lean conditions, the measured data are well within the uncertainty limits of simulations. At fuel rich conditions, the uncertainty limits are lower and the experimental data are outside the uncertainty limits, showing a major applicability problem of the mechanism at these circumstances. There was good agreement at all conditions between the variance of NO concentrations calculated by local and global (Monte Carlo) methods.

We have determined that at stoichiometric conditions the uncertainty of the calculated NO concentration is mainly due to the uncertainty of kinetic parameters. Changing the equivalence ratio to lean and especially to rich conditions, the contribution of the thermodynamic data to the uncertainty significantly increased. The lists of reactions and species were determined, belonging to the kinetic parameters and enthalpies-of-formation that cause high uncertainty of NO production. These parameters included the enthalpy-of-formation of NNH at lean conditions; kinetic parameters of reactions $NO+NH=N_2O+H$, $O+NNH=NH+NO$, $H+CH_2=CH+H$ and $H_2O+CH=CH_2O+H$ near stoichiometric conditions; and $H_2O+CH=CH_2O+H$ at fuel rich conditions.

In combustion systems, NO can be formed in four parallel pathways; these are the thermal, prompt, via N_2O and via NNH formation routes. The relative contribution of these formation pathways and their uncertainty was investigated as a function of equivalence ratio. Based on the Monte Carlo analysis results at three equivalence ratios, NO-formation histograms for each route were generated.

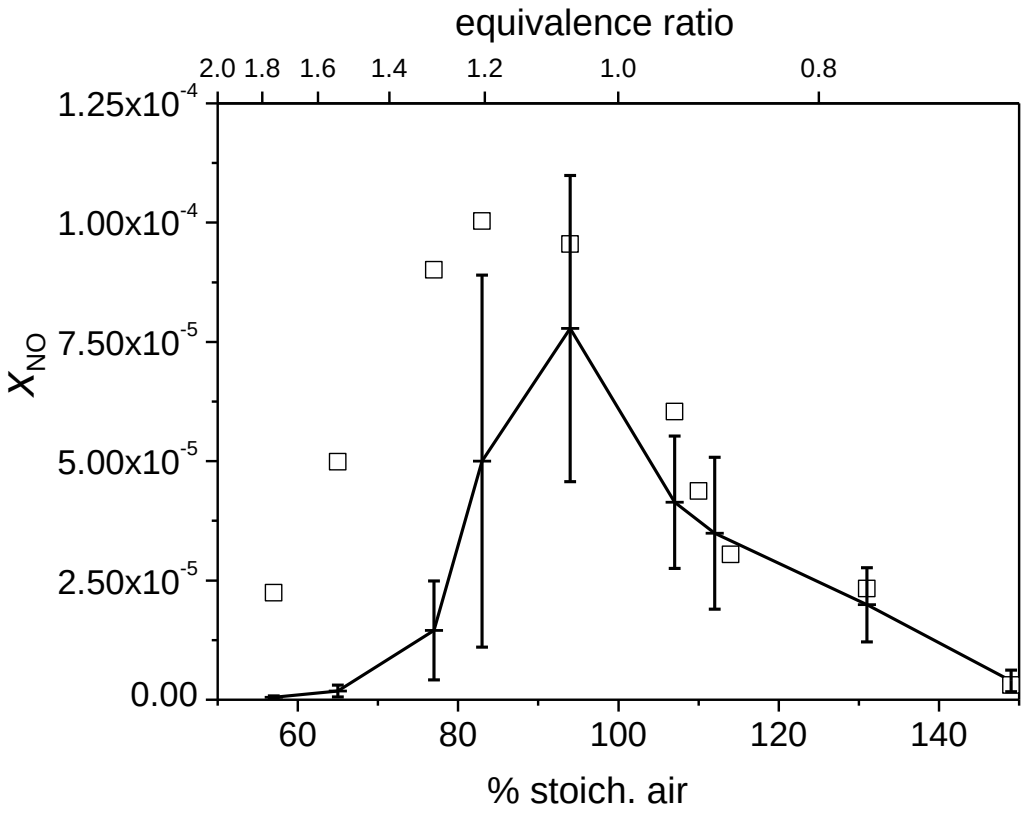

Figure 1: Comparison of the experimental data of Bartok et al [4] (squares), the simulation results (line) and the 1σ uncertainty of the simulation results.

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A GLOBAL SENSITIVITY STUDY OF SULPHUR CHEMISTRY IN A PREMIXED METHANE FLAME MODEL USING HDMR

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The use of accurate computational models describing combustion processes is crucial for the design of low emission technologies. Trace amounts of sulphur in the fuel can have an impact on the extent of nitrogen oxide emissions and therefore suitable models describing the interaction of sulphur containing compounds with other species within flames are required [1]. Sulphur chemistry is however, quite poorly understood at high temperatures, with many reaction rates and thermochemical parameters being estimated in previous studies. An assessment of the resulting uncertainty in predictions of nitrogen oxide emissions is therefore of interest. Identifying the main sources of uncertainty provides useful information for further experimental and *ab initio* kinetic studies. Combustion models provide a challenge for uncertainty analysis since they often contain a large number of uncertain parameters such as reaction rate coefficients and heats of formation. If such parameters are estimated then their uncertainty ranges can be quite large [2]. Combustion models also tend to be highly nonlinear. The use of traditional methods for global uncertainty and sensitivity analysis such as Monte Carlo simulations therefore becomes problematic due to their computational expense and the difficulty in interpreting the results for large parameter sets. Commonly a screening method such as the Morris method [3] is first applied in order to identify unimportant parameters if the input space dimension is very high. This can help with the interpretation of Monte Carlo outputs, but does not necessarily reduce their computational expense [2]. Recently the method of high dimensional model representation (HDMR) [4] was developed to provide a model replacement that can be easily employed within global uncertainty analysis. HMDR methods provide a straightforward approach to explore the input output mapping of a model without requiring large numbers of full model runs. Furthermore, sensitivity indices can be determined in an automatic way in order to rank the importance of input parameters and to explore the influence of parameter interactions.

The effectiveness of the Random Sampling (RS)-HDMR [5] approach is shown in this work via application to a premixed methane flame model describing the influence of fuel trace elements, such as sulphur containing compounds, on the formation of nitrogen oxides in combustion devices. The modelling process is carried out by the CHEMKIN [6] package and the simulation has been performed using PREMIX [6]. The SOx extension of the methane/NOx mechanism studied here consists of 156 reversible reactions and 24 species [2]. The uncertainty study focuses on reactions of sulphur containing species and their heats of formation. Due to the poor categorisation of many of the thermo-kinetic parameters, uncertainty ranges are defined according to a minimum and maximum possible value with equal probability of the values across the range.

An optimisation method was introduced in [7] as an extension to the existing set of RS-HDMR tools. The RS-HDMR component functions can be approximated by analytical basis functions such as orthonormal polynomials which reduces the sampling effort dramatically [5]. Usually the first and second-order component functions are approximated by orthonormal polynomials all of the same order. The idea of the optimisation method is to decide which component function is approximated best by which polynomial order. In [7] a maximum polynomial order of three has led to very satisfactory results. This approach has been extended here to further improve the accuracy of the mapping process by applying a maximum polynomial order of seven. The optimisation method also provides a possibility to exclude HMDR component functions, which have only a very small contribution to the overall output uncertainty, by introducing a threshold. This provides an automatic way to identify unimportant parameters within the analysis, thus removing the necessity to employ screening methods, even for a problem with such a high dimensional input space. For comparison, the results obtained from the extended RS-HDMR method are compared with widely used methods, such as Morris One at a Time and Monte Carlo simulations.

The computational effort required for the construction of the HDMR model replacement is considerably lower than for traditional global uncertainty analysis methods. A total of only 1024 full model runs were sufficient to produce a model replacement with very high accuracy. The model replacement can then be used to assess the output uncertainty of the model and to calculate sensitivity indices. In this study we explore the sensitivity of nitrogen oxide emission to possible changes in the kinetic rate parameters and the thermodynamics of sulphur containing compounds.

The three highest ranked reactions identified by the HDMR method are SO+NH=NO+SH, SO+N=NO+S and SO+OH=SO_2+H. The Morris method identifies the same reactions in the same order. The final NO concentration is mainly influenced by first-order effects, which means that input parameters are acting independently upon the output. Plots of the HMDR component functions are shown to reveal useful information about the input output relationships of the model and can be used to calculate first and second-order sensitivity indices without the need for additional full model runs. Some of the first-order effects are identified as being very non-linear as shown in Figure 1. The results indicate that several parameters show high sensitivity in some parts of their input ranges but that their effect is much reduced in other regions. Local sensitivity coefficients would therefore be strongly affected by the nominal values chosen.

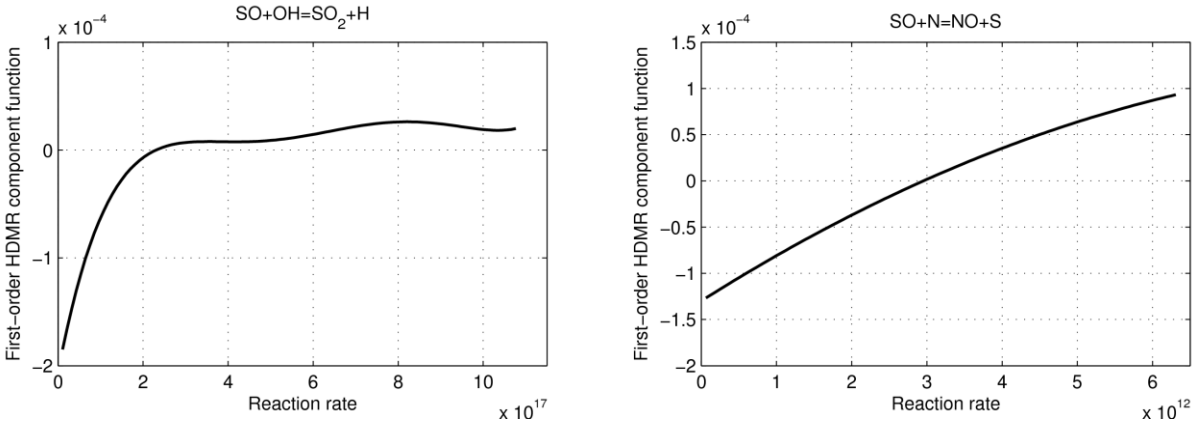

Figure 4: First-order RS-HDMR component functions approximated by orthonormal polynomials.

The output statistics of the full model are shown to be well represented by the model replacements. The proposed HDMR method therefore provides a powerful tool for general application to global uncertainty and sensitivity analysis of chemical models and can be applied without using a screening method in advance in order to identify unimportant parameters.

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POLYNOMIAL CHAOS EXPANSIONS FOR UNCERTAINTIES QUANTIFICATION AND SENSITIVITY ANALYSIS

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The purpose of the paper is to show that polynomial chaos expansions can be effective in modelling uncertainties and dealing with sensitivity analysis based on the analysis of the variance. We show the connection between Sobol's decomposition and generalized polynomial chaos expansion for sensitivity estimates for non linear mathematical models.

1. Polynomial Chaos expansions

Polynomial Chaos (PC) expansions are derived from on the original theory of Wiener [1] for the spectral representation of stochastic processes using Gaussian random variables. PC expansions have been used for uncertainty quantification by Ghanem and Spanos [2] and extended by Xiu and Karniadakis [3] to non-Gaussian uncertainty input. Any well-behaved process y (e.g. second order process) can be expanded in a convergent (in the mean square sense see Cameron and Martin [4]) series of the form :

$$y(x,t,\xi) = \sum_k y_k(x,t)\Psi_k(\xi)$$

where ξ is a set of d independent random variables with a known joint density $p(\xi)$, ψ_k are orthogonal polynomials and $y_k(x,t)$ are the PC coefficients or stochastic modes of y. Denoting with the brackets "<.>" the expectation operator and taking into account orthogonality of Ψ_k we have :

$$y_k(x,t) = \left\|\Psi_k\right\|^{-2} < y(x,t).\Psi_k > (1)$$

For practical use, the PC expansions have to be truncated in term of polynomials order. Several approaches can be used to estimate PC coefficients. The first is based on Galerkin projection of the model equations, leading to a set of coupled equations for the coefficients $y_k(x,t)$. This approach requires an adaptation of deterministic solvers. Opposing approaches, of simpler implementation, are based on Monte-Carlo simulations or quadrature formulas to evaluate PC coefficients from equation (1), see for instance Le Maître *et al* [5]. When the number d of variables is large, quadrature formulas based on tensor product of 1D formulas, requires too many numerical evaluations and sparse grids integration based on Smolyak's constructions [6] are preferred. PC coefficients are therefore evaluated from a set $\left\{\left(\xi^i,\omega^i\right), i=1,2,\cdots,n\right\}$ of points and weights by formulas of the form

$$y_k(x,t) \cong \hat{y}_k(x,t) = \left\|\Psi\right\|^{-2}\sum_1^n y(x,t,\xi^i)\psi_k\left(\xi^i\right)\omega^i$$

The projection on the PC basis results in a surrogate model approximating the numerical model of uncertainties :

$$y(x,t,\xi) \cong \sum_{k=0}^p \hat{y}_k(x,t)\psi_k(\xi)$$

The mean and the variance are derived from the PC expansion respectively by the first coefficient $\hat{y}_0(x,t)$ and by $\sum_{k=1}^p \hat{y}_k^2(x,t)\left\|\Psi_k\right\|^2$. Fractiles can also be calculated by Monte-Carlo simulations of the PC surrogate model.

2. Sensitivity analysis from PC expansions

Now, we consider the global analysis, like named in Saltelli *et al* [7] based on analysis of variance and we use Antoniadis's notations [8]. To simplify notations, let us consider a random variable and a Sobol-like decomposition of a PC expansion of y :

$$y(\xi) = \sum_{k=0}^{\infty} y_k\Psi_k(\xi) \cong \hat{y}(\xi) = \sum_{k=0}^p \hat{y}_k\Psi_k(\xi_1,\xi_2,\cdots,\xi_d) = \sum_{u\subseteq\{1,2,\cdots,d\}} f_u(\xi_u)$$

where f_u gathers the terms of the PC expansion which depend only of the components of $\xi_u \subseteq \xi$ whose index is in u with $f_\varnothing = \hat{y}, \Psi_0 = \hat{y}_0$. Let us note K_u the subset of the set of indexes $K = \{1,2,\cdots,p\}$ such as $K_u = \left\{k \in K \middle| \Psi_k(\xi) = \Psi_k(\xi = \xi_u)\right\}$.

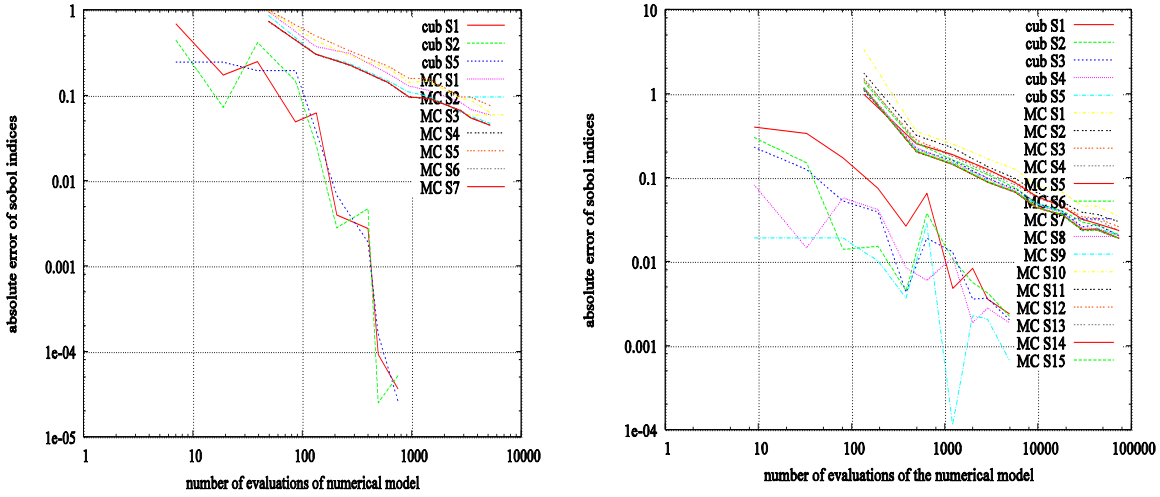
Taking into account orthogonality of f_u and Ψ_k, we have :

$$f_u(\xi_u) = \sum_{k \in K_u} \hat{y}_k \Psi_k(\xi) \Rightarrow \int f_u^2(\xi) p(\xi) d\xi = \sum_{k \in K_u} \hat{y}_k^2 \left\| \Psi_k \right\|^2 = \sigma_u^2$$

and we obtain the ANOVA decomposition and the Sobol's sensitivity indices :

$$\sigma_{\hat{y}}^2 = \sum_{u \subseteq \{1,2,\cdots,d\}, u \neq \varnothing} \sigma_u^2 \Rightarrow S_u = \sigma_u^2 / \sigma_{\hat{y}}^2$$

We have applied PC expansion to two classical test using Petras's toolbox [9] for sparse numerical quadrature.



The figures show absolute error of sobol indices according to the number of evaluations of the numerical model, Homma-Saltelli model (left) : $\sin(\xi_1) + a\sin^2(\xi_2) + b\xi_3^4 \sin(\xi_1), a = 7, b = 0.1, \xi_i \approx U(-\pi, \pi)$ and Saltelli-Sobol model (right) : $\prod_{i=1}^{d} \left(\left|4\xi_i - 2\right|\right)/(1+a_i), a_i = (i-1)/2, d = 5, \xi_i \approx U(0,1)$. We can observe that the error decreases in $1/\sqrt{n}$ for MC simulations. PC requires less numerical evaluations than MC simulations. Nevertheless, the difference in efficiency PC-MC reduces when the stochastic dimensions increases. Current efforts focus on the construction of sparse grids and adaptive methods to improve the precision on the integral evaluations and improve the convergence of PC expansions [10].

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MOMENT-INDEPENDENT GLOBAL SENSITIVITY ANALYSIS WITH CORRELATED INPUT FACTORS: AN APPLICATION TO A CHEMICAL REACTOR

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Recent works have proposed the use of a moment independent measure of uncertainty importance by looking at the entire distribution of the model output (Borgonovo [1] and [2]). Let $\underline{X} \in E \subseteq R^n$ be a set of (correlated) input factors characterized by the joint p.d.f $f_{\underline{X}}(\underline{x})$, and Y=g($\underline{X}$) be the output of the model of interest. The δ-importance of X_i is defined (Borgonovo [1] and [2]) as:

$$\delta_i = E_{X_i}\left[\int \left| f_Y(y) - f_{Y|X_i}(y)\right| dy\right] \quad \textbf{(1)}$$

where $f_Y(y)$ is the joint unconditional density of Y and $f_{Y|X_i}(y)$ is the conditional density of Y given X_i.

The works of Borgonovo [1] and [2] have estimated and compared δ and Sobol's sensitivity indices for models in the absence of correlations. We recall that Sobol's global sensitivity indices are defined starting from the following high-dimensional model representation of Y (Sobol' [3], Alis and Rabitz [4]):

$$g(\underline{X}) = \sum_i g_i(X_i) + \sum_{i<j} g_{i,j}(X_i, X_j) + \ldots + g_{1,2,..n}(X_1, X_2, \ldots, X_n) \quad (2)$$

The decomposition in eq. (2) is unique under the assumption that $f_{\underline{X}}(\underline{x}) = \prod_i f_{\underline{X}}(\underline{x})$, i.e., when the X_i are independent.

Correlations (and dependencies in general) lead to a number of issues in performing global sensitivity analysis, as highlighted in the works of several authors. Bedford [5], evidences that correlations cause loss of uniqueness of eq. (2). Saltelli and Tarantola [6] treat the computation of variance-based importance measures by introducing two "*Settings.*" In the first setting they identify the factor that, if determined, would lead to the greatest reduction in the output variance . The corresponding sensitivity measure is:

$$V_i = V\left[E(Y \mid X_i)\right] \quad (3)$$

V_i coincides with the first order terms of Sobol's variance decomposition in the absence of correlations. The second setting of Saltelli and Tarantola [6] consists in identifying the smallest set of factors that leads to a target variance reduction.

In this work, we study the effects of correlations in the computation of the δ importance measure, as they have not been dealt with yet, and compare them to the effects on the variance-based measure in eq. (3). We proceed as follows. We tackle the issue of the computation first. We develop a numerical algorithm based on Replicated Latin Hypercube for the generation of the correlated samples. We inspect the effect of correlations using three test cases: a linearly additive model, a multiplicative model and the Ishigami test function (see [1] and [2]). On all the models analytical expressions for V_i importance measures were available. We investigate the effect of increasing correlations in the parameters on the sensitivity analysis results. We obtain first the results for the independence case; we then examine the effect of a 0.25, 0.50, 0.7 and 0.9 correlation on the parameters. The utilization of the linear case has the advantage of making transparent the effect of correlations, as no interactions are present in the model. We then analyze how results change as a function of model complexity, starting with a model which is completely characterized by interactions. This allows us to study how interactions and correlations interfere. This approach gives us the possibility of studying the relationship between δ-additivity and interactions. We recall that interactions are defined based on Sobol' function decomposition and they can be appreciated by the sensitivity indices (Sobol' [3]):

$$S_{i,j,\ldots,m} = \frac{\int \cdots \int \left[g_{i,j\ldots,m}(X_i, X_j, \ldots, X_m)\right]^2 \prod_{k=i,j,\ldots,m} dX_k}{V} \quad (4).$$

If a model does not entail interactions and the parameters are independent, then all the $S_{i,j\ldots,m}$ are null and the first order sensitivity indices sum to unity ($\sum_{i=1}^{n} S_i = 1$.) One says that the model is additive. Similarly, if $\sum_{i=1}^{n} \delta_i = 1$ holds, we say that δ-additivity holds. Considering different model structures, we explore what are the conditions under which a model is δ-additive and analyze whether the same conditions assure additivity of variance-based sensitivity results. We are then left with investigating the effects of dependencies on δ-additivity. Finally, we apply these procedures to a model for the stability of a chemical reactor, whose global sensitivity analysis has been discussed in Saltelli et al [7] for the independent input case.

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SIMPLEX SCREENING

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This paper presents a new screening method which takes up the principles of Morris' method, without the "one at a time" (OAT) constraint. We will show why, in particular cases, OAT designs should be avoided.

The increasing use of computer experiments has gone along with a larger number of model parameters to analyze and control. In high dimension, it is uncommon that the number of computer simulations is sufficient to correctly characterize the model. The usual procedure is then to reduce the number of dimensions by considering the group of factors that are known to be the most influent. To this end, screening techniques are used to "prune" models at a low computational cost.

Screening is a preliminary phase in the study of a computational model. Typically a metamodel is estimated in order to perform studies that would not be possible directly on the simulator: sensitivity analyses, optimization… Reducing the number of dimensions of the metamodel decreases its variance of estimation, thereby improving its quality.

Among the screening methods, the method of Morris [2,3] is often applied when a reasonably large number of simulations can be done (more than *5p* simulations, where *p* is the number of factors). Although this number is very low, it is high compared to other screening methods (for example, supersaturated designs that require less than *p* simulations). The method of Morris has two main advantages. Firstly, in most cases all influent factors are screened, and this thanks to its "high" computational cost. Secondly, it provides very rich information: in addition to the main effects it gives indications on nonlinearities and interactions.

In this work, we consider that screening has exhausted the simulation budget. We then have no other choice than estimating the metamodel with the screening design points. We note $\vec{x}_i = (\vec{u}_i, \vec{v}_i)$ the design points, with $\vec{u}_i$ and $\vec{v}_i$ the influent and the non influent factors, respectively, and $y_i = f(\vec{x}_i)$ the responses. We are seeking a metamodel *g* such that $y_i = g(\vec{u}_i) + \varepsilon_i$. This means that the orthogonal projection of the original points onto the subspace formed by the influent factors is considered.

Figures 1 and 2 represent two screening designs in 2D. The first is a well known Morris' OAT design [2,3]. The second is the "simplex screening design" which we introduce in this paper. The projections of the points on the *u*-axis are represented in dotted lines.

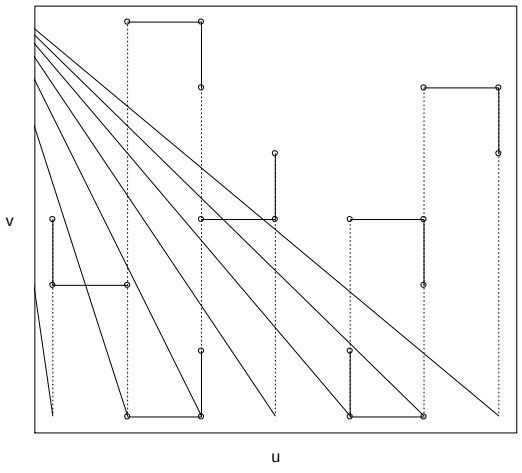

Figure 1 : Morris' OAT design

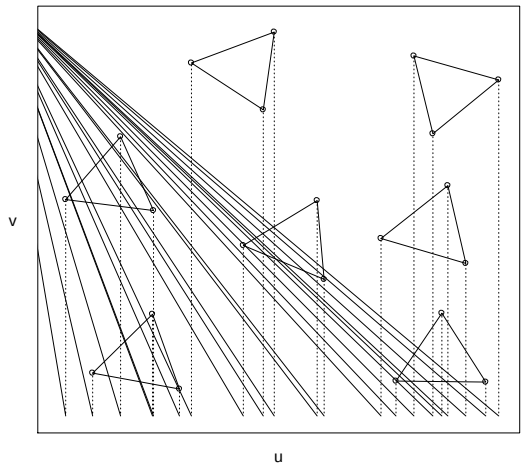

Figure 2 : simplex screening design

In figure 1, vertically aligned points superimpose onto each other through projection. For a regression on the first dimension, this leads to a loss of information. It is not a loss of points: all the points will be used for the regression, but one projected point could match several points of the design. In figure 2, the projections give a

better coverage of the *u*-axis. For the same kind of regression, uncertainty upon the regression will be lower with the design of figure 2 than with that of figure 1. This illustrates why the simplex design can be more informative in projection than Morris' OAT.

The simplex design of experiments does not have a structure as rigid as that of Morris, but it makes it possible to calculate as efficiently the same sensitivity indices. Indeed, one elementary effect per factor can be computed for each simplex by interpolating a first order polynomial (Snee and Marquardt [5]):

$$Y = d_0 + \sum_{i=1}^{p} d_i X_i$$

The elementary effects are given by the coefficients d_i. Then, the sensitivity indices μ^* and σ are calculated according to the Morris' method (Campolongo [1]):

$$\mu_i^* = E|d_i|$$

$$\sigma_i = \sigma(d_i)$$

where the mean and the standard deviation are computed on the population of simplexes. The simplex screening method generalizes the Morris' OAT design since it is a particular case of a simplex design.

As the simplex design is used for metamodel estimation and because it has a reduced number of points, it is important that it covers the space well, i.e. it should be a space filling design (see Santner et al [4]). In recent work, Campolongo et al. [1] have proposed a method for improving the sampling strategy in Morris' designs. It consists in maximizing the distances between the OAT trajectories. We use this method without modification in the simplex sampling strategy.

The simplex screening method is compared to Morris' OAT on several standard test cases (Morris function, Sobol g-function…). Monte Carlo validation shows that:

- for screening, the simplex designs give as good results as Morris' OAT: the two methods identify the same set of influent factors.
- for metamodel estimation, the simplex designs are better than Morris' OAT: the metamodel residual variance is smaller with the former than with the latter.

A study on an industrial simulator from petroleum exploitation will also be shown. Given 51 initial factors, only 255 simulations are permitted to: 1. identify that only ten factors were influent, and 2. estimate a kriging metamodel upon the subset of influential factors.

The simplex screening method also makes it possible to perform a screening with any kind of design of experiments. Indeed, for estimating the sensitivity indices, it is sufficient to be able to extract some simplexes from the design. This strategy yields worse results than with a specific design (like regular simplexes), but it makes it possible to carry out a screening on existing databases of simulations without having to deal with a metamodel.

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GLOBAL SENSITIVITY ANALYSIS OF COMPUTER MODELS WITH FUNCTIONAL INPUTS

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Introduction

This work addresses the problem of global sensitivity analyses of numerical models when some input parameters ε are not scalar but functional: $\varepsilon(\mathbf{x})$ is a one or multi-dimensional stochastic function where $\mathbf{x}$ can be spatial coordinates, time scale or any other physical parameter. This work focuses with models which depend on scalar parameter vector $\mathbf{p}$ and use some stochastic processes simulations or random fields $\varepsilon(\mathbf{x})$ during their running. The output value Y of the computer code depends on the realizations of these random functions. For example, the oil reservoirs production evaluations depend on geostatistical simulations of the heterogeneous geological media (Zabalza-Mezghani et al. [7], Ruffo et al. [4]), the environmental assessment on soil models use spatially distributed maps affected by random errors (Tarantola et al. [6]), the thermo-mechanical behaviour of the fuel rod under nuclear irradiation depends on temporal parameters modelized as stochastic processes (Iooss and Ribatet [1]), … These models are typically non linear with strong interactions between input parameters. Therefore, we concentrate our methodology on the estimation of the variance based sensitivity indices; that is, the so-called Sobol indices (Sobol [5]).

To deal with this situation, a first natural approach consists in the discretization of the input functional parameter $\varepsilon(\mathbf{x})$ or its decomposition in an appropriate basis of orthogonal functions. Then, for all the new scalar parameters which represent $\varepsilon(\mathbf{x})$, sensitivity indices are computed. However, in the case of complex functional parameters, this approach seems to be rapidly impracticable as these parameters cannot be represented by a small number of scalar parameters (Tarantola et al. [6]). Moreover, when dealing with non physical parameters, sensitivity indices interpretation would be quite difficult. Indeed, most often, physicists would prefer to obtain one global sensitivity index concerning $\varepsilon(\mathbf{x})$.

In this work, four strategies to resolve this problem are presented. The advantages and drawbacks of each approach are discussed and some applications will be shown during the conference presentation.

1. Sobol indices by Monte Carlo calculations.

To resolve the problem of correlated input parameters in the Sobol indices calculations, Jacques et al. [2] have proposed to use the multi-dimensional sensitivity indices (Sobol [5]): each group of correlated parameters is considered as a multi-dimensional parameter. The simple Monte-Carlo algorithms (Sobol [5]) can then be used to calculate the different Sobol indices (first order, second order, …, total). In our case, this solution is fully applicable by considering the input functional parameter $\varepsilon(\mathbf{x})$ as an unique input multi-dimensional parameter. However, it is supposed that $\varepsilon(\mathbf{x})$ is not correlated with any other input parameters. Moreover, the calculation of Sobol indices by the simple Monte-Carlo method requires more than thousand model evaluations for one input parameter. In complex industrial applications, it is often unrealisable.

2. Using an intermediate "trigger" parameter governing the random function simulation.

Tarantola et al. [6] have proposed another solution by introducing a scalar input parameter $\xi \sim U[0,1]$ governing the simulation of the random function. For each sample simulation, if $\xi < 0.5$, the functional parameter $\varepsilon(\mathbf{x})$ is fixed to a nominal value $\varepsilon_0(\mathbf{x})$ (for example the mean $<\varepsilon(\mathbf{x})>$); if $\xi > 0.5$, the functional parameter $\varepsilon(\mathbf{x})$ is simulated. Therefore, the sensitivity index of ξ quantifies the influence of the random function on the model output variable. Contrary to the previous case, various sensitivity analysis methods can be applied (regression, FAST, Sobol, …). However, as the previous method, it also requires the use of the computer model to perform the sensitivity analysis. Moreover, ξ reflects only the presence or the absence of the stochastic errors on $\varepsilon_0(\mathbf{x})$, and the term $\mathrm{Var}[E(Y|\xi)]$ does not quantify properly the contribution of $\varepsilon(\mathbf{x})$ to $\mathrm{Var}(Y)$.

3. Using a metamodel.

To perform a variance-based sensitivity analysis on long running time model, some work propose to replace the computer code by an approximate mathematical function, called a metamodel (Ruffo et al. [4]). For metamodels with sufficient prediction capabilities, the bias due to the use of the metamodel instead of the true model is negligible. Several choices of metamodel can be found in the literature: polynomials, splines, Gaussian

processes, neural networks, … Therefore, a first solution would be to fit a metamodel including the multi-dimensional scalar parameters representing $\varepsilon(\mathbf{x})$ (*i.e.* its discretization or its decomposition in an appropriate basis). However, this seems to be impracticable due to the potential large number of scalar parameters. A second solution consists in replacing the continuous parameter ξ by a discrete parameter $\xi' = 1_{\xi > 0.5}$, which can correspond to the scenario parameter of Ruffo et al. [4] (where the number of geostatistical realizations is finite and fixed, and where each different value of the discrete parameter corresponds to a different realization). However, the situation differs in our context; as the previous method, the term $\mathrm{Var}[E(Y|\xi')]$ does not quantify properly the contribution of $\varepsilon(\mathbf{x})$ to $\mathrm{Var}(Y)$.

The last solution considers $\varepsilon(\mathbf{x})$ as an uncontrollable parameter and a metamodel is fitted in function of the other scalar parameters $\mathbf{p}$: $Y_m = E(Y|\mathbf{p})$. Therefore, using the relation $\mathrm{Var}(Y) = \mathrm{Var}[E(Y|\mathbf{p})] + E[\mathrm{Var}(Y|\mathbf{p})]$, it can be seen that the total sensitivity index of $\varepsilon(\mathbf{x})$ corresponds to the expectation of the unexplained part of the metamodel $E[\mathrm{Var}(Y|\mathbf{p})]$. However, classical parametric metamodels are not adapted to correctly estimate $E(Y|\mathbf{p})$ because of the heteroscedasticity of this situation (some examples are shown in Iooss and Ribatet [1]). This can cause some misspecifications of the sensitivity indices.

4. The joint modeling approach

Zabalza-Mezghani et al. [7] have proposed a solution by using a theory developed for experimental data: the simultaneous fitting of the mean and the dispersion by two interlinked generalized linear models (McCullagh and nelder [3]). This approach, called the joint modeling, has been recently extended by Iooss and Ribatet [1] to non parametric models. This generalization allows more complexity and flexibility while fitting the data. They propose to use generalized additive models (GAMs) based on penalized smoothing splines. The GAM allows model and variable selections via quasi-likelihood function, statistical tests on coefficients, graphical display, … Its restriction, compared to other complex metamodels stands in the additive effects hypothesis.

Therefore, two metamodels are obtained: one for the mean component $Y_m = E(Y|\mathbf{p})$; and the other one for the dispersion component $Y_d = \mathrm{Var}(Y|\mathbf{p})$. The sensitivity indices of $\mathbf{p}$ are computed using Y_m with the standard procedure, while the total sensitivity indice of $\varepsilon(\mathbf{x})$ is computed from $E(Y_d)$. Using the explicit formula on Y_d and the associated regression diagnostics, qualitative sensitivity indices for the interactions between $\varepsilon(\mathbf{x})$ and the scalar parameters of $\mathbf{p}$ can be deduced.

Acknowledgement:

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AN INFORMATION-THEORETIC FRAMEWORK FOR GLOBAL SENSITIVITY ANALYSIS

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For many areas of interest, models of complex systems can be taken to have the form of a deterministic mapping from a set of *n* inputs to one or more output(s) (Figure 5). The outputs can be considered separately, so that for each output Y_k there is a map

$$f_k : (X_1, \ldots, X_n) \mapsto Y_k.$$

Usually, the input-output mapping is not available in explicit form but can be evaluated numerically for any given inputs.

Global sensitivity analysis aims to rank the inputs $X_1, \ldots, X_n$ according to the degree to which they influence the output, individually and conjointly. Here 'inputs' may also refer to intrinsic model parameters whose influence on the output is to be determined, as in Fig 1B. This type of global sensitivity analysis is commonly performed in a probabilistic manner by evaluating the model for multiple sets of randomly and independently selected input values drawn, for instance, from uniform distributions over suitable intervals. The output, being a function of the randomised inputs, thus also becomes a random variable. If the inputs are sampled independently, the variance of the output distribution can be decomposed into contributions by individual inputs, pairs, triplets, and so forth. This procedure is well known in statistics as 'analysis of variance' (ANOVA) (e.g. [1]), and several authors have contributed to improving its computational efficiency for sensitivity analysis (e.g. [2] and [3]).

Rather than analysing the *variance* of the output distribution, we take a different route, measuring output uncertainty in terms of Shannon's entropy [4]. Our starting point is the concept of the 'communication channel' [5], which enables us to view the model as a transmitter of information between inputs and outputs (Fig 1B).

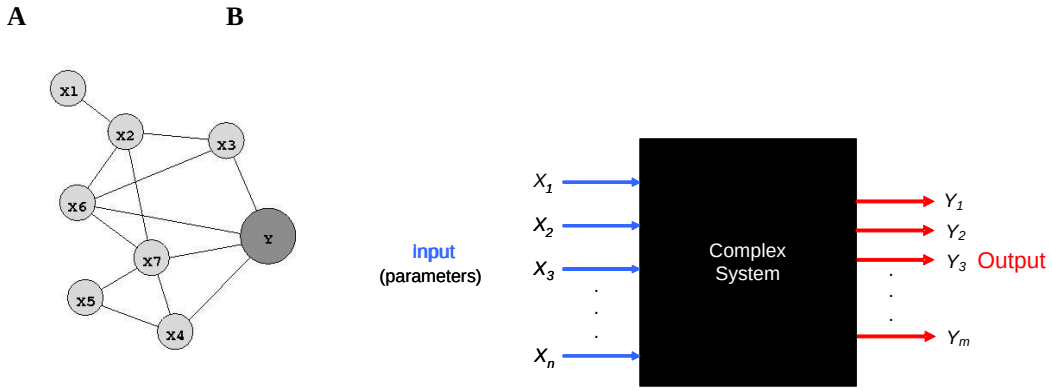

Figure 5. *A complex system with multiple inputs and outputs. This is a typical situation in systems biology. For instance, pathway models (**A**) are described by sets of coupled non-linear ordinary differential equations (deterministic or stochastic). Input-output relations can only be elucidated by numerical evaluation of the system output, e.g. a flux, for various configurations of the input parameters. Global sensitivity analysis aims to determine the degree to which these inputs control the output, and how they interact. In most applications, the input-output mapping is non-linear and not given in closed form; hence the system is a 'black box' (**B**).*

The *mutual information* of two variables is a quantity that measures their mutual dependence [5]. Determining the mutual information $I(X_i;Y)$ between random sampling sequences of individual inputs X_i and their output counterpart can elucidate first order input-output relations. Mutual information provides a general measure of association that is applicable regardless of the shape of the underlying distributions and – unlike linear or rank order correlation – insensitive to non-monotonic dependence among the random variables. Further insight can be obtained by unravelling *conditional dependencies* among the system inputs. We here define novel and general sensitivity measures of second and higher order by evaluating input correlations induced by

conditioning on the output. To our knowledge, only a first-order information-based analysis has been discussed in the literature to date [6; 7, *pp. 402 – 407*].

As does variance, the output entropy *H(Y)* quantifies the variability of a distribution, but differs from it in that, while variance essentially assumes Gaussian distributions, the entropy is more general. We therefore further develop an information-theoretic framework for the sensitivity measures thus derived, based on the observation that their sum is bounded from above by the output entropy $H(Y)$. From this viewpoint, the (information-theoretic) sensitivity indices quantify the amount of output uncertainty removed by the knowledge of individual inputs and combinations thereof.

Sensitivity analysis of this kind is also an analysis of the *total* mutual information $I(X_1,\ldots,X_n; Y)$, which subsumes *all* input-output associations including interactions. The resultant summation theorem for the sensitivity measures is an information balance in which the sum equals $I(X_1,\ldots, X_n; Y)$. Although in practice only effects of up to third or fourth order can easily be calculated explicitly, the joint impact of all higher order terms is provided by the remaining difference to $I(X_1,\ldots, X_n; Y)$. We can therefore assign credit or influence fully to all the parameters of a system over a wide range of operating conditions.

For all variance-based approaches, the absence of input correlations is a critical prerequisite for the uniqueness of the variance decomposition [8, 9]. As will be demonstrated, in our methodology independent inputs merely simplify the analysis. If input correlations exist (e.g., due to non-orthogonal sampling), their effect can easily be taken into account. We apply the methodology successfully to a model of the NFκB signaling pathway and thereby define how to modify its behaviour to provide a designed maximum effect.

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POSTER PRESENTATIONS

SCALAR AND GEOMETRICAL DESCRIPTION OF 3D-CYCLE STOCHASTIC SENSITIVITY

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The small random disturbances of nonlinear dynamical system can decisively affect its behavior and lead to rich variety of regimes. Consider stochastic system $\dot{y} = f(y,\mu) + \varepsilon\sigma(y)\dot{\omega}$. Here y is n-dimensional vector, f is vector-function, μ is real parameter, ω is n-dimensional standard Wiener process, σ is n x n – matrix disturbances function, ε is a small parameter (noise intensity). The most general probabilistic description of this forced system is given by the Kolmogorov-Fokker-Planck equation. As a rule the main interest is connected with the regime of stochastic auto-oscillations steadied in dynamic system. Analytical research of stationary distribution density ρ(y,ε) is possible only for 1-dimensional dynamical systems and in some infrequent cases for 2-dimensional systems. For 3-dimensional systems the construction of numerical solution of Kolmogorov-Fokker-Planck equation is connected with significant computational difficulties.

The case of steady rest point is widely discussed in the literature for stochastic dynamics and is fundamentally developed. The main attention in presented paper is devoted to the limit cycle. It is supposed that the deterministic system $\dot{y} = f(y,\mu)$ has T-periodical solution ξ(t) with corresponding exponentially stable phase curve (cycle Γ). It means that value of deviation Δ(y) of the forced trajectory state y from the cycle Γ tends exponentially to zero as time increases. External random perturbations force the trajectory of dynamical system to leave the deterministic orbit and form some stochastic bundle around it. Empirical study of cycle stochastic sensitivity based on direct numerical simulations is very difficult due to considerable time consumption and computational resources.

1. Stochastic sensitivity function

In presented work, the method based on quasipotential function $v(y) = -\lim_{\varepsilon\to 0} \varepsilon^2 \ln \rho(y,\varepsilon)$ is given. This function is an asymptotic of stationary density ρ(y,ε). Qausipotential has been actively used in last years for stochastic dynamics problems research and appeared in papers of Wentzell A.D. and Freidlin M.I. [1]. With the help of first approximation of quasipotential *v(y)* in a small vicinity of cycle Γ the stationary density can be written in following form of normal distribution [2, 3]:

$$\rho(y,\varepsilon) \approx K \exp\left[-\frac{\left(\Delta(y), \Phi^{+}(\gamma(y))\Delta(y)\right)}{2\varepsilon^2}\right],$$

where "+" means pseudo-inversion. Function Φ(γ) is so-called stochastic sensitivity function (SSF). SSF characterizes a dispersion of the intersection points of random trajectories with hyperplane orthogonal to cycle Γ at the point γ ∈ Γ. SSF describes a sensitivity of the cycle to the small random disturbances. Using SSF one can successfully research different phenomena connected with the influence of random perturbations on the limit cycle without empirical modeling.

The stochastic sensitivity matrix Φ(γ) is singular (all distribution points are concentrated in one hyperplane). It is convenient to search for a function Φ(γ) in parametrical form. The solution ξ(t) connecting the points of cycle Γ with points of an interval [0, T) gives the natural parametrization Φ(ξ(t)) = W(t). Then the following system, consisting of linear matrix differential Lyapunov equation and two corresponding conditions, can be written as

$$\begin{cases} \dot{W} = F(t)W + WF^{T}(t) + P(t)S(t)P(t) \\ W(0) = W(T) \\ W(t)r(t) = 0 \end{cases},$$

where $F(t) = \dfrac{\partial f}{\partial y}(\xi(t))$, $S(t) = \sigma(\xi(t))\sigma^{T}(\xi(t))$, $r(t) = f(\xi(t))$, $P(t) = P_{r(t)}$,

$P_r = I - rr^{T}/r^{T}r.$

This system has an unique solution [2, 3]. Corresponding numerical algorithms for calculating of this solution were suggested in [3].

Let us consider the three-dimensional case (n = 3). Then spectral decomposition of SSF can be written in the following form: $W(t) = \lambda_1 v_1 v_1^{T} + \lambda_2 v_2 v_2^{T}$, where λ_1, λ_2 are eigenvalues and v_1, v_2 are corresponding

normalized eigenvectors of matrix W(t). Scalar analysis of 3D-cycle stochastic sensitivity is based on research of two scalar functions $\lambda_1(t)$ and $\lambda_2(t)$.

2. Geometrical description of 3D-cycle stochastic sensitivity

The constructive way for complete description of cycle stochastic sensitivity is the following. Eigenvalues λ_1, λ_2 and corresponding normalized eigenvectors v_1, v_2 of matrix W(t) specify in normal plane $\Pi(t)$ (build in some point on the cycle orbit) some confidence ellipse Y(t). This ellipse with some chosen value of fiducial probability defines in plane $\Pi(t)$ a confidence domain for intersection points of stochastic bundle. These ellipses specify on the system phase space around the cycle some torus , which defines a confidence domain for stochastic cycle.

This torus plays a role of a simple 3D-model for stochastic cycle. Visualization of this torus gives detailed and evident description of stochastic cycle orientation and form and fully characterizes its stochastic sensitivity. In the paper, the following algorithm for constructing of confidence torus is presented:

- value of SSF is calculated for each of base points. Using eigenvalues λ_1, λ_2 and eigenvectors v_1, v_2 of SSF matrix confident ellipse Y is constructed;
- base points on ellipses are chosen;
- with the help of triangulation the carcass of torus is constructed. Triangles apexes are base points of ellipses. Using normal vectors to triangles directing vectors to each apex are build;
- torus carcass and directing vectors are used to create the 3D-scene image. Realized numerical algorithm of enveloping of torus surface relies on implementation of graphic library OpenGL and uses Gouraud smooth shading method.

3. Stochastic sensitivity analysis of Roessler system

Method of stochastic sensitivity analysis based on SSF was applied for researching different 2-dimensional and 3-dimensional dynamic models [2 - 4]. In this paper analysis for stochastically forced Roessler system

$$\begin{cases} \dot{x} = & -(y+z) + \varepsilon\dot{\omega}_1 \\ \dot{y} = & x + \alpha y + \varepsilon\dot{\omega}_2 \\ \dot{z} = & \alpha + z(x-\mu) + \varepsilon\dot{\omega}_3 \end{cases},$$

is demonstrated . Here $\alpha = 0.2$, $\mu \in (0.4 ; 4.2)$.

The designated parameter interval is period doubling bifurcation zone for Roessler system. While parameter μ changes on this interval, stable limit cycles double their period. At $\mu \approx 4.2$ system changes its state and undergoes from order to chaos.

Deterministic cycles of Roessler system and random trajectory bundles around them are examined. With the help of SSF the stochastic sensitivity of cycles is researched in details. Scalar analysis is performed. Good coincidence with results, based on direct numerical simulation, is achieved. An exponential growth of stochastic sensitivity for period doubling bifurcation zone is found. The value of growth coefficient is obtained. For some different values of parameter μ confidence tori are built to demonstrate the possibilities of geometrical description of stochastic sensitivity. The modeling of Roessler system torus under raising of noise intensity is performed.

Achieved results show that SSF is a useful analytical tool in researching thin phenomena observed in stochastically forced systems with limit cycles. Geometrical description of stochastic cycle sensitivity is demonstrated.

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MULTIDIMENSIONAL SENSITIVITY ANALYSIS FOR MULTI-ATTRIBUTE DECISION MAKING UNDER PREFERENTIAL UNCERTAINTY

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Complex decision situations require the consideration of technical, economic, ecological, socio-psychological as well as political aspects. Approaches from Multi-Criteria Decision Analysis (MCDA) can help to take into account various incommensurable aspects and subjective preferences of the decision makers and thus contribute to transparency and traceability of decision making processes (see e.g. Geldermann et al. [10]; Belton and Stewart [1]).

An important and challenging area of applying multi-criteria methods is nuclear emergency and remediation management involving various stakeholder and expert groups in the decision making process with diverse background knowledge and different views, responsibilities and interests. Hence, the focus of this research is to highlight the role of MCDA in nuclear emergency and remediation management on the basis of a hypothetical case study.

Providing methods to structure and analyse decision problems by means of attribute trees and to elicit the relative importance of criteria in such a tree, multi-attribute value theory (MAVT, see Keeney and Raiffa [12] for an overview) has proven to suit for application in the later phase of nuclear emergency management (see Geldermann et al. [10]; Hämäläinen et al. [11]; French [8]). In MAVT, preferential information is modelled by weighting factors (i.e. inter-criteria comparisons) and value functions (i.e. intra-criteria preferences).

However, the uncertainties that can arise in a decision making process are often underestimated. The occurring uncertainties can be classified in many different ways, see for example Mustajoki et al. [13]; Bertsch et al. [4]; French [6]. According to their respective source, a distinction can be made between "data uncertainties" (uncertainties of the input data to a model), "parameter uncertainties" (uncertainties related to the model parameters, such as the weighting factors of a MCDA model) and "model uncertainties" (uncertainties resulting from the fact that models are ultimately only simplifications/approximations of reality, see French and Niculae [9]).

The modelling of the decision makers' preferences is a crucial part in any multi-criteria analysis. In this paper, special emphasis is placed on handling the uncertainties associated with these preferential parameters. While methods such as SWING and SMART (see Von Winterfeldt and Edwards [14]; Edwards [5]) seek to support decision makers (or their advisers) in eliciting appropriate weights for the different criteria in MAVT by allowing the assignment of weight ratios instead of direct weights, the most difficult problem is often the determination of precise weights or weight ratios. Experiences gained from conducting scenario-focused decision making workshops and also training courses on the use of decision analysis, have shown that the participants do in general appreciate the benefits from applying MCDA but that they need more guidance. They were often unsure about an exact quantification of the modelled preferences. Hence, an appropriate handling of the so-called "preferential uncertainties" is of particular importance.

Classical one-dimensional sensitivity analysis can help to assess the robustness of a decision with respect to variations of preferential parameters (e.g. a weight). However, the major drawback of the procedure is that it is limited to varying one weight at a time. Considering the impact of the simultaneous variation of several weights of a decision model by allowing the assignment of weight intervals instead of precise values could contribute to facilitate the weight elicitation process. Similarly, investigating the impact of the simultaneous variation of the value functions' shapes can facilitate the process of determining appropriate value functions for each attribute, see Bertsch et al. [2]. Besides varying the value functions' shapes it is also interesting to investigate the effect of varying their domains' boundaries. In practice, the boundaries are often defined by the minimum and maximum scores actually achieved by the different alternatives (with respect to the considered attributes). By following this approach, theoretically possible better or worse outcomes are neglected. However, the estimation of reasonable values for these theoretically possible boundaries is a difficult task. An analysis whether or not the variation of the boundaries has an impact on the results can help a decision making group to cope with this task.

In general, the problem of preferential uncertainties is closely interconnected with the field of group decision processes (see e.g. Zhang [15]). We think that it could be easier for groups to agree on parameter ranges (intervals) instead of precise values. Furthermore, it should be noted that preferences may certainly vary according to value systems that are influenced by culture which, in particular, has to be accounted for when decision groups involve persons with different cultural backgrounds. Using approaches for sensitivity analysis that allow to find out whether or not the variation of certain preference parameters has an impact on the ranking of the alternatives, disagreements which do not affect the results can be eliminated from debate and the group can focus on discussing the differences that do matter in terms of the results (Bertsch et al. [3]; French [7]).

In this paper, a Monte Carlo approach is presented that allows to perform multidimensional sensitivity analyses for the different preferential parameters. The main objective is to explore the sensitivity of the results of decision processes to simultaneous variations of these subjective parameters and consequently to contribute to a facilitation of the preference modelling process by comprehensibly visualising and communicating the impact of the preferential uncertainties on the results of the decision analysis.

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OPTIMIZATION OF COMPRESSOR VALVE DESIGN FOR MINIZIMATION OF GAS PULSATIONS USING UNCERTAINTY ANALYSIS

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Gas pulsation in the suction manifold of reciprocating automotive compressors is a common problem. These are mainly caused by the periodic impact of the valve against the seat and because of the unbalance due to piston kinematics. The focus of this research is to initially perform a parametric based study and utilize Uncertainty Analysis techniques to optimize the compressor valve design by taking into account the inherent variability in the operational and design simulation parameters. This research is a continuation of earlier work, where an entire simulation model for a multi-cylinder automotive compressor was developed to predict the gas pulsations in the suction manifold. From these studies it was determined that the main factors that contribute towards gas pulsations are the reed valve, the net pressure and its distribution across the valve, mass flow rate, and certain operational parameters.

First, a parametric study will be done of the different important geometric parameters of the compressor valve together with some material and stiffness properties using Finite Element Analysis Software and Matlab. The geometric dimensions of the valve are based on a number of parameters that need to be optimized keeping in view the over all geometric constraints of the suction manifold. The main purpose is to increase the mass flow rate and to reduce the low frequency noise in the suction manifold. Second, important factors that have a significant impact on the net pressure acting and its distribution across the valve will be considered. The pressure distribution can have a significant effect on the valve opening time and consequently on the mass flow rate resulting in higher gas pulsations. The exact way in which the pressure is distributed across the valve is not known but different pressure profiles will be assumed in order to analyze the response. Third, certain operating parameters will be varied based on probability density functions. The objective here will be to show how the mass flow rate profile affects the gas pulsations in the suction manifold.

The gas pulsations in the suction manifold are highly dependent on the proper valve design. The estimated gas pulsation obtained from the above methods will be quantified in terms of a distribution and the affects on the output distribution by changes in valve geometry will be explained. The results will also be compared with the pressure pulsation obtained from the experimental data. It will be shown that a good compressor valve design can be achieved by parametric study of the valve geometry profile and could be easily combined with other compressor design and operating parameters using uncertainty and sensitivity analysis to better predict the gas pulsation behavior in the suction manifold.

SENSITIVITY ANALYSIS OF STATE-TRANSITION MODELS OUTPUT: THE RIVM CHRONIC DISEASE MODEL

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State-transition models are employed to trace future trends of risk factors and disease prevalence rates within populations [1,2]. The reliability of these models is based on the validity of the assumptions made in the model and on the accuracy of the input data they require. Uncertainty and Sensitivity Analysis should be performed to assess the reliability of the results and to detect the input variables that contribute most to the output variability. Often the number of state-transition model input variables is so huge and the computer code in which they are written required running-time that are so large that not all the methods to perform uncertainty and sensitivity analysis are practically available. Because of that, this kind of analysis is rarely applied to state-transition models. Here we describe how to deal with these limitations in practice.
We first present the RIVM Chronic Disease Model [3] that is a multistate-transition model describing the trends of several risk factors and of the related diseases within the Dutch population. It is also an important tool for health economics [4,5] but our analysis will focus only on its epidemiological applications.
The model involves thousands of input factors depending on the choice of the output of interest, and each model run is quite time consuming. For these reasons any sophisticate and complex uncertainty and sensitivity analysis cannot be performed on the Chronic Disease Model output without having performed before a screening method to exclude all non influential input variables from the subsequent analysis.
Our outputs of interest will be the prevalence projections of never smokers/smokers/former smokers and of several diseases related to smoking such as lung cancer and coronary heart disease within the Dutch population older than 15 years.
The input factors we decided to include in the analysis are the prevalence rates of smokers, the starting rates, the quitting rates and the relapse rates (that are the rates governing the transitions from never smokers to smokers, from smokers to former smokers and from former smokers to smokers respectively) and the relative risks for all cause mortality and for disease specified by risk factor class (smoking state). All these input are specified by gender and within gender by five-years age classes.
We performed a simple one-at-a-time experiment and the more informative Morris's OAT design [6,7]. We will compare the results and point out some difficulties in dealing with very different kinds of input factors like those we investigated. Since all input factors are age dependent and specified by gender and the outputs are functions of time, these sensitivity analysis methods prove to be also very effective methods to detect possible errors and to check the coherence of the model structure.
We also suggest a possible way of performing sensitivity analysis to quantitatively attribute the output uncertainty to the uncertainty in the input factors as a further step to assess the reliability of the model results.

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TOWARDS A REDUCTION OF A TITAN IONOSPHERIC CHEMISTRY MODEL

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Chemical models of Titan's ionosphere are presently involving hundreds of reactions, and the ion mass spectra obtained on site by the Cassini spacecraft indicate that they are far to be sufficient to explain the observed molecular growth [1]. It is thus unavoidable that the complexity of the models will increase. In parallel, there is a strong demand for reduced chemistry modules to include in 2D or 3D atmospheric models.

In a first time, we focussed on the reaction database used to describe bimolecular ion-molecule reactivity. Our target observable was the ion mass spectrum with it's 90% confidence interval, as generated by Monte Carlo uncertainty propagation with the full chemistry model. We wished to estimate how many reactions, among the 582 presently included in the database, were necessary to reproduce this mass spectrum without significative alteration (Fig. 1).

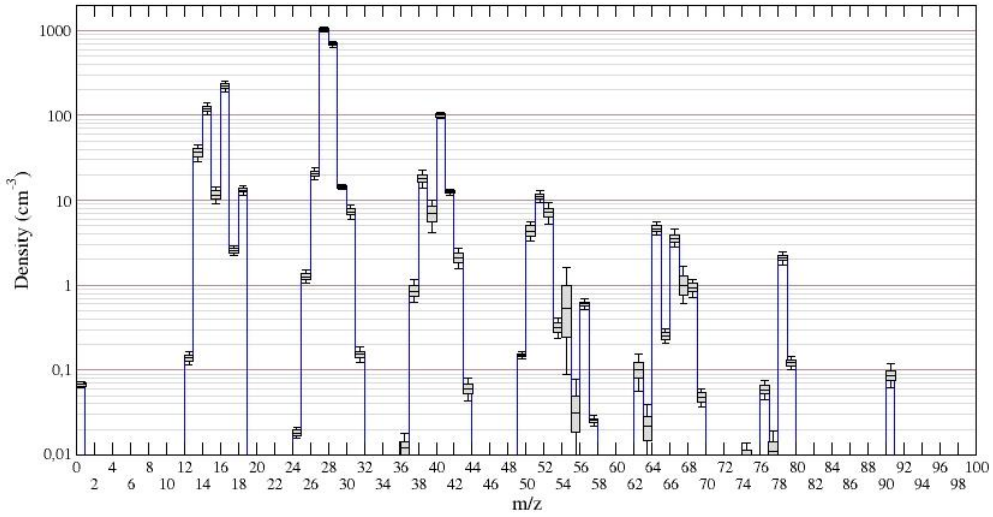

Figure 3: Ion mass spectrum simulated with the full reaction database, with uncertainties resulting from bimolecular reactions parameters (rate constants and branching ratios).

We compared two methods to reduce the reaction scheme:

5. A brute-force screening method: we systematically subtracted the reactions in the chemical network and checked whether the resulting mass spectrum reproduced the target observable. All the reactions which, when suppressed, led to a nominal prediction out of the 90% confidence interval of the target were kept in the model.
6. A global sensitivity analysis method, based on input-output correlations, to identify major reaction paths leading to the target mass spectrum. All reactions having rank correlation coefficients below a chosen threshold with the observed mass peaks were discarded.

A similar efficiency was found in both cases, reducing the initial chemical network by a factor of 5-6: 95 reactions with the brute-force method *versus* 117 reactions with the global sensitivity analysis method (Fig. 2). However, notable discrepancies were observed in the minimal lists of reactions produced by both methods. Moreover the brute-force pruning method appears to be dependent on the screening order: substantially different reduced lists were obtained according to the starting point of the screening process. This might be due to non-linearities and/or compensations in the network bifurcations when subtracting the reactions one-by-one. At the opposite, the global analysis, although slightly less effective than the brute-force method, is probably more adequate for such a non-linear and complex chemical network.

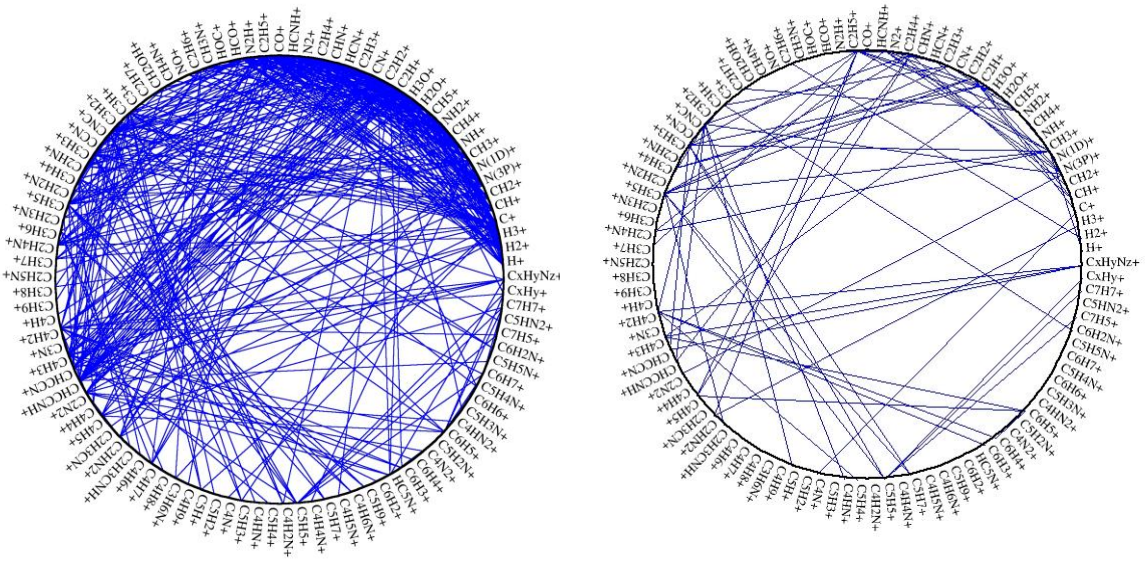

Figure 4: Left: "full" ion-molecule reactions network (582 reactions); right: reduced network after global sensitivity analysis, reproducing the target ion mass spectrum within uncertainties (117 reactions). The lines join ions related by an ion-molecule reaction; neutral species are not specified.

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PARTIAL DERIVATIVES AND SINGULAR VALUE DECOMPOSITION FOR THE ANALYSIS AND CONTROL OF TIME-DEPENDENT SPATIALLY DISTRIBUTED SYSTEMS

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The mathematical representation of natural and industrial systems frequently requires the use of time-dependent spatially distributed models. Although differential methods are intrinsically local, they are perfectly suited for some settings and may prove very informative. Suppose that the transformation between the independent variables $\boldsymbol{x} = (x_1, x_2, ..., x_n)$ and the dependent variables $\boldsymbol{y} = (y_1, y_2, ..., y_m)$ is represented by a function $f : R^n \rightarrow R^m$. The response to be analysed can be a scalar but the study of a vectorial response tend to increase the understanding of the transformation. When function *f* is linearized at the given point of the input space (defining a trajectory in the model phase space), the partial derivatives are organized in the $m \times n$ Jacobian matrix $\boldsymbol{J}$.
For instance, if the vector $\boldsymbol{y}$ accounts for the temporal evolution of an output variable of interest, each column of $\boldsymbol{J}$ is the result for all the time steps composing the response of an infinitesimal perturbation on one of the input parameters x_i. Conversely, each line of $\boldsymbol{J}$ can represent the contribution of the different parameters x_i (spatially distributed) on an aggregated response y_j. While one can propose a physical interpretation for the lines and/or columns of the Jacobian matrix, a very interesting view angle is provided by its singular value decomposition (*SVD*). This factorization is widely used for the analysis of linear ill-posed problems [5] and its potential extrapolation to nonlinear systems is spreading in various disciplines (ex. [1], [3], [6]) . When applied to the Jacobian matrix of the transformation, it provides very relevant information for the analysis and control of the system under study. The first singular vectors in the input space describe the sub-space from the original control space maximizing the spread of the outputs, in the output space they identify the output variables really informative for the estimation of the model control variables. Together with the singular value spectrum, they are valuable elements to assess and enhance the sensitivity and identifiability of the independent variables. Going back to the illustration mentioned previously, if y accounts for the temporal evolution of an output variable and if a given spatially distributed parameter is composing the vector $\boldsymbol{x}$, the parameters really influencing the response (spatial location) and the measurements really constraining the parameters (temporal location) are identified.

Although different techniques can be employed for the evaluation of the Jacobian matrix, algorithmic differentiation is very efficient in providing accurate derivatives. Tremendous advances have been made in this domain Griewank [4] and consequently the code based approach is facilitated by the advent of powerful automatic differentiation (*AD*) engines (see http://www.autodiff.org). The derivatives computed by means of algorithmic differentiation are accurate to the machine precision. Considering the computer code implementing the direct model as a concatenated sequence of instructions, algorithmic differentiation is based on a rigorous application of the chain rule, line by line. The application of the chain rule from the inputs to the outputs of the function is denoted as the forward mode of *AD* whereas the reverse mode operates from the outputs to the inputs. Because the computational cost of the reverse mode (discrete equivalent of the adjoint state method [2] from optimal control theory) is independent from the dimension of the input space, for vector valued response functions, it can be shown that when the ratio between the dimension of the input space and the dimension of the output space is greater than one, the reverse mode is more efficient in computing the Jacobian.

Independently from the *curse of dimensionality* high-dimensional input spaces can be investigated while the use of sampling based approaches would imply a prohibitive computational cost. The described methodology is applied an catchment scale hydrological model representing the transformation of rainfall into runoff. Using the information provided by the *SVD* of the Jacobian matrix, it is shown that adjoint sensitivity analysis provides an extensive insight into the relation between model parameters and the hydrological response and enables the use of efficient gradient-based optimization techniques.

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NUMERICAL SENSITIVITY AND EFFICIENCY IN THE TREATMENT OF EPISTEMIC AND ALEATORY UNCERTAINTY

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1. Introduction

Nowadays, the need to treat both epistemic and aleatory uncertainty in a unified framework is well recognized [1]. One method to do so is to mix probabilistic convolution (for aleatory uncertainty) and fuzzy calculus (for epistemic uncertainty). Existing propositions either concern simple models [2] or are computationally very costly [3] (a luxury not always affordable, especially in nuclear safety, where models can be very complex). Here, we propose a numerical treatment of such methods, based on Monte-Carlo sampling technique, which greatly reduces the computational costs and can be applied to complex models. Moreover, using well-known results from order statistics [4], we propose to integrate the notion of numerical accuracy to our results. Our proposition mainly consists in setting some decision step before the propagation is done, rather than after it has been done. Section 2 recalls theoretical basis of the propagation technique used here and discusses previous practical solutions proposed to put this method in practice. Section 3 explains our propagating method (called the RAndom FUzzy method, or RaFu) and how it is applied. The RaFu method, implemented in SUNSET software for uncertainty analysis, is currently used and developed at IRSN

2. State of the art

Let us consider a set of K parameters $X_1,\ldots,X_K$ tainted with aleatory uncertainty (i.e. X_i i=1,…,K takes a random value and is modelled by a probability distribution p_i, or equivalently by a cumulative distribution F_i), and a set of L parameters $X_{K+1},\ldots,X_{K+L}$ tainted with epistemic uncertainty (i.e. X_i i=K+1,…,K+L has a deterministic value which is imprecisely known). Let $M(X_1,\ldots,X_K, X_{K+1},\ldots,X_{K+L})$ be the mathematical model of interest depending on our K+L uncertain parameters.

The aleatory uncertainty of a parameter X is faithfully modelled by a probability distribution p. Epistemic uncertainty, on its side, is more faithfully modelled by intervals encompassing the imprecisely known true value of a parameter. Nevertheless, we often have more information than just a minimal and a maximal values (e.g. an expert can give intervals with different confidence levels). Possibility distributions are mappings $\pi : \mathbb{R} \rightarrow [0,1]$ that can be seen as a collection of nested confidence intervals (thus extending the notion of intervals), which are the α-cuts $[x_\alpha,x^\alpha] = \{x, \pi(x) \geq \alpha\}$ of the distribution π. The degree of confidence that the interval $[x_\alpha,x^\alpha]$ contains the true value of the parameter X is then 1- α. Thus, the K first parameters of the model M are modelled by probability distributions p_i, while the last L are modelled by possibility distributions π_i

Parameters are then propagated through the model. Guyonnet's proposition [5] (which makes no assumption about the complexity of the model) is to first propagate the K first parameters through usual Monte-Carlo simulation, thus getting N probabilistic samples (eventually integrating some information about correlation by usual techniques [6]), and then to propagate the L last parameters by using fuzzy extension principle for each N-uple. By using the fact that the extension principle is equivalent to make an interval computation for each α-cut, he proposes to approximate the resulting fuzzy number by making computations over a limited number of α-cuts. He then gets a collection of N fuzzy numbers ${}^M\pi_i$, each of them occurring with probability 1/N. To each α-cut of the random fuzzy number ${}^M\pi$ corresponds a collection of N intervals ${}^M\pi_i^\alpha = [{}^M\pi_{i,inf}{}^\alpha , {}^M\pi_{i,sup}{}^\alpha]$, from which can be built 2 cumulated distributions $[F_\alpha,F^\alpha]$. To build a summarized representation, Baudrit et al. [3] propose a post-processing that consists in taking the mean of the cumulated distributions $[F_\alpha,F^\alpha]$, while Ferson and Ginzburg [2] propose to take the double pair $[F_0,F^0]$ and $[F_1,F^1]$. In the two propositions, authors suppose that the fuzzy random number is built before giving one of these two representations. This supposition is computationally costly. For example, let us suppose that 100 samplings are done on the K first parameters, and that for each of them, the corresponding fuzzy number is approximated by taking twenty α-cuts (α = 0,0.05,…0.95,1). 2100 interval computations are then needed to build the final result.

In some applications, assuming one can afford so much computations is clearly unrealistic. Moreover, although it is proposed in [2] and [3,5] to use numerical sampling for complex models, the question of numerical accuracy is not considered in any of them. This is why we propose a method where numerical accuracy is integrated and where the decision step is set before the propagation (thus reducing computational cost). Let us note that the two post-processing methods mentioned above can be found back with our propagating method.

3. The Random Fuzzy (RaFu) method

The RaFu method uses the same theoretical framework as the one recalled in section 2. It is designed so that both epistemic and stochastic uncertainties are simultaneously sampled and propagated through the model, with the aim of building a given response. The main originality of the RaFu method is that this response is pre-defined by a triplet of parameters (γ_S,γ_E ,γ_A) specified by a decision maker (DM) :

- Parameter γ_S corresponds to the statistical quantity chosen for modelling the stochastic uncertainty of the response
- Similarly, parameter γ_E corresponds to the fuzzy quantity used for modelling the epistemic uncertainty of the response
- Finally, parameter γ_A measures the desired numerical accuracy on the final result.

According to the DM values for (γ_S,γ_E ,γ_A), the RaFu method then determines the minimal sample size and the nature of the required sampling to build the wished response. Number of calculations is thus reduced to its minimal number, in accordance with the DM choice. Moreover, computation cost can be easily evaluated, allowing the DM to eventually revise its choices before uncertainty propagation. For example, if the DM want to have an upper limit of the response 95% percentile, to be hyper-cautious about epistemic uncertainty (i.e. concentrate on α-cuts $[x_0,x^0]$) and to have a numerical certainty of 99% to cover the true value, he or she chooses the triplet (γ_S,γ_E ,γ_A)=(0.95,0,0.99). By using results from order statistics [4] (an use often quoted as Wilks formula [7]), the RaFu method derives the minimal sampling size to satisfy the DM's choice (in our example, 90 calculations) and the nature of this sampling. Let us note that parameters (γ_S,γ_E ,γ_A) are not forcefully numbers (i.e. γ_E can be "every α-cut, from 0 to 1").

It is interesting to note that the post-processing methods proposed in [2] and [3] can both be translated in term of a decision on parameter γ_E. The Post-processing of Baudrit et al. [3] can be interpreted as "I want the mean pair of cumulated distribution taken over every confidence degree (i.e. α-cut) of epistemic uncertainty". The proposal from Ferson and Ginzburg [2] can be translated by "I want the most optimistic and the most pessimistic pair of cumulated distributions".

Let us get back to the example given in the previous section. With the RaFu method, knowing the desired final quantity before propagation allows to reduce computations from 2100 to 100 in the case of Baudrit et al. method (100 samples are made, and one random α-cut is chosen each time. This randomised α-cut insures us that we converge to the mean, without having to make the propagation for 21 α-cuts each time). In the same way, Ferson and Ginzburg's result can be obtained by reducing computations from 2100 to 200 (here, 2x100 computations are required, one set of 100 calculations for a fixed α-cut of level 0, and another one for a level of 1). Detailed algorithm and convergence proof will be provided in the full length paper.

4. Conclusions

Mixing fuzzy calculus with probabilistic propagation to get fuzzy random variable allow one to take into account both aleatory and epistemic uncertainties. A limitation of such methods is often the high computational complexity, which, according to us, is not always justified in practice. Thus, we propose a method (the RaFu method) that brings forward some decision step and can greatly increase numerical efficiency. The final results of usual post-processing methods can be found back with the RaFu method, as well as many other possible methods. Finally, we have proposed to add considerations about numerical accuracy in the process, an important point in sampling processes that is, to our knowledge, almost never mentioned in works trying to cope both with epistemic and aleatory uncertainties.

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EFFICIENT ESTIMATION OF FIRST-ORDER SENSITIVITY INDICES

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The method of Sobol' [6] or the FAST method [1] are classical techniques to compute sensitivity indices (see [5] for a wide and thorough review). Although specifically designed to estimate these indices, both require many function evaluations. Recently, other approaches based on nonparametric estimation tools have been proposed to overcome this computational time problem by working on reduced samples of the inputs. One of them is the Bayesian approach of Oakley and O'Hagan [3] which relies on approximating the function with kriging ideas. Another one is the method of Da-Veiga, Wahl and Gamboa [2] depending on conditional moments estimation through local polynomial techniques. Such nonparametric methods allow to significantly reduce the number of function evaluations needed to accurately estimate sensitivity indices. However from a statistical point of view, though computationally efficient, these estimators share the problem of a nonparametric rate of convergence induced by the use of nonparametric techniques.
We propose here a new estimator for first-order sensitivity indices which attains the optimal rate of convergence. The main idea comes from the work of Laurent [4] on efficient estimation of integral functionals of a density. It is based on a Taylor expansion and on the estimation of a quadratic functional. We have followed the same scheme and adapted it to the estimation of first-order sensitivity indices which appear to be more general functionals of a density than those studied in the work of Laurent. Proofs of convergence and efficiency are presented and we underline the notable simplification which appears due to the intrinsic structure of the conditional expectation.
We then present simulation results on analytical examples to compare this approach to the standard techniques and to the nonparametric methods aforementioned.

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A SENSITIVITY BASED APPROACH FOR DETERMINING THE EXTREME PROFITS AND LOSS CONTRIBUTION INDEX

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In this article, we propose a new performance index adjusted for risk, which allows the comparison of an asset's contributions to a portfolio's favorable and unfavorable events. This index, called the Extreme Profits and Loss Contribution Index (EPLC), in combination with portfolio theory, allows the evaluation of more volatile portfolios within the Markcowitz efficiency frontier [1], and thus the recommendation of choosing or rejecting portfolios through considering the efficiency of their more volatile assets.
The EPLC index, defined in monetary terms like the Value at Risk (VaR) [2], considers the two main concepts from portfolio theory: the correlation among assets and the risk premium. However the main contribution of the proposed index is that it considers simultaneously extreme favorable and unfavorable events. Classical portfolio theory deals with a criterion based on average and variance, while VaR methodology considers only one percentile of the profit distribution. Thus EPLC provides additional information to the decision-maker.
The EPLC index is built by using the importance measure (IM) $\eta^2 = \frac{Var_x[E(Y \mid x)]}{Var[Y]}$ [3-5]. First, a sensitivity analysis based on a Monte Carlo simulation is performed to quantify the IM of each asset in both extreme favorable and unfavorable regions (extreme profits γ_j and extreme losses λ_j are defined by the user as a percentile of the profit distribution). Then the index is built as the ratio of the two IMs weighted by expected values of each region, as suggested in [6].

The use of the EPLC is presented through several examples where assets that explain extreme profits or extreme losses have greater participation in losses than in profits, or vice-versa.

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MERGING IMPORTANCE MEASURES USING AN ORDERED WEIGHTED AVERAGING BASED FRAMEWORK

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Sensitivity indexes or Importance measures (IM) are valuable tools that have been used to quantify and rank the contribution of a variable of a model with respect to their contribution to a considered measure of variability. To quantify the impact of a variable, different IM based on different definitions have been proposed, like SRC, SRRC, PCC, PRCC, SPEAR, PEAR or η^2 indexes [1-3]. In general, each of the IM takes into account different perspectives and the final idea is that variables can be ranked with respect to the impact they have on a model characteristic.

This means that different IM may rank variables in a different order. For example, a component that is the most important with the importance measure A may not necessarily be the most important component with respect to importance measure B, even if the two IM evaluate or quantify a similar model characteristics [4].

In order to produce a single final ranked list, the Decision-Maker (DM) has to combine the results, that is, to "fuse" those ranked lists produced by each IM, taking into account his/her preferences such that optimal performance is achieved as a result of the aggregation. If IM are considered as experts that judge the behavior of each component, then the aggregation problem to be solved can be considered as a Multi Expert-Multi component decision Problem. Different authors [5-8] discuss this kind of problem in some other contexts.

In this paper a result-merging algorithm is proposed based on the Ordered Weighted Averaging (OWA) [6]. OWA operators were initially introduced in the area of decision making in order to provide a means for aggregating scores or ranks associated to the satisfaction of multiple criteria. To our best knowledge, there are no reports on the use of OWA applied to aggregation of multiple IM. An example shows the benefits of such combination.

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VARIANCE-BASED SENSITIVITY ANALYSIS IN UNBALANCED FACTORIAL DESIGNS

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Variance-based sensitivity analysis has been extensively discussed for models in which the inputs can be regarded as independent, uniformly distributed random variables. In this case, there are generally recognized methods for attributing the variance to main effects, higher order terms and random variation. Here, we will address the case of nominal inputs for an unbalanced, possibly incomplete, design for a model without interaction.

The correlation ratio $\frac{Var(E[Y|\mathbf{x}])}{Var(E[Y|\mathbf{x}])+E[Var(Y|\mathbf{x})]}$ is a widely used measure of variance-based sensitivity. We examine three estimators of this ratio in a simple case—a balanced one-factor design. The three approaches are: (i) to estimate each of the three components of the correlation ratio, without bias, from ANOVA mean squares, (ii) to estimate the variation between factor levels by use of margin means, and (iii) to estimate the correlation ratio by use of the coefficient of multiple determination. We discuss the bias, if any, in the components and correlation ratios obtained with the three approaches.

When dealing with unbalanced designs, we assume that the imbalance reflects an intention to give the factor levels different weights, based on logical considerations or a known true representation. Given that assumption, we define theoretical measures of variation and combine them into correlation ratios in unbalanced one-way designs and multi-way designs for which the number of observations in each cell is proportional to the product of the margin numbers. We also show that the component-wise unbiased approach is easily extended from the perfectly balanced case to the latter form of imbalance.

In the case of a truly unbalanced two-factor design, we argue that there are only three sources of variation: effects in the first factor, effects in the second factor, and random variation. The imbalance, however, makes it difficult to separate these sources, as discussed by Saltelli *et.al*[1]. The theoretical measures of variation must be redefined in order to achieve the desired properties of correlation ratios, i.e. ratios summing to one and being non-negative. For the redefined measures, we prove that the technique of solving variation components from ANOVA mean squares can not be used, and at the same time we also show that the coefficient of multiple determination can not be used for estimating the correlation ratio. We suggest a method for estimating variation components by replacing the theoretical factor level effects by their estimators and then combine them into estimators of correlation ratios. This design and the suggested method do not require any thorough discussion of sampling and integration techniques; the method uses only well-known ANOVA calculus and simple calculations based on margin means or estimated effects. We discuss mainly two-way designs, but the method can easily be extended to multi-way designs. It is not component-wise unbiased, but the bias decreases with increasing sample size.

The methods discussed have been successfully applied to data sets representing outputs from models of road traffic emissions. We have studied a selection of pollutants for gasoline and diesel-powered private cars. Emission data were generated by the COPERT III model [2] using a new computer program [3] that can quickly compute emissions for each input value over a grid of input combinations. This program can read and write data on text files for subsequent use in statistical software.

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SIMENV - A FLEXIBLE FRAMEWORK FOR SENSITIVITY AND UNCERTAINTY ANALYSES OF LARGE-VOLUME MODEL OUTPUT

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Modelling and simulation are essential techniques in global change research. One of the challenges in this research field is the development of integrated models which is being achieved mainly by combining models for individual systems and fostered by the availability of increased computing power. Such integrated simulation models are often based on legacy source code applications written in a programming language rather than in a model design language. They typically produce large amount of multi-dimensional model output that has to be handled in the course of a model analysis. These aspects hamper the application of quality assurance techniques since source code is not always well known by model users and intensive code manipulations are normally beyond the scope of the work. Additionally, the computational costs for models in global change research are often very high which demands structured experimentation approaches. Dealing with uncertainty and communicating it to decision makers and the general public is crucial in climate change research [1], [2]. For instance, increasing computing power enabled sensitivity and uncertainty studies of climate projections [3], [4].

For these purposes, a structured and integrated approach for simulation model verification, validation as well as sensitivity and uncertainty analyses is required. This comprises planning experiments, distributing simulation load, post-processing experiment output, and visualizing analysis results. Typically, existing tools supply these functionalities only partially. Furthermore, their interfaces to the model potentially imply limitations concerning usability and flexibility. There is a demand from the modeller's perspective to manipulate a model as less as necessary. Finally, modellers and model users often need guidance in sensitivity and uncertainty related aspects of modelling and simulation.

To handle these problems we developed the simulation environment SimEnv [5] as a flexible framework for sample-based model evaluation that integrates most of the standard techniques normally used by non-expert user. It focuses on sensitivity and uncertainty analyses. SimEnv offers a well-structured and user-friendly approach to interface models, to define und run experiments, to post-process them, to derive quantitative measures, and to qualitatively evaluate them by interactive visualization techniques. It is designed to cope with multi-dimensional, large-volume data in all of these processing steps. Access to the system is facilitated by easy-to-use interfaces.

Experiment definition: The challenge for experiment definition from the developer's point of view is to cover a broad range of tasks for sensitivity, uncertainty and error analyses, numerical verification and validation as well as control design. As a solution we designed pre-formed experiment type templates representing different sampling plans for a subset of model factors (formed from parameters, initial and/or boundary values of the model). SimEnv supplies the following six experiment types: (1) a flexible deterministic screening of the model's behaviour in high-dimensional factor spaces, (2) a global sensitivity analysis based on the Morris method [6], (3) a local sensitivity analysis in the vicinity of the default factor values, (4) Monte Carlo experiments with built-in probability density functions for random and Latin hypercube sampling, (5) an uncertainty analysis to determine total and first order effects of factors on model output by the Sobol' method [7], [8], and (6) an optimization technique based on simulated annealing [9] to minimize a cost function derived from model output over the factor space.

Model interface: Crucial for the applicability of a model experiment framework is a flexible interface to plug in models easily. Thus we designed a model interface that allows with only minimal model modifications (1) to transfer the sample factor values into the model, and (2) to store model variables as SimEnv experiment output for later post-processing. Model interfacing is done at the model language level for C/C++, Fortran and Python by incorporating SimEnv interface function calls into model source code. The basic approach is to include per experiment factor and per model output variable field a SimEnv function call. Additionally, there are special interfaces for Matlab, Mathematica and GAMS models, for shell script models, and an interface to directly transform native ASCII model output to SimEnv experiment output.

Load distribution: Hardware resources are the main bottleneck for studies of large ensemble simulations. Factor values are sampled during experiment preparation which allows performing the single runs of an experiment in parallel. This is supported by SimEnv on workstation clusters by a single run distribution mechanism, applying the Message Passing Interface.

Post-processing: Analysis of large-volume experiment output requires efficient strategies for navigating the high-dimensional factor space and for processing / reducing the model output data. Therefore, SimEnv provides

an interactive post-processor with more than 100 filters / operators. Secondary model output functions can be derived by applying chains of general-purpose operators to model output and reference data. Run ensemble related aggregated measures are calculated by experiment-specific operators. SimEnv supplies built-in operators and an interface for user-defined operators.

Visual evaluation: A further challenge is to analyse and communicate multi-dimensional experiment output and measures. Therefore, a tailored interactive visualization module has been developed and integrated. To handle the diversity of experiment data, this module provides both methods for spatial data sets (graphs, maps and 3D displays) and for data sets with abstract experiment dimensions (scatter plot matrices, parallel coordinates, histogram displays). This diversity of techniques with a variety of interaction mechanisms enables model evaluators to get deeper insight into the behaviour of their models and to communicate the results. However, a problem comes along with the number of visualization techniques and their numerous parameters. Thus, to help non-expert users to generate expressive and effective graphical representations, a mechanism to design appropriate visualizations that is based on data characteristics and user goals has been integrated (see [10] for an overview).

For most of its components, SimEnv offers data interfaces to NetCDF, IEEE compliant binary, and ASCII format. Its strength is to efficiently handle multi-dimensional, large-volume output fields. Due to the flexible and modular framework design, additional sampling strategies / experiment types can be integrated easily into the environment by implementing the corresponding modules for experiment preparation, post-processing, and visualization. The system has proved its applicability in a number of sensitivity and uncertainty case studies, ranging from conceptual qualitative models [11] to large scale climate models [4]. In the paper we will illustrate the capabilities of the system by a practical study.

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TRACER BTC SENSITIVITY W. R. TO FRACTURE – MATRIX PARAMETERS IN SINGLE-WELL PUSH-PULL TESTS WITH CHANGING HYDRAULIC REGIME

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Fluid residence times and transport-effective fracture densities (or specific heat-exchange areas) are two important parameters of subsurface flow systems in fractured-porous formations (or geothermal reservoirs). To determine them, tracer tests are indispensable. Hydraulic and geophysical testing methods cannot reliably determine the two parameters, because the signals on which these methods rely do not depend on, or do not correlate unambiguously with fluid motion and with solute (or heat) fluxes across fracture surfaces. Fluid temperature variations accompanying hydraulic operations do, in principle, reflect the two parameters, but usually high thermal diffusivities make temperature signals rapidly reach quasi-equilibrium values, obliterating parameter dependencies (especially those that would become critical in the long run).

In general, tracer BTCs (breakthrough curves) from single-well push-pull tests exhibit much lower sensitivity to advection-related parameters, than tracer BTCs in flow-path spikings. However, unlike sometimes stated in mainstream literature, a single-well push-pull procedure is not able to reduce the sensitivity of BTCs w. r. to hydrodynamic dispersion, and it does not really contribute to reducing that famous 'empirical indiscernability' between the various processes (hydrodynamic dispersion, matrix diffusion, sorption, multiple-compartment flow and exchange, 'heterogeneity' in general) whose added effects produce BTC tailings.

At the German site of ICDP (Deep Continental Drilling Program), known as the KTB (*Kontinentale Tiefbohrung*), two boreholes are available in the crystalline basement: 4-km deep pilot hole, and 9-km deep main hole, penetrating different, regionally non-intersecting, yet hydraulically slightly communicating faults. The pilot hole is known to screen a highly-permeable fault in 3.8 – 4 km depth, and is fully cased except for this interval. Here, a sequence of short- and long-term spikings could be applied in parallel with a long-term hydraulic, geophysical and seismic testing program: solute and heat push-pull tests were conducted in the depleted, the stimulated, and the early post-stimulation state, with a late outflow phase in the still weakly pressurized, late post-stimulation state (fig. 1); tracer sampling could be performed at this hole only.

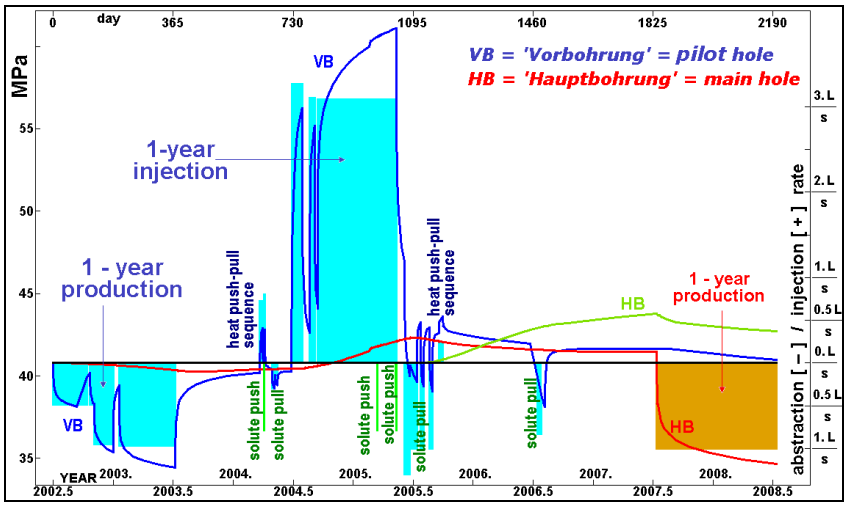

Fig. 1: Sequence and concurrence of various hydraulic and tracer tests at the KTB site

Tracer BTCs from solute push-pull tests (fig. 2), or temperature responses from heat push-pull tests (fig. 3), either, enabled to estimate two parameters: a transport-effective contact-surface area per volume between fractures and rock matrix (or a transport-effective fracture density) deemed as σ, and an effective radial extension *R* of the accessed reservoir (or the space scale 'seen' by the tracers), while other flow- and transport-related parameters are assumed as known, or the tracer BTCs exhibit such poor sensitivity w. r. to these parameters that their values do not matter for the estimation of σ and *R*. In general, this estimation will slightly depend upon the type of conceptualization used for the fracture network, and upon the kind of exchange processes or fluxes assumed across or close to fracture surfaces.

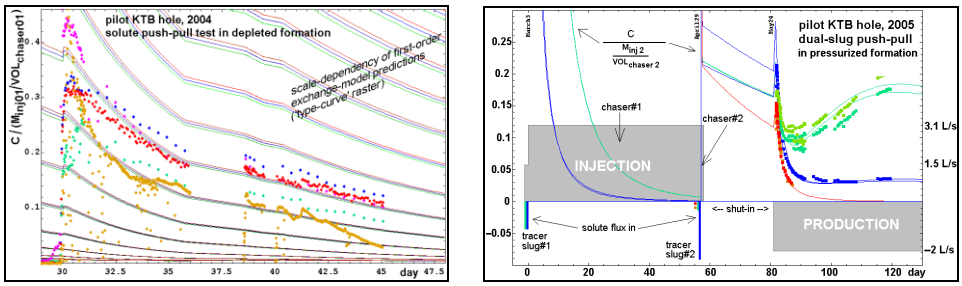

Fig. 2: Solute tracer push-pull tests in depleted vs. stimulated state: measured tracer BTCs, and model fitting

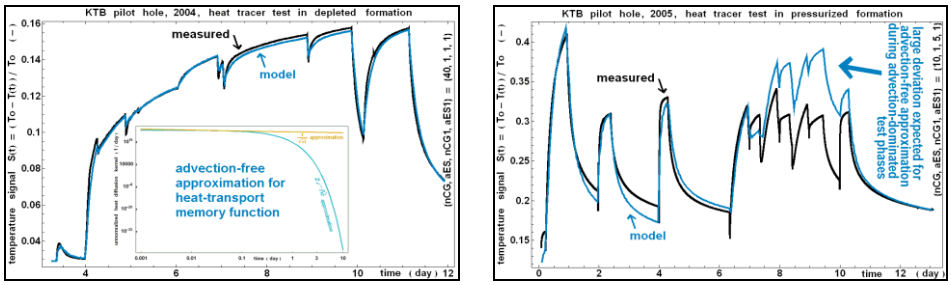

Fig. 3: Heat push-pull sequences in depleted vs. stimulated state: in-situ temperature signal, and model fitting

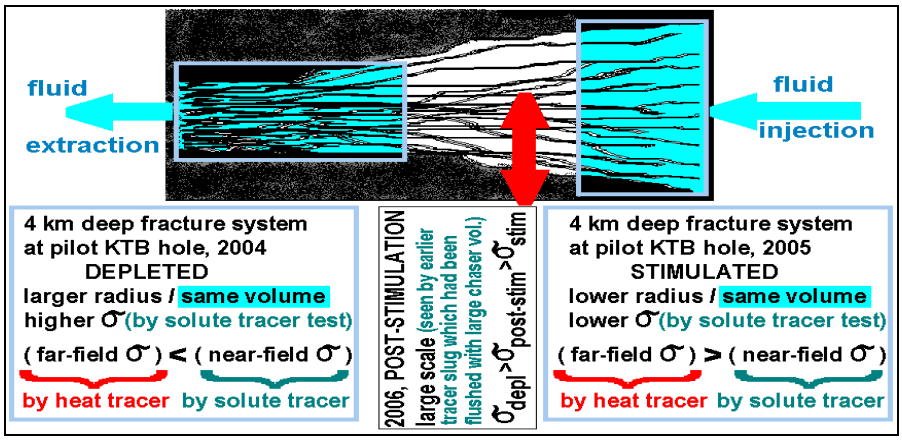

Fig. 4: Interpretation of fracture-system parameter changes during depletion or stimulation. Shaded areas represent equal reference volumes; the same fluid volume means a larger radial extension in depleted, than in stimulated state. During depletion, even some fractures becoming hydraulically inactive may still contribute non-negligible tracer fluxes, thus indicating a higher fracture density.

The effects of long-term depletion (by fluid abstraction) and of long-term stimulation (by cold-fluid injection) on the fracture system were sensitively reflected by solute and temperature signals in terms of σ and *R*, with good sensitivity especially w. r. to σ. For an equal flushing volume, the solute tracer test in depleted state indicates higher values of σ and *R*, than in stimulated state (the post-stimulation, still weakly pressurized state being characterized by intermediate values of σ and *R*). Further, in such low-porosity crystalline rock, heat diffusivity exceeds solute diffusivity by several magnitude orders; as a consequence, heat push-pull tests produced more 'rapid' signals in time and they could 'see' a larger scale in space, thus yielding 'far-field' values in contrast to the near-field values derived from solute tracer tests:

$$\sigma_{\text{stimulated, far-field}} > \sigma_{\text{stimulated, near-field}} \quad , \quad \sigma_{\text{depleted, far-field}} < \sigma_{\text{depleted, near-field}}$$

$$R_{\text{stimulated}} < R_{\text{depleted}} \quad , \quad R_{\text{solute tracers}} < R_{\text{heat}}$$

This implies (cf. fig. 4) that the prevailing effect of long-term, moderate-rate, cold-fluid injection was to enlarge pre-existing fractures, rather than creating new ones – despite some expectations that cooling-induced cracking would prevail; even though (micro-)cracking might have occurred extensively, these (micro-)cracks' contribution to heat and solute transport was overwhelmed by the contribution of pre-existing fractures.

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USE OF SENSITIVITY ANALYSIS TO IMPUTE DATA ON WAGE AND SALARY

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Wages and salaries by social characteristics (sex, age, occupation and educational level) and also in relation with non-standard forms of paid employment are essential to analyse and understand the labour market. These data will allow analysing how wages and salaries accrue to different categories of employees as a result of their involvement in different kinds of paid employment. We tested the possibility of collecting data on wages and link this information with other relevant information from the LFS.

Analyses also concerned wages for which there is a higher frequency of non-response to this item depending on profession and branch of economic activity.

The fact of using the data regarding the employees' monthly wage has drawn the attention on the problem of treating the non-responses, which affect almost a fifth of all respondents. We articulated the imputation procedure according to the following phases:

1) Identification and elimination of the *outliers*;
2) Imputation of the exact value in the case of respondents providing wage in bands;
3) Imputation of missing values.

As regards the identification of the *outliers*, the purpose was to identify the abnormal values so high or so low that there is a sufficiently high probability they are wrong. Likewise, it is relevant to identify the values that, despite their very low relative frequency, could perturb the estimation of the regression coefficients for imputing the missing values, due to their distance from the distribution centre. Applications by means of the multivariate techniques will be used.

The imputation phase was carried out through the INPUTE module of the IVEware packet, developed by the Institute for Social Research of the University of Michigan. The module consists of a generalised procedure of multivariate imputation that can treat even relatively difficult data structures under the MAR hypothesis (missing at random). IVEware applies the stochastic regression imputation methods. The results of the methods of regression imputation are strongly influenced by the specification of the regression model and by the set of covariates that we choose to include. In particular, the auxiliary variables must be strongly correlated to wages.

Furthermore the results are also influenced by the model's function, linear or logarithmic, and by the imputation's range.

In order to choose the best set of covariates we conducted a simulation using data of respondent to wage and salary. So it was possible to compare imputed data with the answers. In particular we compare the difference of results about 4 models:

1.linear model with large bounds
2.linear model with small bounds
3.logarithmic model with large bounds
4.logarithmic model with small bounds.

So we tested how the model selected influence the final distribution, both the descriptive statistics and the distribution curve.

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SOME ASPECTS OF SENSITIVITY IN GAUSSIAN BAYESIAN NETWORKS

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Gaussian Bayesian networks are graphical probabilistic models that provide a graphical framework of complex domains with lots of related variables with the same Gaussian structure.
We develop a method to perform a one-way sensitivity analysis for Gaussian Bayesian networks useful to evaluate the network's output and the impact of model inaccuracies, being the network's output the results about the variable of interest and considering each time the impact of only one inaccurate parameter.
This sensitivity analysis is based on computing a divergence measure, as the sensitivity measure, that compares the network's output with and without a perturbation that quantifies model inaccuracies (Gómez-Villegas [1]).
Moreover, the effect of the evidence propagation is considered because the sensitivity measure is computed after this propagation.
In this work we generalize the obtained results computing a n-way sensitivity analysis to evaluate a set of model inaccuracies over the network's output. In this case, a set of variables of interest are also considered.
We illustrate the proposed methods with some examples.

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THE ARPEGE/ALADIN LIMITED AREA ENSEMBLE PREDICTION SYSTEM: SENSITIVITY EXPERIMENTS USING GLOBAL SINGULAR VECTORS

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By perturbing the initial state of a numerical weather prediction (NWP) model it is possible to take into account the impact of the errors in the initial conditions (the fully exact description of the initial state is not achievable due to observation errors, errors in the data assimilation techniques etc). Then the model is integrated from these different initial conditions forming an ensemble of numerical weather predictions. The spread of this ensemble provides useful information on the predictability of the atmospheric state and on the probability of different weather events. One possible way to create such an ensemble is to use the singular vector method [1] to perturb the initial conditions of the model. The aim is to find perturbations for a given initial state which grow most rapidly according to the chosen norm (e.g. total energy norm) focusing on a specific area (the optimization area) during a given time interval (optimization time). In this study sensitivity experiments were carried out in order to explore whether or not it is possible to optimize an existing global ensemble system (based on the French global NWP model ARPEGE) for Central Europe by changing only the optimization area and optimization time used for the global singular vector computations. With this purpose several optimization areas and times were defined and tested through case studies and longer test periods. Global ensemble forecasts were downscaled with a limited area NWP model (called ALADIN). Verification results show that the proper choice of the singular vector optimization domain and optimization time can increase the spread of the ensemble and (on average) improves the skill for the Central European area. This conclusion was found to be valid for the global forecasts and the limited area predictions (i.e. the simple downscaling of the global model) as well.

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DESIGN OPTIMIZATION AND RELIABILITY ASSESSMENT OF PASSIVE AND ACTIVE STRUCTURAL SYSTEMS VIA SENSITIVITY ANALYSIS

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In this paper the application of variance based sensitivity measures to numerical models of passive and active structural systems is evaluated. Sensitivity Analyses (SA) are performed for the purpose of design optimization, reliability and durability assessment.

In modern engineering, the Finite Element Method (FEM) has become a widely accepted tool to assess the mechanical behavior of technical components and structures, whereas the reliability and structural durability of systems is assessed mostly using experimental test methods. With increasing complexity of the structures and especially integration of electronic components and smart materials, e.g. piezoceramic actuators and sensors, experimental costs become exceedingly large. Thus, great effort is undertaken to replace these traditional test methods by computational simulation tools, which have to be able to reproduce the complex system performance and also account for various failure and fatigue scenarios.

The combination of FEM modeling and global SA methods seems to be very promising for this purpose. Uncertainty inherent to such systems can be implemented and interacting parameters can be identified. Using an accordingly well defined model output and failure modes designed as uncertain distributed input parameters, SA can be used to identify and classify the importance of the different input values and thus assess the reliability of the system with respect to each implemented failure mode.

The methodology used is exemplified by the analysis of a simple passive structure. Subsequently the application to an active complex system is presented. At first a notched axisymmetric component part is considered, which can be found in many technical structures. The component is exposed to a pressure load and the system failure is characterized by plastic deformation and the formation of structural cracks. To avoid failure and to secure a long lifespan, components like this are often overdesigned which contradicts the objective of energy efficient lightweight design. In order to optimize the component design and still secure the operational reliability a variance based SA is performed to identify the parameters which contribute strongly to the component failure defined as a certain threshold of plastic deformation. Several uncertain parameters are considered, where variations in the material parameters and abrasion of the machine tools, influencing the geometrical shape, are taken into account. A parallel probabilistic analysis is performed and correlation coefficients obtained. The results of the variance based SA and the probabilistic analysis are presented and discussed.

A second application scenario for SA is presented, with the analysis of an active oilpan system. Sound radiated from the oilpan is one of the main contributions to the noise emission of combustion engines in cars and dominates the noise contribution in most urban traffic scenarios. For several technical reasons, passive solutions for the reduction of noise emission are not feasible. Therefore, active noise suppression systems are designed, comprising piezoelectric actuators and sensors, which are subject to more or less severe degradation depending on operating conditions, applied control algorithm and load-time history. The performance of the active system, characterized by a defined reduction of noise emission in a particular frequency range, is simulated in different failure and fatigue scenarios. These include sensor and actuator degradation and malfunction. In order to choose an optimal design, including the most fault tolerant control algorithm, a SA is conducted, to incorporate uncertainties and variations in the positioning and performance of sensors and actuators and geometrical and material parameters. The results are shown and discussed. The application of variance based sensitivity measures on models based on the FEM is shown to be a valuable tool to assess an optimized design with respect to reliability and robustness.

A STOCHASTIC PERTURBATION SCHEME TO REPRESENT MODEL RELATED ERRORS IN NUMERICAL ATMOSPHERIC FORECASTS

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It has been demonstrated that ensemble (Monte Carlo) forecast systems can describe forecast uncertainty associated with errors in the initial conditions of chaotic dynamical systems. The realistic description of model-related forecast errors is a more challenging task. Despite the development and application of various related techniques (see, e.g., Toth and Vannitsem [1]), ensemble forecast systems in general are under-dispersive and cannot properly account for model-related uncertainty.

To represent model-related forecast uncertainty in numerical atmospheric general circulation models, a stochastic perturbation scheme has been developed for and tested with the National Centers for Environmental Prediction (NCEP) Global Ensemble Forecast System (GEFS). The scheme is based on the time evolving perturbations in an ensemble forecast system. The stochastic perturbations are defined based on the total conventional forcing, including the grid scale processes and the sub-grid scale parameterizations. Specifically, the stochastic perturbation (i.e., an extra forcing term) for a particular ensemble member is a weighted combination of the tendencies of the ensemble perturbations, i.e the differences in tendency between the ensemble members and the control forecast. The combination coefficients (see Fig. 1) are generated through a temporally correlated stochastic process using constraints that keep the perturbations quasi-orthogonal. The resulting flow dependent perturbations are applied to all model state variables.

The scheme will be assessed in the context of how well it captures forecast errors that cannot be explained by perturbing the initial state of the system. Initial tests with the stochastic perturbation scheme show a significant reduction in the number of outliers (i.e., cases when the verifying truth lies outside of the ensemble of forecasts), and an increase in the spread of the ensemble, reaching the level of root mean square error of the ensemble mean forecast. Also, a marked decrease in systematic errors is observed, along with an improvement in probabilistic forecast performance. Interestingly, the positive effects of the stochastic perturbation scheme are complementary to the effect of statistical post-processing used for reducing systematic errors. When statistical bias correction is applied on the stochastically perturbed ensemble, the performance significantly surpasses that of an ensemble that is either only statistically bias-corrected or only stochastically perturbed.

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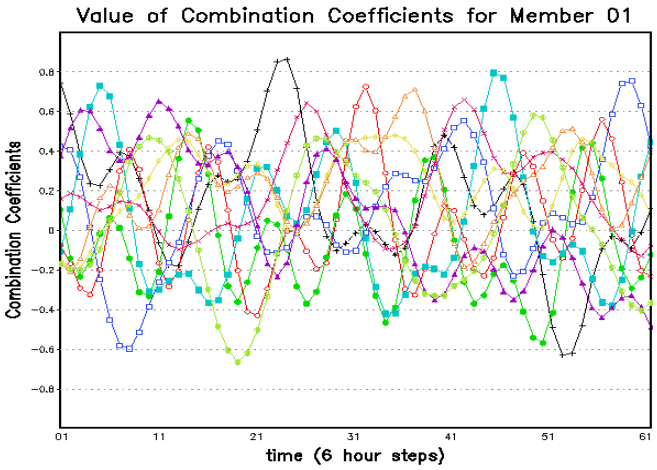

Fig. 1. Linear coefficients used to combine tendency perturbations for stochastic forcing to be applied on a particular ensemble member, based on all members of the ensemble (lines with various colors), as a function of forecast lead time

THE USE OF G.I.S. AND P.C.A. FOR MAPPING PRECIPITATIONS IN ARID AREA: CASE OF ZIZ ET RHERIS WATERSHEDS, MOROCCO

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This works aims to presents a statistical analysis and a spatial modelling of a G.I.S platform of the precipitation data in the semi-arid area of south-east Morocco, which corresponds to watersheds of the Ziz and Rheris rivers. This analysis is a kind of statistical treatment of rainfall data series which provides cartography with the precipitation data (Fig.1). Thus, we propose an equation explaining the precipitation value by means of four variables determined from a model of multiple regressions. This approach of modelling, based on the construction of continuous spatial information in raster format from the punctual data issued of the variable density observation networks, leads to search for the laws and the statistical properties. These last, permit to understand well the spatialization of precipitations with physiographic environment (MNT, slope, exhibition, geology, proximity of the Sahara, latitude and longitude).

The use of the statistical techniques notably the analysis in main constituents (AMP), and the multiple regression, as well as the cartographic capacity of a G.I.S seems well adapted to criticizing and analysing the continuity and spatial modelling of rainfall data in semi-arid climate.

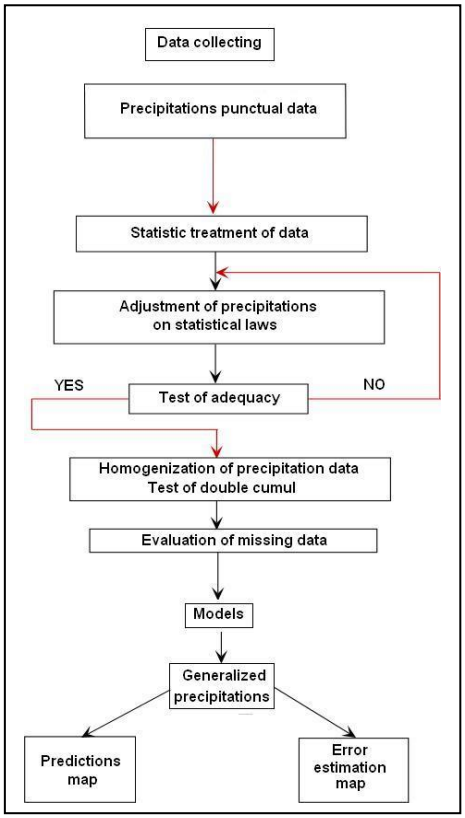

Fig.1: Modelling approach used to spatialize climatic data

SENSITIVITY ANALYSIS OF STEEL STRUCTURES WITH IMPERFECTIONS

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Sensitivity analysis methods in application to the analysis of the influence of imperfections of steel structures on their reliability are presented in the paper. The aim of sensitivity analysis is the assessment of the influence of input random variables on the variability of output random variables. In regard to the limit states of structures, the load carrying capacity (or deflection at selected section) is frequently considered as the output variable. In mass produced products (e.g. steel hot–rolled profiles, etc.) it is possible to according to the relative sensitivity determine those variables that the monitored output (e.g. load carrying capacity) is especially sensitive to. It is then possible to concentrate control activity on these variables with aim at securing sufficient stability in statistical parameters or at lowering their random variability.

Sensitivity analysis can be generally divided into two groups:

a) Deterministic sensitivity analysis (design sensitivity) is relatively well known, frequently used during structural design. The most frequent type of sensitivity analysis is a parametric study utilizing a computational model, which accompanies the design process [1]. This study may be simply realized as a sequence of calculations with gradually varying values of a certain input parameter X_i in each calculation step $j (j = 1, 2,\ldots,K)$ in a certain real range. The influence of parameter X_i on the response Y_j can be observed through the comparison of the calculative results Y_j (the set of the structure response). Certain more advanced computational programmes include such an option and everything is performed automatically. Quantified data on sensitivity is however not obtained.

b) Stochastic sensitivity analysis offers more complex and quantified information on the influence of parameters. It is however necessary to utilize more sophisticated numerical methods. Different procedures of stochastic sensitivity analysis are frequently implemented in reliability based software. Input parameters are considered as random variables, described by their probability distributions with given statistical parameters: mean value, standard deviation, respectively by their skewness and kurtosis. The procedure for the determination of sensitivity is to a certain degree similar to the deterministic sensitivity analysis. The parameter is also gradually changed, however, within the framework of the applied simulation technique. The influence of this change on the output variable is observed. The change in input variable is performed with respect to its distribution (the frequency of its occurrence), i.e., other valuable information, which is neglected in the deterministic sensitivity analysis, is utilized. The sensitivity analysis is a suitable supplement of every level of reliability analysis. It is usually performed in connection to utilized reliability analysis.

It would be very valuable to perform the stochastic sensitivity analysis utilizing experimental results. This is however practically impossible especially due to economic restraints. Only certain characteristics of beams can be reliably measured by non–destructive methods. It is better to use numerical sensitivity analysis. Particularly due to large diversity of initial imperfections and possibilities of their mutual combination it is more suitable to utilise the so–called numerical sensitivity analysis. During which it is possible to utilize valuable results of long term research e.g. [4, 5].

The subject of the article is the numerical stochastic sensitivity analysis of the influence of imperfections on the load carrying capacity of steel structures. Imperfections are generally random variables, only very little statistical information of these variables from measurements on real structures is available. Typical examples include system imperfections of plane frames; see Fig. 1 and Fig. 2. The loading type of steel frames in Fig. 1 predicts large influence of system imperfections on the load carrying capacity. System imperfections are depicted by a dashed line in Fig. 1. The influence of boundary conditions on the sensitivity of the load carrying capacity to the imperfection is studied. Boundary conditions were considered as hinged and clamped end in the numerical study. These represent limit variants of reality. Additionally considered imperfections include strut imperfections of columns, geometric deviations of profile dimensions, material and geometric characteristics.

The output load carrying capacity was evaluated by means of the geometric non–linear solution of the finite element method. Input random imperfections were considered according to results of experimental research [2] and [3]. The random load carrying capacity was evaluated utilizing the Latin Hypercube Sampling method, which is an improved version of the Monte Carlo method. 800 simulation runs were utilized. The sensitivity analysis was performed in the form of Spearman's rank–order correlation coefficient. A frame of height 6m and span 6m with cross beam IPE 360 and columns IPE 270 was solved.

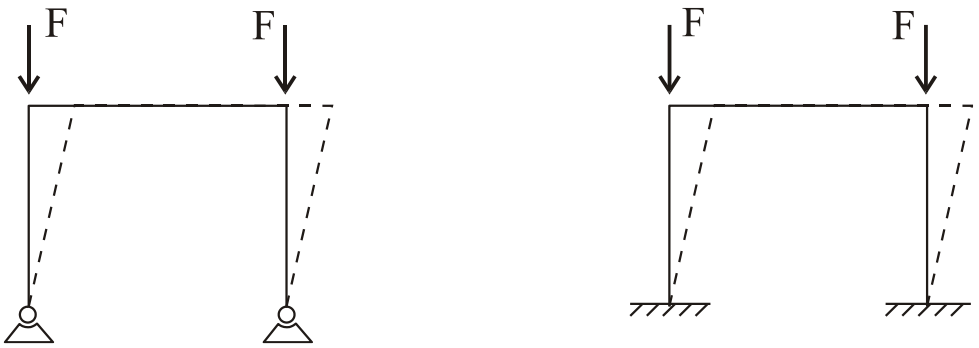

Fig. 1: System imperfections of steel plane frames

The influence of input variables on the load carrying capacity was evaluated by means of sensitivity analysis. Sensitivity analyses results illustrate varying sensitivity of the load carrying capacity to the system imperfections of both frames depicted in Fig. 1. The variability of the load carrying capacity is more sensitive to the variability of system imperfections in the left frame. Conversely, the dominant variables of the right frame are the yield strength and residual stress. Relatively high correlation between the load carrying capacity and the flange thickness of the columns was observed in practically all of the analysed problems.

Statistical characteristics of the dominant input variables should be determined and checked with increased care [2]. Input random variables can generally be divided into two basic groups – imperfections, whose statistical characteristics can be positively influenced in production (yield strength, residual stress, geometrical characteristics), and imperfections, which are not sensitive to changes in the technology of production (e.g. variability of Young's modulus E) [2]. The first group of variables may be further subdivided into two subgroups: (i) variables for which both the mean value and the standard deviation can be changed by improving the quality of production, e.g. the yield strength; (ii) variables whose mean value cannot be significantly changed because it should approximately correspond to the nominal value (geometric characteristics of profile dimensions) [2].

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SENSITIVITY ANALYSIS OF FATIGUE CRACK PROPAGATION

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One of the inherent parts of the design of new or existing structures under the influence of many times repeated loading is the assessment of fatigue. A part of design is the stipulation of the criteria of limit states, i.e. the stipulation of conditions to be fulfilled so that the structure is reliable in all situations and all loading cases and failure does not occur. During the analysis of complex problems of structural behaviour in addition to the final result we generally may be interested in further matters, such as: in what way the input parameters influence the result, or in other words, the sensitivity of the response to a change of the input parameter. The identification of these quantities and their constitutive relations is performed utilizing the methods of sensitivity analysis.

Sensitivity analysis methods enable the quantification of the influence and the assessment of the significance of individual input variables on structural response. In view of the fact that input variables are generally random, it is necessary to take their variability into account during the determination of their influences. The output variable of the computational model is then also a random variable, for which we can determine the mean value, variation coefficient, distribution type, etc. similarly as for the input variables. In the event that information on the variability of input and output variables is available, the quantification of sensitivity of output variables on the input variables can be performed. In this regard we speak about the so-called stochastic sensitivity analysis. The stochastic sensitivity analysis enables the assessment of the relative sensitivity of random variability of the studied phenomenon to the random variability of individual input variables [1].

The aim of the presented study is a sensitivity analysis of the effect of factors influencing the fatigue crack propagation in a steel element under bending moment. The linear elastic fracture mechanics based on Paris-Erdogan's formula was used.

$$\frac{da}{dN} = C\left(\Delta K\right)^n \tag{1}$$

where a – crack size, N – number of cycles, C, n – material constants, ΔK is the amplitude of the stress intensity coefficient. C, n are material constants which can be determined by statistical processing from a set of experimentally determined data pairs (da/dN, ΔK). From acquired results it is possible to make recommendations which input random variables have the greatest influence on the fatigue resistance and should thus be checked with increased accuracy in production of new structures and during the examination of existing structures.

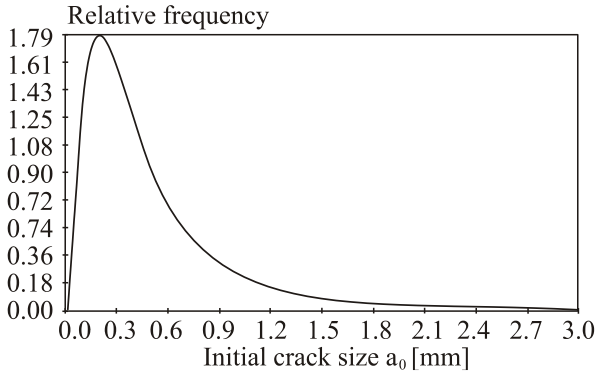

Fig. 1: Density function of initial crack size a_0

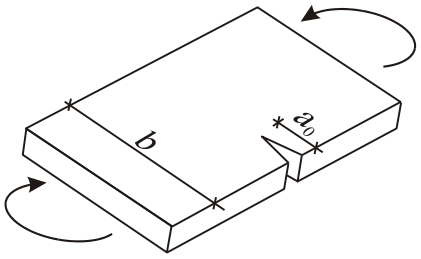

Fig. 2: Element with initial crack size a_0

From measurements of crack propagations in the surface of welded joints it was determined that the lognormal distribution with mean value $m_{a0} = 0.526$ and standard deviation $S_{a0} = 0.504$ can be considered for the initial crack [4]. Further random variables considered include the width of steel element b and the critical length a_{cr} that the crack approaches without reaching macro plastic instability. Mean value $m_b = 400$ mm and standard deviation $S_b = 25$ mm [2] were considered for the width of the steel element. In the case of the critical crack length a_{cr} mean value $m_{acr} = 200$ mm and standard deviation $S_{acr} = 20$ mm [2] were considered. The coefficient n, which represents a function of a whole array of factors [3], was also implemented as a random variable. The coefficient n increases with decreasing fracture toughness. The parameter n was assumed to have a Gaussian

distribution with mean value m_n=3 and variation coefficient v_n=0.01 in our study. The strong correlation between parameters C and n was confirmed experimentally [3]. In the event that exponent n does not represent a universal constant, it stems from the analysis of Paris-Erdogan's relation (1), that the physical size of constant C generally changes too. The interrelationship between C and n can be expressed according to [3] as $\log(C) = c_1 + c_2 n$. Parameters c_1<0 and c_2<0 are constants for given material grade. We considered in accordance with [3] for our example for steel of grade S235 c_1= -11.141, c_2= -0.507. The realizations of input random variables were generated utilizing the LHS method for 400 runs. The fatigue resistance, which is the maximum number of cycles N during which the crack with initial size a_0 reaches the critical size a_{cr}, was considered as the output random variable.

The sensitivity analysis was evaluated by monitoring the Spearman rank-order correlation coefficient between the input and output, see Fig. 3a. The method based on the evaluations of the ratio of second order of variation coefficients between input and output was chosen as a second alternative, see Fig. 3a.

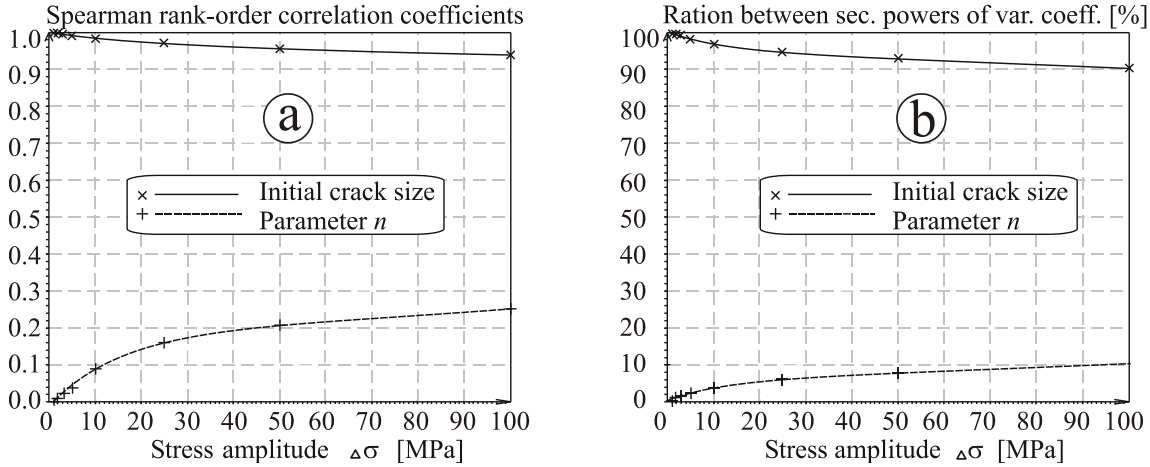

Fig. 3: Results of sensitivity analysis

The variability of initial crack size a_0 has the greatest influence on the variability of fatigue resistance [2]. The sensitivity coefficient value decreases with increasing stress amplitude $\Delta\sigma$. Since the initial crack size has a large influence on the fatigue resistance, its statistical characteristics should be determined with maximal precision. The second dominant variable is parameter n. Determination of satisfactorily accurate statistical characteristics of parameter n is of major importance for further application in probability analyses. The sensitivity coefficient of parameter n increases with increasing value of $\Delta\sigma$. The variability of the width of the steel element b and of the critical length a_{cr} has no influence on the variability of fatigue resistance and hence can be considered as deterministic variables. This may significantly simplify modelling.

Acknowledgement:

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REDUCTION OF A GAS-PHASE REACTION MECHANISM DEVELOPED FOR THE ANODE CHANNELS OF SOLID-OXIDE FUEL CELLS

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Fuel cell technology is one of the most promising opportunities for generating energy with decreased environmental impact. Several types of fuel cells have been developed in the past decades. One of the great advantages of solid-oxide fuel cells is their absolute tolerance to CO, unlike the other types of fuel cells *e.g.* solid polymer electrolyte fuel cells (SPEFCs). Furthermore, in solid-oxide fuel cells several available fossil fuels can be used, thus there is no need to build a hydrogen delivery infrastructure. In hybrid systems, where a gas turbine is built in the SOFC, the efficiency can reach 75-80 % [1].

The core of the solid-oxide fuel cell (SOFC) is a solid electrolyte, which is a conductor for oxide-ions at the operating temperature. During the operation of the solid-oxide fuel cell, oxygen is reduced at the cathode, the formed oxygen anion diffuses across the oxide-ion selective electrolyte, which is insulating for electrons. Although solid-oxide fuel cells have so far been operated with methane, propane, butane, fermentation gas, gasified biomass and paint fumes [2], the hydrocarbon fuel is first converted mainly to CO and H_2 by steam reforming, either within the anode region or externally. In the three-phase region, hydrogen is electrochemically oxidized and forms water and electrons. This water then participates in the water gas shift reaction to convert CO to CO_2 and H_2, and this H_2 is subsequently oxidized in the three- phase region.

The operating temperature is about 800-1000 °C and therefore the homogeneous gas-phase reactions are significant before the fuel mixture reaches the anode. These reactions convert the initial hydrocarbons to H_2, CO, H_2O and other products, and also may lead to the formation of polyaromatic hydrocarbon deposits. Air and water steam may be added to the initial fuel to prevent deposit formation. Deposit formation can be related to the concentration of species having more than four carbon atoms, denoted by C^{5+}.

Anthony Dean and his group study the homogeneous gas-phase anode channel reactions of solid-oxide fuel cells. Recently, a detailed reaction mechanism was created and tested [3] that is applicable at solid-oxide fuel cell operating conditions. It can model the reactions of methane and natural gas, with air and/or steam added. In this study, a further developed (2006 May) version of the mechanism was investigated which contains 6874 irreversible reactions of 350 species. This mechanism is too large for an industrial optimisation process and therefore reduction is needed. Our purpose was to find a reduced mechanism, which contains less species and fewer reactions, but its simulation reproduces the results obtained using the original mechanism within a few percent. We intended to investigate the effects of the composition and temperature on the formation of the main products and the C^{5+} species.

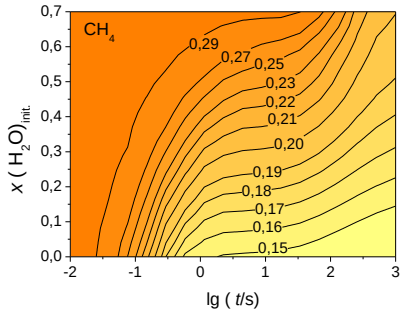

Figure 6 Mole fraction of methane in a methane – air – steam mixtures

The CHEMKIN 4 program package was used for the simulations. The effect of the various initial compositions was investigated in two series of simulations using the original mechanism. The operating conditions of a solid-oxide fuel cell can vary across a wide range of conditions, and we selected initial parameters that generally represent well the SOFCs. Thus, temperature and pressure were chosen to be 900 °C (1173.15 K) and 1 atm (101325 Pa), respectively. In both series of simulations, the initial mole fraction of methane was 0.3. Results are illustrated on a series of contour plots showing mole fractions of species as a function of residence time (*x* axis) and the initial mole fraction of steam (*y* axis).

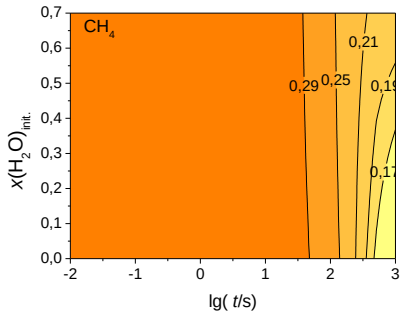

Figure 7 Mole fraction of methane in methane – carbon dioxide – steam mixtures

In the first series of simulations, the initial mixture consisted of methane, air and steam. Mole fraction of steam was varied from 0.7 to 0. Accordingly, the initial mole fraction of air changed from 0 to 0.7. The mole fraction of methane is viewed in Figure 1. In the second series of simulations, the initial mixture consisted of methane, steam and CO_2. Mole fraction of steam was varied from 0.7 to 0, and thus the initial mole fraction of CO_2 changed from 0 to 0.7. The mole fraction of methane is viewed in Figure 2.

It's visible that the composition of the original mixture has a great importance. The curves have very different characteristics: presence of oxygen makes the reaction much faster. In air rich mixtures the decay of mole fractions of oxygen and methane are fast. In methane – air – steam mixtures there are significant

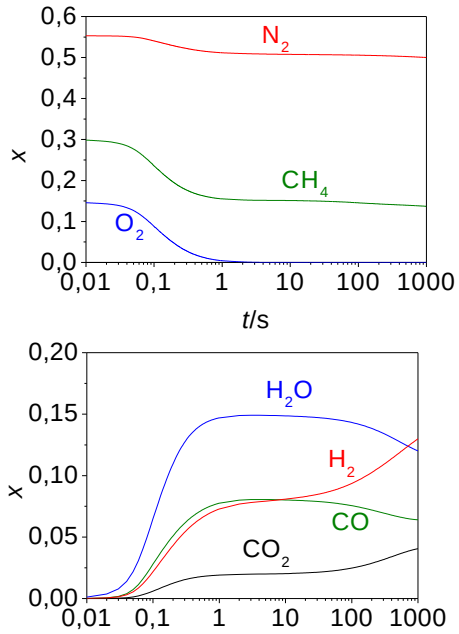

Figure 8 Mole fraction-time curves

differences in the behaviour of air rich and steam rich mixtures. In methane – steam – carbon dioxide mixtures the changes are much slower and the dependence on the initial composition is less.

The mechanism reduction was carried out at isothermal and isobaric conditions. The composition of the initial mixture was 30.0 % v/v methane and 70.0 % v/v air. The assumed composition of air was 79 % v/v nitrogen and 21 % v/v oxygen. The mole fraction of CH_4, O_2, N_2, CO, CO_2, H_2CO, H_2, H_2O, C_2H_6, C_2H_4, C_2H_2 and benzene (C_6H_6) reaches or exceeds 0.001. The mole fraction-time curves of major species can be seen in Figure 3.

Two ways of mechanism reduction were applied. In the first manner, the reduction was carried out in two steps: first the redundant species, then the redundant reactions were eliminated. In the second manner some disadvantages of the original method were eliminated.

A possible algorithm for the detection of redundant species can be based on the inspection of the normalized Jacobian $\tilde{\mathbf{J}}_{ij} = (y_i / f_j)(\partial f_j / \partial y_i)$. An element of the normalized Jacobian provides information about how the production rate of species *j* changes, if the concentration of species *i* is perturbed [4,5]. In the next step, redundant reactions were eliminated. A possible method for the elimination of redundant reactions from detailed reaction mechanisms is the principal component analysis of the rate sensitivity matrix **F** (PCAF method) [5,6]. Both analyses were done by program KINALC [7].

The reduced mechanism contains only 1834 irreversible reactions of 168 species. We observed good agreement of the mole fractions of the important species, when their mole fraction was higher then 0.001. Thus, good agreement was observed for species CH_4, N_2, CO, CO_2, H_2, H_2O, C_2H_4 and C_2H_2 during the whole time-scale; O_2, H_2CO and C_2H_6 till 1 s, and benzene (C_6H_6) from 100 s. The average error was less than 1 %, the largest difference was 6.90 % for the mole fraction of benzene at t = 970 s.

The original species/reaction elimination method has some disadvantages. Species, having either non-zero initial concentration, or an introduction term, or an effective production reaction (a reaction route back to initialized or introduced species) is called a living species. The original method allows that a species is indicated to be necessary, but this species is not necessarily living. Addition of one species to the set of important species not necessarily makes any reaction selected, thus the connection of those species or set of species should be investigated, which make at least one reaction selected. Minimal sets closely connected to the group at every times are identified and ranked according to their strengths of link. At every time point there can be many minimal sets with strong link to the group, therefore it is reasonable to try more of them to find the optimal way to reduce error. Each of the added sets is checked whether its species become living when added to the group. After this a numerical test determined, which effective set of species are the most efficient in improving agreement with the full mechanism. The obtained skeletal mechanisms are integrated, and their species and global errors are stored. At every size, the set of necessary species with smallest error are taken under PCA to find important reactions. One of the reduced mechanisms contains 50 species, its maximal error is 5 %, and the simulation process is 92 times faster.

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THE PRINCIPAL VARIANCE-BASED SENSITIVITY INDICES CAN BE ESTIMATED WITHOUT ASSUMING INDEPENDENCE BETWEEN THE INPUT VARIABLES

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The two principal types of variance-based sensitivity indices, the "first-order effect" index and the "total effect" index, are well known and often used in global sensitivity analyses of results from computational models. However, originally, the definition and interpretation of these sensitivity indices as well as the sampling-based computational procedures, e.g. the "Homma-Saltelli" method, have been based essentially on the assumption of stochastic independence between the input variables involved. Particularly, it is well known that Sobol's variance decomposition, a crucial point of the original representation of the variance-based global sensitivity analysis, is valid only in case of independent input variables. Modifications of the method, e.g. assuming independence only between variables from disjoint subsets but not necessarily between variables inside each subset, have slightly mitigated but not fully eliminated this restriction.

This paper will show that the assumption of independence is essentially unnecessary and can be dropped. The "first-order effect" and the "total effect" sensitivity indices can consistently be defined and interpreted without this restriction and without reference to Sobol's variance decomposition as well. Moreover, a slight modification of the original "Homma-Saltelli" sampling-based computational procedure is suggested with which the two types of sensitivity indices can be estimated in the dependent case in nearly the same way and at exactly the same moderate computational cost as in the independent case. It therefore provides a practicable alternative to the computationally much more expensive "nested" "double-loop" calculations so far necessary for the global sensitivity analysis in the general non-independent case. Any type of dependence between the input variables can in principle be accounted for by this method as long as it can be represented by tractable conditional probability distributions. In the independent case, i.e. when the joint probability distribution of the variables is the product of their marginal distributions, this method of course coincides with the traditional "Homma-Saltelli" method.

GLOBAL SENSITIVITY ANALYSIS FOR SIMULATION MODELS WITH MULTIPLE OUTPUTS: AN APPLICATION TO A DYNAMIC CROP MODEL

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Dynamic crop models are used by agronomists for crop management and for predicting the effects of farmers' practices on crop characteristics, assuming various climate and environment conditions. Many crop models predict plant growth (wheat, corn...) on a daily basis through detailed mechanisms in function of daily climatic inputs like daily radiation and temperature. Their outputs can be expressed as time series. Such models are dynamic, complex and often over-parameterized with respect to the available observations [4]. Indeed, they can include up to 200 parameters which need calibration. In general, it is impossible to estimate all parameters of such models. The strategy of selecting a subset of parameters to be calibrated and fixing the others to their nominal values is reported in [1], [2] and is based on sensitivity analysis.

For a dynamic crop model, sensitivity analysis can be applied separately on each daily output but there is a high level of redundancy between close dates and, on the other hand, interesting features of the dynamic may be missed out [5]. As an alternative, Campbell and McKay [3] proposed to decompose time series upon a complete orthogonal basis and to compute sensitivity indices on each component of the decomposition. In this paper, we follow on this proposal and present the multivariate sensitivity analysis under a global framework coherent with classical multivariate methods. A global index is deduced which synthesizes the decomposition of the total output inertia between parameter main effects and interactions. It may be used to select a subset of parameters to be calibrated. In addition a quality criterion is proposed for any approximation associated with the decomposition.

Crop models are usually deterministic and they can be written in the mathematical form

$$Y(t) = f(X, t), \qquad (1)$$

where X is here the parameter vector and $Y(t)$ is the output at time t, for $t=1 \ldots T$. $Y(t)$ may represent, for instance the wheat biomass observed at day t. Each parameter is unknown but is supposed to vary within an uncertainty interval.

Consider, for simplicity, a complete factorial design on the uncertain parameters. Simulations using equation (1) generate the outputs matrix $\mathcal{Y}$. Each column $\mathcal{Y}(t)$ of $\mathcal{Y}$ represents the simulated values of the output variable at a given time t. Each row of $\mathcal{Y}$ is an individual dynamic output for a given set of input values and the rows of $\mathcal{Y}$ constitute a sample of dynamics in R^T over the uncertainty domain of the input factors. The quantity $\sigma 2 = \text{Trace}(\mathcal{Y}'\mathcal{Y})$ is called the total inertia of $\mathcal{Y}$. In practice, the columns of $\mathcal{Y}$ are often centered and standardized so that $\sigma 2 = T$. When a Principal Component Analysis (PCA) is applied to the matrix $\mathcal{Y}$, global sensitivity analyses can be performed on each principal component via ANOVA decompositions. The 'Sum of Square (SC)' associated with any factorial term W (a main effect or an interaction between parameters included in X) and any principal component H_j can be expressed as $SC_{Wj}=\text{Trace}(\mathcal{Y}'S_W\mathcal{Y}v_jv_j')$, where S_W is the orthogonal projection matrix on the subspace associated with W and v_j is the eigenvector associated with H_j. This quantity becomes $SC_W^P = \text{Trace}(\mathcal{Y}'S_W\mathcal{Y}\sum v_jv_j')$ when summing for j over the first P principal components and $SC_W = \text{Trace}(\mathcal{Y}'S_W\mathcal{Y})$ when summing over all principal components. By then summing SC_W (resp SC_{Wj}, SC_W^P) over all factorial terms W, one obtains $\sigma 2$ (resp λ_j , $\sum\lambda_j$), where λ_j is the inertia associated with H_j. Thus SC_W represents the inertia accounted for by W and SC_{Wj} the variance due to W on the principal component H_j. In consequence, the Sensitivity Global Index of W is defined as $SGI(W) = SC_W/\sigma 2$, whereas $SI_j(W) = SC_{Wj}/\lambda_j$ is the classical Sensitivity Index of W on H_j.

In practice, the model is often approximated by the first P principal components and by restricting the ANOVA models to the main effects and a few interactions. Thus the "approximate" Sensitivity Global Index $\widetilde{SGI}$ is defined as

$$\widetilde{SGI}(W) = SC_W^P / \sum_{j=1}^{P} \lambda_j \qquad (2)$$

In this case, $\sum_W SC_W^P / \sigma 2$ quantifies the percentage of inertia preserved by the approximation. In order to assess the approximation directly on the $\mathcal{Y}(t)$s, a dynamic coefficient of determination at date t is also proposed.

This approach was applied to the crop model WWDM (Winter wheat Dry Matter Model) which simulates wheat dry matter at a daily time step in function of 7 parameters. Table 1 shows the Sensitivity Global Indices when one considers only the first 3 principal components and the first order interactions. These indices were computed by using the sums of square SC_W^3. The radiation use efficiency parameter Eb appears to be the most important parameter and it is worth investigating in its calibration. By using the first 3 principal components and only the first order interactions, 91% of the total inertia is accounted for. The dynamic coefficient of determination is shown in Figure 1.

Factorial Term (W)	Sensitivity index per component			Sensitivity Global Index	
	PC_1	PC_2	PC_3	$\widetilde{SGI}$	SGI
Eb	0.446	0.089	0.002	0.294	0.282
A	0.013	0.482	0.026	0.184	0.178
TI	0.104	0.164	0.154	0.128	0.126
Lmax	0.139	0.016	0.007	0.088	0.085
A:B	0.083	0.009	0.088	0.057	0.060
B	0.058	0.010	0.083	0.042	0.041
A:TI	0.016	0.028	0.298	0.034	0.036
Eb:A	0.002	0.085	0.005	0.032	0.031
Eb:Ti	0.018	0.029	0.027	0.023	0.022
Lmax:A	0.016	0.017	0.052	0.018	0.018
PCInertia (%)	56.1	34.9	4.6	95.6	100

Table 1: Sensitivity Indices for the top ten WWDM factorial terms.

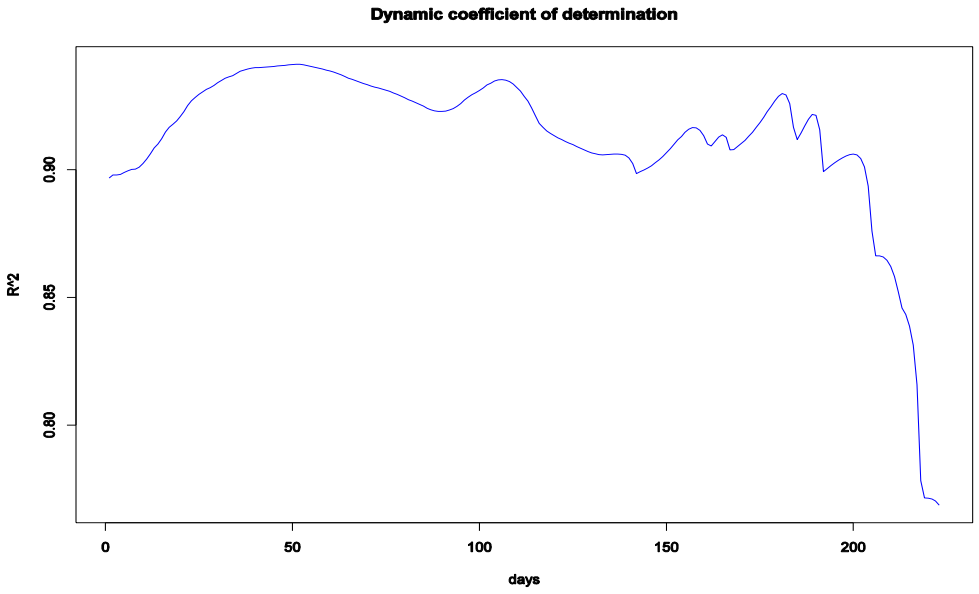

Figure 1: Dynamic coefficient of determination for WWDM model

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ENTROPY-BASED SENSITIVITY ANALYSIS IN HEALTH RISK ASSESSMENT

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For realistic decision-making in risk management, the reliability and quality of exposure and risk model outputs, which depend on uncertainty, must be known. Therefore, sensitivity analysis is a central point to study the problem of *how the output Y is sensitive to the uncertainty of the input variables* $X_1, X_2, \ldots, X_p$. Usually, output uncertainty is described in terms of variance. Variance is popular in sensitivity analysis because of its simplicity and its historical development; statisticians also use it as a reference measure of the dispersion.

Other measures may be used to characterize the uncertainty of a model output related to an input variable. Krykacz-Haussmann [1] has criticized the use of variance as a measure of output uncertainty and proposed to use the entropy. Entropy is an information criterion which measures the amount of uncertainty or information content that is implied by a probability distribution. It has the advantage of depending on many more parameters than just the second moment which allows only to measure a dispersion around the mean. Moreover, the conditional variance $V(Y|X_i = x_i),\ i = 1,\ldots,p$ can be larger than $V(Y)$ while the entropy $H(Y)$ verifies $H(Y|X_i = x_i) < H(Y)$. Shannon's entropy of a random vector $\boldsymbol{X} = (X_1,\ldots,X_p)$ of IR^p with probability density function $f(\boldsymbol{x})$, is defined as:

$$H(\boldsymbol{X}) = -\int_{IR^p} f(\boldsymbol{x})\log[f(\boldsymbol{x})]d\boldsymbol{x}.$$

Note that the entropy of continuous random variables is not invariant under a continuous invertible transformation of variables.

To anticipate the impact of input vector variations to the output in terms of entropy, the following result [2] is very useful when the dimensions of the two vectors are the same: Let $\boldsymbol{X} = (X_1,\ldots,X_p)$ and $\boldsymbol{Y} = (Y_1,\ldots,Y_p)$ be two random vectors of p variables, and $t(.)$ a continuously differentiable transformation such that $\boldsymbol{Y} = t(\boldsymbol{X})$, then:

$$H(\boldsymbol{Y}) = H(\boldsymbol{X}) - \int_{IR^n} f(\boldsymbol{x})\log[J(t(\boldsymbol{x}))]d\boldsymbol{x},$$

where $f(\boldsymbol{x})$ is the probability density of $\boldsymbol{X}$ and $J(\boldsymbol{y})$ is the Jacobian of the inverse transformation $t^{-1}(.)$. Unfortunately, such a result is not yet available for vectors of different dimensions: $\dim(\boldsymbol{X}) \neq \dim(\boldsymbol{Y})$. Furthermore, unlike in the univariate case, many entropy expressions aren't calculable in multivariate situation.

Comparatively to the variance for which the expression $V(\boldsymbol{Y}) - E_{\boldsymbol{X}}(V(\boldsymbol{Y}|\boldsymbol{X}))$ is used, the "mutual information" $I(\boldsymbol{X},\boldsymbol{Y})$ between two random vectors $\boldsymbol{X}$ and $\boldsymbol{Y}$, is an invariant (under one-to-one transformations), symmetric and natural measure of the dependence between $\boldsymbol{X}$ and $\boldsymbol{Y}$, and corresponds to:

$$I(\boldsymbol{X},\boldsymbol{Y}) = H(\boldsymbol{X}) + H(\boldsymbol{Y}) - H(\boldsymbol{X},\boldsymbol{Y}) = H(\boldsymbol{Y}) - H(\boldsymbol{Y}|\boldsymbol{X}).$$

Sensitivity indices based on mutual information seems to be as much attractive as variance-based sensitivity analysis one, to obtain "importance measure" on input variables.

There is no universal relationship between entropy and variance "orderings of distribution". Mukherjee and Ratnaparkhi [3] presented some relationships between the two for some particular univariate distributions. Writing the entropy in terms of variance, Ebrahimi and al. [4] find the orderings across some families of univariate distributions. Also, "$\text{var}(X) < \infty$" implies that "$H(X) < \infty$" but the converse may not hold. That means entropy measures could exist even if variance ones are infinite or not defined. For example, the variance of the Cauchy distribution, or the T-Student distribution one for some parameters, does not exist, while their entropy always does. The entropy $H(\boldsymbol{X})$ is a dimensionless scalar measure of a distribution; consequently in the multivariate case, entropy rankings can be easily obtained. On the contrary, the variance $V(\boldsymbol{X})$ approach leads to a matrix of order $\dim(\boldsymbol{X})$ and variance rankings are based on arbitrary measures, such as the determinant or the trace of the variance-covariance matrix. We show that entropy depends on much more information about a vector of random variables than its variance.
A copula $c(\boldsymbol{x}) = c(x_1,\ldots,x_p)$ is a multivariate probability density function defined on the unit cube $[0,1]^p$ (each

marginal law is a uniform $U[0,1]$ dependent to each other). The copula approach has the advantage of characterizing, splitting and modelling the whole dependence structure between the p random variables $X_1,\ldots,X_p$, whatever the marginal distributions.

In the bivariate case, we have examined entropy (and mutual information) and variance orderings of parametric copulas families $c(x,y)$ with respect to some functions of margins, such as sum and product. We present and discuss some analytical formulas and graphical relationships between variance and entropy of several bivariate copulas, such as Farlie-Gumbel-Morgenstern, Gamma-Exponential or Dirichlet. We also compare joint, conditional and marginal entropies and variances using the following property:

$$H(\boldsymbol{X},\boldsymbol{Y}) = H(\boldsymbol{X}) + E_{\boldsymbol{X}}\left(H(\boldsymbol{Y}|\boldsymbol{X})\right) = H(\boldsymbol{Y}) + E_{\boldsymbol{Y}}\left(H(\boldsymbol{X}|\boldsymbol{Y})\right).$$

As a practical application, the U.S. Environmental Protection Agency's Integrated Exposure Uptake Bio Kinetic (IEUBK) model for lead in children allows to estimate children's blood lead levels by integrating exposure from lead in air, food, water, soil, dust and other sources with pharmacokinetic modelling. Unfortunately, the model doesn't assume any probability distribution for the input variables. Thus, we have coded the model to carry out Monte Carlo simulations on input variables corresponding to children's disparity in order to obtain the blood lead concentration's distribution which conveys the output variability. Empirical simulation results and entropy-based sensitivity analysis appear to be helpful in focalising on the major aspects of the IEUBK model to take into account the input distributions. Our results are compared to variance-based sensitivity analysis in terms of "expected reduction" of the uncertainty.

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STRUCTURAL UNCERTAINTY IN A QUASI-2D HYDRODYNAMIC MODEL FOR THE TRANSPORT OF CONTAMINATED SEDIMENTS IN INUNDATED AREAS DURING RIVER FLOODING

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There are many sources of uncertainty in modelling systems including uncertainty due to parameter estimations, input data and structure of the system. In this paper, modelling system structure is understood to be the algorithms and equations used to describe and calculate processes. This talk places emphasis on structural uncertainty in models and modelling systems since this topic has received very little attention in research compared to the wealth of literature on parameter and input data uncertainty. This imbalance is partly due to the difficulty in quantifying structural uncertainty and an example is given in this talk on how the structural uncertainty can be calculated. Here, a hydrodynamic model is used to simulate the flooding of a river and an adjacent-lying inundated surface area, such as a polder or the hinterland behind a dyke breach, using two different discretisations schemes: i) the flooded area is considered as a single tank which is filled and emptied during the flood, or ii) the area is discretised using a finer two-dimensional representation. Monte Carlo simulations are run with varying parameter and input data sets on both models and the variation in the output results are compared for both. The difference between the probability distributions in the state variables between the two models can be attributed to the uncertainty in the structure of the model representation of the inundated area.

Another objective of this paper is to describe the development of the quasi-2D model used to simulate floods. In flood modelling, many one-dimensional (1D) hydrodynamic and water-quality models are too restricted in capturing the spatial differentiation of processes within the inundated areas and two-dimensional (2D) models are too demanding in data requirements and computational resources. The latter is an important consideration when uncertainty analyses using the Monte Carlo techniques are to complement the modelling exercises. Hence, a quasi-2D modelling approach is pursued which still calculates the dynamic wave in 1D but the discretisation of the computational units is in 2D, allowing a better spatial representation of the flow and substance transport processes in the inundated areas without a large additional expenditure on data pre-processing and simulation processing. The models DYNHYD (1D hydrodynamics) and TOXI (sediment and micro-pollutant transport) from the WASP5 modelling package (Water quality Analysis Simulation Program), developed by the US Environmental Protection Agency, was used as a basis for the simulations. The models were extended to incorporate the quasi-2D approach and were coupled in the HLA (High Level Architecture) platform to enable interactions between the models during simulations. This platform allowed ease of implementing Monte Carlo simulation runs, which were used for the uncertainty analyses. A flood event on the middle reach of the Elbe River in Germany was simulated as a test case. The results show a more realistic differentiation of suspended sediment and zinc concentrations between the inundated areas and the main channel. The results also show that for flood simulations, uncertainties in boundary conditions are higher and should be given more attention than uncertainties in model parameters.

MATHEMATICAL MODELLING OF MESENCHYMAL STEM CELL PROLIFERATION AND DIFFERENTIATION

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The bone marrow contains a subpopulation of cells called Mesnechymal Stem Cells (MSCs) which are able to renew themselves repeatedly and have the ability to differentiate into multiple cell lineages. For example, MSCs can give rise to osteoblasts, chondrocytes, adipocytes and hematopoietic-supporing stroma. Given their multipotency and the ease with which they may be cultured, MSCs have high therapeutic potential.
As a consequence of the ageing population the demand for replacement tissues is increasing. MSCs are present in adult organisms and they may act as a source of such tissues. However before MSCs can be used in clinical therapies for tissue regeneration, experimentalists must be able to produce specific cell types. While tissue engineering is a large and rapidly expanding area of experimental research, many questions still remain. For example, optimal environmental conditions for culturing MSCs to maximise the yield of osteoblasts have yet to be identified. This is partly due to the fact that it is difficult to measure reliably system parameters and that there is no universal label for MSCs. Several laboratories have developed different methods for isolating MSCs but it is difficult to compare their results.
By building simple mathematical models (deterministic and stochastic) of stem cell proliferation and differentiation we aim to provide insight into the mechanisms that control these processes [1]. In particular, by performing sensitivity analyses we can identify model parameters whose variation has a significant effect on the system dynamics. Such results can be used to guide experimentalists by suggesting which parameters should be manipulated in order to increase the yield of the desired cell type.

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ANALYZING THE EFFECT OF INTRODUCING A KURTOSIS PARAMETER IN GAUSSIAN BAYESIAN NETWORKS

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Gaussian Bayesian Networks are graphical models that represent the dependence structure of a multivariate normal random variable with a DAG (directed acyclic graph); see, for example, Cowell et al. [2], Shachter and Kenley [4]. This qualitative aspect of the model has to be put with a quantitative part made up by the conditional distributions of each node given its parents in the graph, which are the preceding nodes. These conditional distributions are also normal distributions and the calculations are easily implemented.
On the other hand the multivariate exponential power distribution (Gómez et al. [3]) is a family depending on a kurtosis parameter that goes from leptokurtic to platykurtic distributions with the normal as a mesokurtic distribution. This distribution is a generalization of the univariate distribution that was considered in Box & Tiao [1] for robustness studies in Bayesian inference and used later with this purpose in many situations. The conditional distributions are elliptical and can be also easily handled for calculations.
The problem of uncertainty about assumption of normality is very common in applications. Thus a sensitivity analysis of the non-normality effect in our conclusions is necessary. The kurtosis parameter of the multivariate exponential power distributions becomes the main tool to deal with deviations from the normal distribution.
The output in Gaussian Bayesian Networks is usually the conditional distribution of the unknown variables of interest given some evidence, that is some known values for the rest of variables. Therefore a more general model can be considered using the multivariate exponential power distribution to describe the joint distribution of the Bayesian Network, with a kurtosis parameter reflecting deviations from the normal distribution. The sensitivity of the output to this perturbation is analyzed using the Kullback-Leibler divergence measure, studying the effect of slight non-normality in different ways. Some applications are also given.

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DETERMINISTIC SENSITIVITY ANALYSIS FOR A MODEL FOR FLOW AND TRANSPORT IN POROUS MEDIA

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This work is devoted to the deterministic sensitivity analysis of a mathematical model for the simulation of flow and transport in porous media. The method used is based on the singular value decomposition of the Jacobian matrix of the mathematical model of the problem. Since the method uses a first order approximation, it provides local results around particular input and output parameters. For this reason we also study the variability of the results of the computation of sensitivities due to the variations of the input parameters of the model. Numerical results are compared with those obtained through a statistical analysis.

The questions of safety and uncertainties are central to feasibility studies for an underground nuclear waste storage site. One of the important points to be considered is the problem of the evaluation of uncertainties concerning safety indicators ("output parameters") which are due to uncertainties concerning properties of the subsoil, such as hydraulic conductivity, or of the contaminants ("input parameters"). Uncertainties about the input parameters are due to imprecisions of measurement techniques or to spatial variability. Safety indicators may be for instance the measure of the water flow through outlet channels or concentration measures.

Two different aspects of the quantification of the influence of the parameters on the safety indicators are uncertainty analysis, which corresponds to the quantification of the uncertainty concerning the indicators (for example in the form of distributions or quantiles) and sensitivity analysis, which corresponds to the identification of the weight of the input parameters with respect to their influence on the indicators. For sensitivity analysis, probabilistic approaches, such as Monte-Carlo methods, can be used. These methods give good results and are relatively easy to implement, but they are expensive because they require a large number of simulations (see for example [1,2]). The deterministic method investigated here is much less demanding in computing time but it gives only local information: for nonlinear problems, the results obtained will be correct only for small variations of the input parameters (relatively to the nonlinearity) around a particular set of input parameters.

For deterministic methods, "first order" uncertainties are computed from the derivatives of the function $\boldsymbol{F}$ relating the output parameters to the input parameters. Different methods can be used for differentiation: divided differences, automatic differentiation, analytic differentiation for possibly implicit problems. For each method, direct mode or reverse mode (reverse mode is equivalent to the adjoint state method), can be used. These derivatives can be used combined with interval arithmetic to evaluate uncertainties in the form of intervals containing the image under $\boldsymbol{F}$ of input intervals, see [3].

The derivatives of $\boldsymbol{F}$ are stored in the Jacobian matrix $\boldsymbol{J}$. The hierarchization of the influences of the inputs of the function upon their influence on the outputs of the function is provided by the singular value decomposition (SVD) of $\boldsymbol{J}$. The Singular Value Decomposition can also be used in probabilistic sensitivity analysis ([4]).

Thus the probabilistic and deterministic approaches are complementary and both deserve to be developed. In our study, we apply both approaches to the same problem.

We will present our discretized model for flow and transport in porous media. The flow equation is based on the stationary Darcy law and is discretized with a mixed hybrid finite element method. The transport equation consists of a mass balance equation for each contaminant and a law of exchange between liquid and solid phases for each contaminant.

We will give some details about the computation of the derivatives used for the deterministic analysis. For the flow equation we use a C++ code which has been differentiated with analytical formulas, using the adjoint state method. For the transport equation we combine manual differentiation and automatic differentiation. For automatic differentiation we use the library AdolC ([5]). The singular value decomposition of the Jacobian matrices, computed with LAPACK, provide a (weighted) hierarchical list of directions in both the space of input parameters and in the space of safety indicators. Then a truncated computation of the uncertainties on the outputs is possible.

For the flow model, various deterministic studies have been computed for a 3 dimensional test case. We observe a weak variability of the local sensitivities when the choice of the input parameters varies in the spectrum of possible input parameters. This is due to the weak nonlinearity of the model, assured by the choice of a logarithmic parameterization. In this case, probabilistic and deterministic studies provide similar results. We

also confront numerical results obtained using a deterministic analysis with those obtained using a probabilistic analysis for the full model.

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APPLICATION OF SENSITIVITY ANALYSIS IN OPTIMIZATION OF BEAD GEOMETRY OF PTA HARDFACED VALVE SEAT RINGS

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Hardfacing is the deposition of a filler metal on the surface of a base metal. Its purpose is to provide the properties or dimensions necessary to meet a given service requirements. The basic requirements are higher wear resistance, resistance to corrosion and resistance to deformation at elevated temperatures. Hardfacing is applied to the contact surfaces of the valve seats and movable guiding elements of valves in order to ensure and maintain for a long period of time "tightness of the body / disc – seating areas of valves" with the functions of closing, opening, throttling and controlling. Hardfacing by means of cobalt base alloys to obtain wear-resistant surfaces has been used in the valve industry since the twenties [1, 2].

Among the various welding processes that are used for the hardfacing of valve seats, plasma transferred arc hardfacing (PTA) is popularly employed because of its inherent advantages like high deposition rate, low penetration and dilution, and smooth weld surface profile with minimum finishing [3]. The selection of appropriate values of process parameters to get the desired quality of hardfaced layer is very important. The successful hardfacing requires optimization of the process parameters to have low dilution and a crack free overlay, which necessiates a thorough understanding of the process characteristics affecting the technological and metallurgical characteristics of the overlays. With a view to solve the above difficulties faced in PTA hardfacing of valve seat rings, an attempt was made to study in detail the various aspects such as mathematical modeling, optimization, and sensitivity analysis.

The independently controllable process parameters affecting the bead geometry and quality were identified to enable the carrying out of the experimental work and developing the mathematical models, these being: Welding current (A); Travel speed (S); Powder feed rate (F); Oscillation frequency (H); and Torch stand off (N). An automatic PTA surfacing system designed and fabricated by M/s Primo Automation System was employed to conduct experiments at M/s KSB Pumps Limited, Coimbatore. Hardfacing was carried out by depositing stellite -6 (Co-Cr.-A) onto carbon steel (ASTM-A105) ring of inner dia 93 mm, outer dia 120 mm and thickness 20.5 mm. The experiments were conducted by depositing a single layer with electrode negative (DCEN). Industrially pure Argon at a constant flow rate of 15 lpm for shielding, 5 lpm for Plasma, and 3 lpm for powder feeding were used. The selected design matrix was a central composite rotatable factorial design [4] consisting of 32 sets of coded conditions. Transverse cut specimens were obtained from the hardfaced valve seat rings and the bead profiles were traced as per the standard metallurgical procedures. Regression analysis was used to develop second order quadratic mathematical models to relate the process variables with the important bead parameters, namely, penetration (P), reinforcement (R), percentage dilution (%D), bead width (W), and total area (TA).

The adequacy of those models was tested using F-test and R-test [5]. Validation of those models was further tested by drawing scatter diagrams, calculating R^2 values and conducting conformity test runs and the average accuracy of the models was found to be about 95%. The direct and interaction effects of the process variables on each of the above response were studied and represented as two-dimensional plots.

The main purpose of this study is to minimize the percentage of dilution of the bead geometry using other important bead parameters with their limits as constraints, in order to retain the metallurgical properties of deposited metal. The model is a nonlinear equation with constraints. The step-by-step procedure for minimization of dilution using the optimization module available in the toolbox of the *MATLAB* version 7.1 software packages was used. The objective function selected for optimization was the percentage of dilution. The bead parameters like penetration, reinforcement, width and total bead area were given as constraints of the equation. The optimum value of the percentage dilution was observed to be 2.05 with corresponding process variables of Welding current = 131 Amps; Travel speed = 124 mm/min; Powder feed rate = 24 grams/min; Oscillation frequency = 53 cycles/min; and Torch standoff = 6.5mm.

The following are the basic parametric changes affecting the optimum solution [6].

1. Changes in the levels of process parameters
2. Changes in the values of the constraints
3. The effect of including additional constraints
4. The effect of including additional variables

A thorough discussion of all the above changes is more tedious. Out of the four changes, the most common change that takes place in many problems are the change in the values of the constraints [7]. i e. the change in the value of the upper or lower limits of constraints. It is important to know what happens to the optimum value of the objective function when the constraint limits are changed. LaGrange multipliers provide

information of sensitivity analysis and for the study on the benefit of relaxing a constraint or the penalty associated with the objective function.

Sensitivity analysis was carried out to predict the direct effects of important bead parameters on percentage dilution and the results are presented in graphical form. The results of the sensitivity analysis are much useful in understanding the interdependence of various weld bead quality parameters in controlling the percentage dilution to enhance the metallurgical properties and hardfacing quality. The sensitivity analysis of percentage dilution due to the change in the limits of constraints were recorded and analyzed.

Acknowledgment:

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CONSTRUCT: A FRAMEWORK FOR CONCEPTUALLY STRUCTURING A MODEL

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A model represents the developer's understanding of a system under research. It encapsulates the builder's knowledge, assumptions and hypotheses that can be tested against a data set of observable phenomena that is collected with similar objectives. In order to reuse or select a model, one must understand its original intentions and assumptions as well as understanding its behaviour. Within the domain of crop modelling, models with different detail consists of many processes that can be modelled differently. In order to understand and compare the different implementations of processes within a crop model, we designed a framework called CONSTRUCT, CONceptually STRUCTuring a model.

The idea behind CONSTRUCT is that a model is built upon concepts: explicitly defined system elements that reflect the understanding of a particular part of the system. The definition of a concept consists of two parts: the semantic meaning of a concept and its interrelations with other concepts. The interrelation of a concept with other concepts is explicitly defined as it holds the assumption and understanding of this particular element within the overall system. A concept can have multiple interrelations, each defining one assumption. Suppose one would like to model the development of biomass among the different plant organs over time. When the framework holds three different algorithms for calculating biomass accumulation and two for partitioning, the framework will yield six models that could model the proposed objective. This outcome can be reduced by refining the objective so that algorithms are rejected based upon the definition of the concepts used.

Models can also be rejected based upon their performance. When a model structure provides an acceptable representation of the researchers understanding of the system, the analysis of model input against a representative data set is the next step in model selection. In order to understand the influence of input variability we propose to use evolutionary algorithms like SCEM-UA to examine the entire range of acceptable inputs for a given set of concepts. The observed phenomena are given a set of statistically independent errors with a zero expectation and a constant variance. The result of this analysis will not yield a single parameter set, but a set of solutions corresponding to a given objective. In general, the objective is to minimise the error between modelled and observed signals. A closer analysis on the outcome of this analysis and the behaviour of the different concepts could also lead to a redefinition of the concept itself, which would then lead to new model structures.

CONSTRUCT provides a tool to analyse and model systems based upon the researchers intentions, hypothesis and system understanding. The framework uses a clear separation between the conceptual and computational aspects of model development in order to reveal the complexity of a system and allow the researcher to assess the appropriateness of a particular model structure by means of its performance, the assumptions made within a model and input variance in relation to the observed phenomena.

SENSITIVITIES FOR FREE: CMA-ES BASED SENSITIVITY ANALYSIS

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We present a novel method for parameter sensitivity identification based on the Covariance Matrix Adaptation Evolution Strategy (CMA-ES) optimization procedure [1]. Our method directly uses the information that is acquired during an optimization process to provide local and global parameter sensitivity estimates with no additional evaluations of the cost function. To demonstrate the performance of the method, we consider a complex example from cell biology, namely a TCR-activated signal transduction network. For this network, different global sensitivity indices are known [2].
The CMA-ES is a powerful evolutionary algorithm for non-linear, non-convex optimization problems. It has successfully been applied in a variety of domains ranging from lens design in optics [3] over computation of Nash equilibria in economics [4] to design of cancer chemotherapies [5]. Moreover, the CMA-ES has demonstrated unique performance in robust parameter estimation for biochemical network models [6].
The CMA-ES comprises a local sampling with a multivariate normal distribution to form the new generation of sampling points. The covariance matrix of the sample distribution is hereby continuously adapted in order to bias the search toward the most likely direction of the global optimum [7]. For each generation, this allows us to estimate a local sensitivity measure, centered around the mean position of the particles at that generation. Our estimator uses the classical coefficient of determination, corresponding to a good measure for a local linearization of the objective function. In order to reconstruct a rank-based measure for first order sensitivity indices we compute a weighted average of the local sensitivities along the CMA search path. The weights are determined by an importance sampling of the local indices. In each generation of the optimizer, the common weight of the sampling points is given by the determinant of the current CMA covariance matrix.

The proposed novel sensitivity measure hence reads:

$$\mathcal{S}_j = \sum_{g=1}^{n_g} det(\mathcal{C}_g) corr(F(x_1^g, \ldots, x_p^g), x_j^g)^2$$

with :

g	Index of the generation
n_g	Number of generation during the search
$\mathcal{C}_g$	Covariance matrix of the gth generation
p	Dimensioniality of the parameter space
$\mathcal{S}_j$	First order rank-based sensitivity index for paramter j
$\{x_1^g, \ldots, x_p^g\}$	Sampling points of generation g
$F(.)$	Objective function

As a benchmark problem, we study a TCR-activated Erk-MAPK signal transduction pathway in biological cells. The pathway model consists of a set of 24 ordinary differential equations with 49 free parameters. After estimating the model parameters with a genetic algorithm, Zhang and Rundell [2] derived parameter sensitivities using a variety of methods, including Sobol's method and Extended FAST [8], using 200 000 sample points. In order to test our parameter sensitivity scheme we evaluate a total of 80 000 sample points. This is done in 20 independent CMA-ES runs. Each run starts at different random points in parameter space, running over 4 000 samples each. All runs are conducted with standard strategy parameter settings as suggested in [7]. The global parameter sensitivity indices of each run are normalized and summed up to give the overall global parameter sensitivity indices as shown in Fig. 1. Given the reduced sample size our results are in good agreement (correlation coefficient 0.8) with the Extended FAST total effect indices (Fig. 2), which are considered the benchmark sensitivity measure. In addition, our CMA-ES optimization has found a new set of model parameters that significantly improve the model quality.

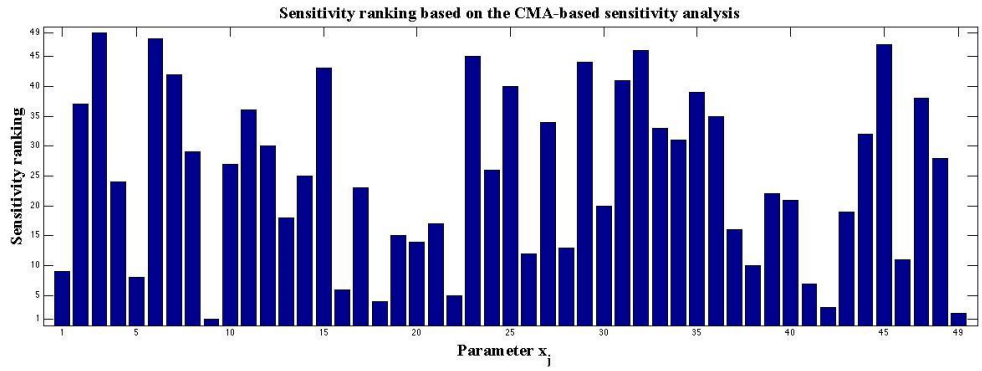

Figure 1: Parameter sensitivity ranks derived from the CMA-based sensitivity analysis given a total of 80 000 sample points

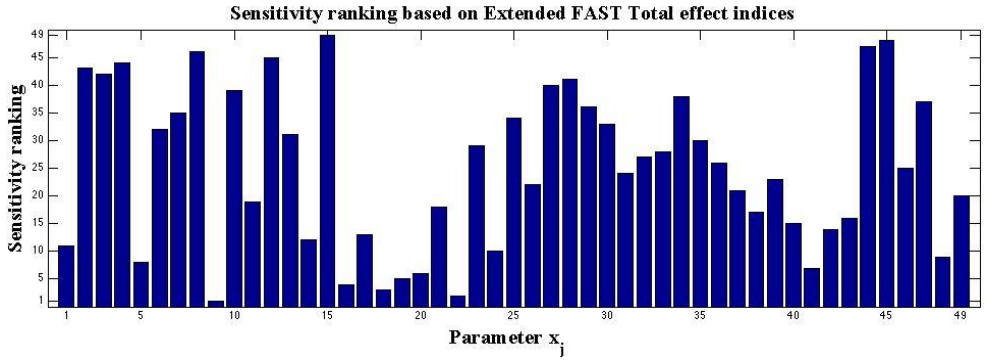

Figure 2: Parameter sensitivity ranks derived from Extended FAST total effect indices given a total of 200 000 sample poins. The indices have been taken from [2].

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STAKEHOLDER PREFERENCE WITH PROBABILISTIC INVERSION: APPLICATION TO COMPETITIVENESS INDICES

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An index over countries is a numerical scale used to compare countries with one another or with some reference number based on one or more specified aspects. Often an index is used in the decision making of policymakers, because it provides policymakers with information about the monitoring of countries progresses in a given policy field. There are several institutions (UNDP, WEF, World Bank, etc.) that elicit indices. When policymakers use an index in their decision making it is important that the index is independent from the institution eliciting it. The index must be a single unambiguous number which captures the facts of the specified aspects and or the different opinions of stakeholders about the specified aspects.

The methods usually applied for eliciting an index often make use of surveys and statistical data. In the surveys respondents are asked to judge the countries based on a specified aspect. The judgment is based on a scale defined by the institutions. The judgments over the specified aspects together with the statistical data are first normalized to uniform scale and then aggregated using an arbitrary set of weights to create an index. This method reflects the preference of the institution rather then the preferences of the stakeholders, even though the preferences of stakeholders may be captured by the use of surveys. The institutions eliciting an index directly impose their preferences of the several aspects of an country by the use of normalization and the selection of a set of arbitrary weights, because they decide what is important and what is not.

The statistical data used may also be irrelevant in the elicitation of an index. Statistical data become irrelevant if either the data do not reflect any of the specified aspects or if the data only reflect the specified aspects for a subset of countries.

These considerations motivated a search for alternative methods for developing indices over countries. In this research the Global Competitiveness Index elicited by the World Economic Forum (WEF) is considered as a test case. Every year the WEF elicits a Global Competitiveness Index (GCI).This index is meant to measure the amount of competitiveness of each country and to shed some light on why some countries grow and others do not in terms of macroeconomics, institution, and technology. Competitiveness is defined as the set of institutions, policies, and factors that determine the level of productivity of a country.

The main objective of this research was to get an index for a set of countries based on preferences of respondents on these countries given the aspect competitiveness. The first phase is to ask respondents to provide us with their preferences on the objects. Initially these respondents will not be actual stakeholders, but are used to test the method of this research. To elicit the preferences of the respondents the Law of Comparative Judgment is used.

In the second phase of this research, the index obtained via the Law of Comparative Judgment is compared with the index from the World Economic Forum to determine if there is any correlation between the two indices. Finally regression is used to select statistical data that are relevant to the aspect competitiveness of the set of countries. The coefficients obtained from the regression analysis can be seen as the weights selected by the World Economic Forum. Finally, new techniques of probabilistic inversion will be used to quantify regression coefficients directly, without recourse to the Law of comparative Judgment.

MONTE CARLO ANALYSIS OF A GENERIC CELL CYCLE MODEL

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The cell cycle is the sequence of events by which a growing cell replicates all of its components and divides them into two sister cells. The eukaryotic cell division cycle is driven by an underlying molecular network, which is centred around complexes of cyclin-dependent kinases (Cdk) and cyclins. In phase G1, the cell is growing in its cytoplasmic mass, which causes a slow but steady accumulation of Cdk/Cyclin activities. The DNA is duplicated in phase S, which is followed by the next growing phase G2. In the subsequent M phase (mitosis), the chromosomes are separated and the cell division takes place.

Csikász-Nagy *et al.* [1] have created a generic cell cycle model that is able to simulate several types of living cells in such a way that for each cell type the differential-algebraic system of equations are identical, but the values of the parameters are different. This common system of differential-algebraic equations contains 14 variables and 86 parameters. In our studies, parameter sets related to budding yeast, fission yeast and mammal cells were investigated. Since measured concentration–time curves are not available for these cells, a parameter set was considered successful, if the corresponding model simulates a proliferating cell. Otherwise, the modelled cell was considered dead. The requirement for a living cell was to produce 4 cell divisions in 1000 minutes and at least one division in the last 280 minutes.

First, the parameters were changed one-at-a-time, while all the other parameters were kept constant at their nominal values. Increasing or decreasing a parameter by four orders of magnitude, the limits were explored where the cell is still alive. Some parameters could be changed by ±4 orders of magnitude; these parameters are non-influential or control the time-profiles of concentrations that are not critical for the cell cycle. Other parameters could be decreased, but increasing them kills the cell, while opposite behaviour was found for another group parameters. Since increasing a parameter may have positive or negative effect on the flux of a pathway, these are typical patterns of parameter influence when the role of a decreased flux pathway can be taken over by another parallel path, but increasing the flux of this pathway causes damage. For the fourth group of parameters, their values could be changed in a narrow window only, indicating their critical role. The results of the classification according to the four groups above were similar for most parameters for each cell type. However, there were 13 parameters with different classification for different types of cells.

To investigate parameter interaction, Monte Carlo analyses of the three cell type models were carried out. For each model, ten thousand parameter sets were generated using Latin hypercube sampling assuming log-uniform distribution, within the limits assigned by the single parameter changes. In the cases of fission yeast, mammal and budding yeast cells only 53, 44, and 69 parameter sets, respectively, were found that produced living cells out of the 10000. In order to explore if increasing a parameter value can be compensated by a systematic change of another parameter to keep the cell alive, correlation of these parameter values was investigated. The ten-based logarithms of the multiplication factors of the nominal parameter values were arranged to a matrix in such a way, that each row corresponded to a living cell and each column to a parameter. Then, the correlations of the column vectors were calculated. The Figure shows a typical example for such correlations for fission yeast cells. The correlation coefficient for parameters *kd20* and *ki20* is –0.48. Both parameters control the concentration of enzyme **Cdc20**. If the values of these parameters are simultaneously low, it causes an early rise of the concentration of **Cdc20**, therefore the cell cycle gets stuck in phase G1. For the definition of parameter names please refer to reference [1].

Correlations with absolute values higher than 0.4 were investigated in details. For the fission yeast model, high correlation was found also for parameters *Jah1* and *kah1p* (correlation coefficient –0.44), both are controlling the concentration of **Cdh1**. Other highly correlated parameters are *Jawee* and *kdapp* (–0.43, both are controlling the length of phase M); parameters *Jatf* and *ksapp* (+0.42, both are controlling the concentration of **active cyclin A**); parameters *ka25* and *ksbp* (–0.42, both are controlling the concentration of **active MPF**); parameters *ksbpp* and *SK* (–0.46, controlling the length of phases G1 and G2).

In the case of the mammal cell model, high correlation was found for parameters *ksepp* and *katfppp* (+0,51), which are indirectly and directly, respectively, control the production of transcription factor **TFE**; parameters *kdepp* and *katfppp* (–0.43), which control the production of **cyclin E**; parameters *J20* and *kitfpp* (+0.43), which both indirectly control the level of **cyclin A**; parameters *kah1pp* and *SK* (–0.53), which affect the activity of **Cdh1**. Increasing the values of both parameters *kdipp* and *SK* (–0.47) increase the decay of **CKI**. If the values of both parameters are low, the high **CKI** concentration results in a halt in phase G1. No high correlation was found between the parameters of the budding yeast model.

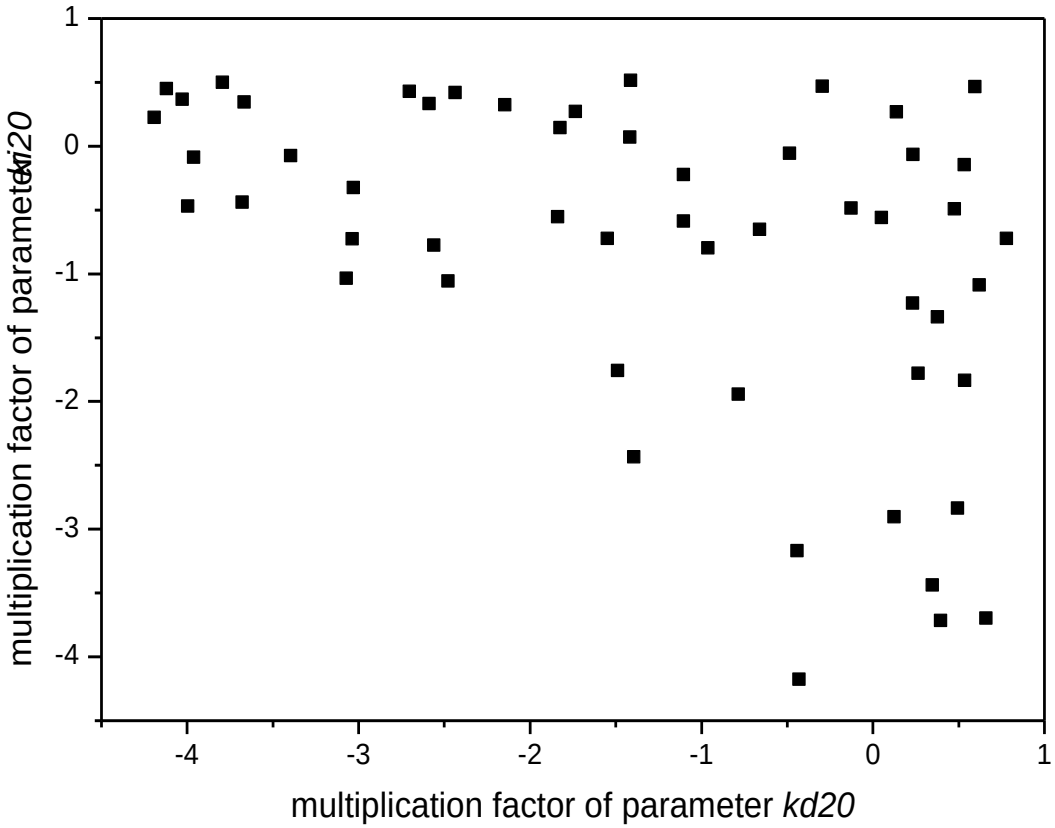

Figure: Values of parameters *kd20* and *ki20* that simulate proliferating fission yeast cells when all other parameters are also changed simultaneously. The axes are the logarithms of the multiplication factors of the original parameter values.

Conclusion: The division cycles of budding yeast, fission yeast, and mammal cells are frequently investigated experimentally and are subjects of vigorous modelling activity. Recently a unified model was published [1] that can simulate the cycles of the above three types of cells using the same system of algebraic-differential equations and different parameter sets. This generic cell cycle model was investigated by systematic changes of parameters. The aim was to find altered parameter sets that also describe living and proliferating cells. Monte Carlo analysis with Latin hypercube sampling was used, and the correlating parameters were identified. For these parameters, either some combinations are not valid or the effect of increasing of one parameter can be compensated by increasing or decreasing another parameter. The identified positive and negative parameter correlations were elucidated knowing the details of the regulating cycles. An unexpected result of this study is that in spite of the common structure of the three models, very different correlations were found for the three types of cells.

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EFFECTS OF INPUT CORRELATIONS IN A COMPLEX CHEMISTRY MODEL

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In a chemistry model, the output concentrations of chemical species are inter-correlated by various constraints: the structure of the chemical network, the conservations laws (mass, energy...). Additional correlations result from uncertain input parameters. For instance, the branching ratios describing the partition of products in multipathway reactions have to obbey a sum rule.

Taking into account correlations of input parameters is known to be essential to quantitative uncertainty propagation and sensitivity analysis. The sum rules for more than two parameters has been recently noted as an issue for complex chemical systems [1].

In this work, we present two aspects of uncertainties correlations in complex chemical systems:

7. the effect of a proper description of the correlations between branching ratios [2,3]. We propose the use of a Dirichlet distribution, and we show that neglecting the sum rule can lead to under- or over-estimation of the output uncertainties, depending on the predicted property (Fig. 1). Globally, the uncertainty budget is quite sensitive to this description.
8. the effect of the correlation between the concentrations of reactants issued from a previous chemistry model [4]. In our system, we observed no effect of this source of input correlation on output uncertainties, but only a correlation transfer from inputs to outputs.

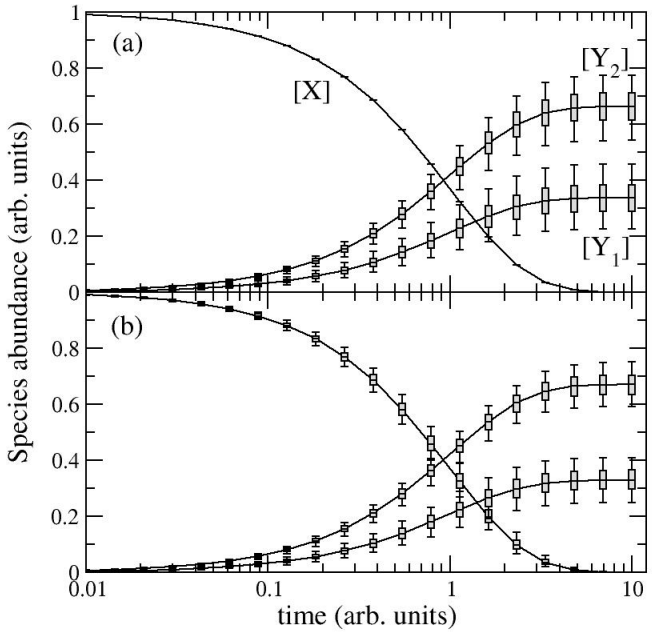

*Figure 5: Time-resolved concentrations for two parallel unimolecular reactions X ✹Y_1 (b_1*k) and X ✹Y_2 (b_2*k), where k is the global rate constant and b_1, b_2 are the branching ratios. (a) exact representation of the branching ratios correlation by a Dirichlet distribution; (b) uncorrelated branching ratios. Whereas the neglect of the correlation leads to an overestimation of the uncertainty about [X], an underestimation is observed for the final products.*

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THE USE OF GLOBAL SENSITIVITY ANALYSIS METHOD IN WELDING SIMULATION

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Control of mechanical effects of welding is one of the main stakes of industrial company and especially in the nuclear field. The robust increase in computer power allows nowadays simulating a complex welded assembly on a personal computer, in order to predict, from the conception stage, if mechanical requirements are reached. For the scientist community, simulation of coupled multiphysic phenomena and model unification are the most challenging to understand. The industrial requirements are more and more numerous: supports to develop new processes, control of mechanical welding effects (in particular, residual stresses and distortions), argument in a nuclear safety analysis reports, etc. Thus, through the use of high-performance computers and advanced models, numerical simulation is expected to become an important tool for innovation in welding engineering.

However, running a welding simulation requires a large number of inputs - about 500 - including for example meshing inputs, boundary and initial conditions as well as material properties and process parameters, and generates several outputs, including spatial distributions of displacements and residual stresses in the weldment. Among inputs those controlling the material properties are one of the key problems of welding simulation. The features of material properties are that they are dependent on temperature and that their full characterization is very expensive, often difficult or even sometime impossible. For instance, it can take several weeks to characterize a specific material without anyway knowing if these data are influent and in which range of temperature. Furthermore, it is quite difficult to use material data published in technical literature, which have almost never been characterized over a sufficiently wide temperature range. To circumvent this problem, most welding modellers content themselves with available material data and use extrapolated values at high temperature. In this context, we think that one of the main stakes is to determine which material properties are the most sensitive in a numerical welding simulation and in which range of temperature.

To bring answers to these questions, one classically performs a local sensitivity analysis on a limited number of materials. This type of study consists in measuring the effect of small variations of input data controlling material properties on the output of the computer code. But validity of the results is limited to the neighbourhood of the studied material(s) and cannot be generalized to others. A more ambitious approach is to perform a global sensitivity analysis [1] to explore the input space covering welding of different steel materials. Using this methodology require some developments to sample hundreds of materials, to schedule launching of the welding numerical experiments, and to realize the linear sensitivity analysis. Several sampling methods were tested and we finally adopted a Latin Hypercube Sampling (LHS) strategy to generate m fictitious material properties ([2], [3]). Because of their dependence on temperature, it has been required to sample each material property at a discrete set of n temperature. Thus, $(m \times n)$ inputs were considered in the global sensitivity analysis. Indeed, each of the m material property used in this model are either monotonically increasing or monotonically decreasing as function of temperature and we have developed a LHS that respect this condition. Finally, hundreds of model evaluations were performed using the Finite Element Method (FEM) and the Cast3M software [4]. We must note that the computer model we address here is deterministic, i.e. replicate observations from running the code with the same inputs give identical outputs. The representativeness of the sample size has been studied using a bootstrap method on empirical statistical moments estimation. We can see in fig. 1 that sample with size 600 or more is reasonable. Sampling of materials properties and global sensitivity analysis were conducted using R software ([5], [6]). Finally, inputs data have been divided in two groups: the group of influent data on which we must concentrate our efforts of characterization and the group of non-influential factor. Thus, inputs having little influence on the output have been fixed and new model evaluations were performed in order to compare the reduced parametrization with the initial one. A good agreement was founded on the distortion output between full parametrized model and the reduced one, with correlation coefficient $R > 99\%$ (fig. 2).

In this work, complete methodology of the global sensitivity analysis has been successfully applied to welding simulation and lead to reduce the input space to the only important variables Contrary to a common idea, this work show that input data controlling high temperature material properties (which are the most difficult and expensive to measure) were not influent on the mechanical effects of welding and can be excluded of the model.

This seams to be a new and useful way of applying sensitivity analysis to validate model and especially mechanical models used in welding simulation. Sensitivity analysis has provided answers to what we consider

one of the probable frequently asked questions regarding welding simulation: for a given material which properties must be measured with a good accuracy and which ones can be simply extrapolated or taken from a similar material?

Acknowledgement
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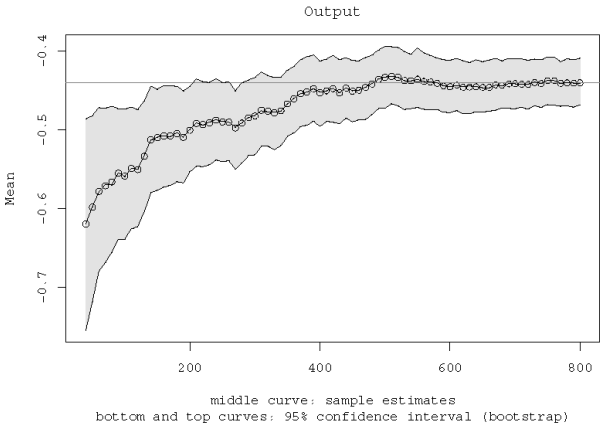
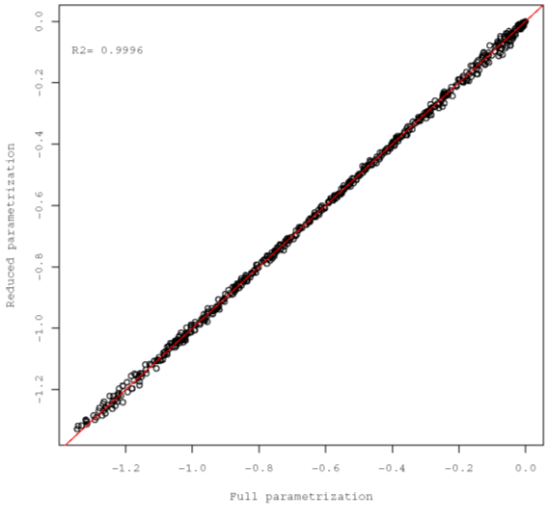
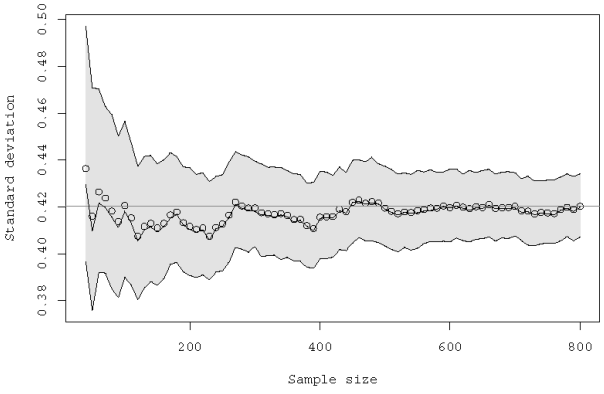


Fig. 1 (right): Convergence of the mean and standard deviation for a distortion output in function of the sampling size.

Fig. 2 (bottom): For a distortion output, comparison of full parametrization ($m \times n$) inputs and reduced parametrization in which less influent inputs have been fixed.





COPING WITH ECOLOGICAL COMPLEXITY: HIERARCHICAL MULT-CRITERIAL, INDIRECT PATTERN ORIENTED MODEL PARAMETERIZATION

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In ecology, due to the accelerated environmental change and increasing negative effects of land use, climate change on ecosystems there is an urgent need both for understanding fundamental processes in ecology and for the development of concepts for long term sustainable land use.

Simulation models in ecology are ideal tools to address ecological questions, as they are able to integrate longer time and spatial scales, formalizing the existing knowledge and to test different hypothesis related both to basic or applied questions.

However, simulation models in ecology in general face several severe problems: they deal with complex, open, and stochastic systems; additionally the details of prevailing processes are often not known, and parameter estimation in general is poor due to lack of empirical data, or due to the difficulties to measure parameters directly. Depending on the investigated question, ecological models have to integrate certain complexity, e.g. if they investigate applied questions. Additionally, to the need to use structural realistic models, a biological plausible parameterization is required to generate results which lie within a realistic range. Such a simulation model may be that complex that it faces severe problems of uncertain parameters and scarce amount of field data to estimate these parameters.

We present a method to face such problems of complexity, using a multi-criterial approach of pattern-oriented modelling (POM, Grimm et al. [1]) to parameterize indirectly a complex simulation model including thirty uncertain parameters. The first approach for such a parameterization was developed by Wiegand et al. [2] for a less complex model, and is now extended to models of higher complexity and uncertainty (Pütz[3]).

The presented pattern oriented parameterization method uses a Monte Carlo Filtering approach, restricting the parameter space by using binary error measures to decide if the inference matches the empirical pattern, which act as a filter for the simulated output. A pattern is defined as a non-random variable, e.g. a trait of one dominant species within an ecosystem, which maybe directly compared to one implemented variable of the simulation model. Due to the scarcity of the data, the patterns are bootstrapped for developing statistical criteria which model parameterization is accepted. These pattern are used from different hierarchical levels of the ecosystem, e.g. from the individual level of one species, to the population, patch or landscape level, using all obtainable of the scarce information.

The advantage of this approach is, that we obtain not only biologically plausible model parameterizations, but we also obtain indirectly information about biological and demographic processes at lower levels, e.g. emergence of new individuals, growth, mortality and other ecological processes, by further sensitivity analysis of the posterior parameter distribution.

The result of this indirect parameterization approach is the gain of strong confidence into the model and the ability to use the model to investigate applied questions. We show the high potential of this approach by means of a grazing model which was developed to investigate the interaction of grazing with stochastic climate in a semiarid ecosystem in Patagonia (Argentine) to assess its degradation risk.

The presented approach bridges the important gap between theoretical and empirical ecology by allowing to tie a simulation model closely to field data and thus leading to reasonable parameter values and ensuring biologically reasonable behaviour.

The presented a multi-criterial, hierarchical pattern oriented approach improves strongly model selection, and thus might be of general interest for simulation models, facing high uncertainties with the need to compare the simulated output with empirical data.

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A NEW METHOD OF SENSITIVITY ANALYSIS FOR INTEGRATED ASSESSMENT MODELLING

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Integrated Assessment Modelling (IAM) incorporates knowledge from different disciplines to provide an overarching assessment of the impact of different management decisions. Such modelling methods generally require the specification of values for numerous parameters from varying sources, many not known with certainty. Rapid increases in model size and complexity, particularly in the case of integrated models for decision-making, pose new challenges for effective sensitivity analysis. As IAM methods are increasingly being used to inform environmental management decisions, it is important that there are sensitivity analysis methods which cater to the challenges posed by these models. Some of the identified shortcomings of existing sensitivity analysis methods in the context of IAM include: computational inefficiency, failure to properly assess parameter interactions, excessive data requirements (e.g. requiring parameter probability distributions), assumptions of model linearity and monotonicity and in particular difficulty of application for models used in decision-making.

The Management Option Rank-Equivalence (MORE) method is a new, rank-equivalence method of sensitivity analysis [1] developed specifically to address the difficulty of applying sensitivity analysis to IAM. While sensitivity analysis methods tend to address the sensitivity of model outputs to the parameter and model inputs, the MORE method investigates the sensitivity of the management decision, which the model is used for, to changes in the model parameters. The method operates on the premise that IAM used in decision-making facilitates the ranking of potential management solutions, based on their efficacy of solving the particular management problem, in order to determine the most effective management solution. When used for decision making, it is important to ensure that the solution is robust and that management option rankings will not alter with small changes in model inputs.

The MORE method of sensitivity analysis incorporates numerical optimization techniques in order to find the minimum and maximum combined change in parameters that will result in the ranking of two management options becoming equal, thus altering the preferred decision. The set of parameter vectors for which the two management options are equally ranked is referred to as the rank-equivalence boundary, as it separates the set of parameter vectors where the management decision would alter from the original solution, from those where it would not. To overcome the difficulty of characterizing the entire rank-equivalence boundary, The MORE method constructs two artificial boundaries based on the minimum and maximum combined change in parameters to reach the rank-equivalence boundary, providing a decision maker with information about the robustness of management solutions given different parameter vector locations as well as characterizing the amount of sensitivity variation in different parameter directions.

While the MORE method enables assessment of the amount of variation of the model sensitivity in different parameter directions, little information is given regarding the change in sensitivity in a particular direction. Further, while MORE sensitivity analysis locates only the minimum parameter change to reach the rank-equivalence boundary, it is possible that there will be several local minima on the rank-equivalence boundary. These locations represent critical points on the rank-equivalence boundary, as they can be reached through small changes in parameter values, which may be similar in value to the minimum combined parameter change, but occur in a different direction in parameter space, thus having different ratios between individual parameter changes. Location of these critical points on the rank-equivalence boundary provides increased information regarding the sensitivity of the decision to changes in individual parameters.

This research proposes an extension to the MORE method, which allows further investigation into the variation of the sensitivity of the model in different parameter directions. In order to locate several critical parameter combinations on the rank-equivalence boundary, a multi-objective, Pareto-optimal search is performed. During the Pareto optimization, the minimization of each individual parameter change is defined as an individual search objective and a constraint is set to restrict solutions to the rank-equivalence boundary. A solution x_2 is then considered to be Pareto optimal if it is at least equal to solution x_1 in all objectives, and better than the solution x_1 in at least one objective. Unlike a weighted combination of the objectives, a Pareto optimal search will identify many locations on the rank-equivalence boundary, thus determining a collection of critical points on the rank-equivalence boundary. These critical points, rather than representing the minimum combined change in parameters, represent the minimum change in a single parameter, with simultaneous minimal changes in other parameters. Hence, this analysis recognizes that while there may be a single minimum change in combined

parameter values, it is likely that there will also be other critical parameter combinations in different directions in the parameter space.

These critical locations can be used to gain further insights into the sensitivity of the decision to the individual model parameters. The collection of critical solutions gives a range of parameter changes to reach the rank-equivalence boundary for each parameter. The frequency of the occurrence of a parameter change within a set range, gives an indication of the decision sensitivity to that particular parameter. A parameter with consistently small changes to reach the rank-equivalence boundary, shows that the decision is consistently sensitive to small changes in that particular parameter. In contrast, a parameter which has varying changes at the critical locations indicates that the decision sensitivity to that parameter is considerably impacted by changes in other model parameters. This allows model users to assess whether parameter uncertainties of individual parameters are within a range that allows confidence in management decisions based on model output.

Use of the Pareto optimization does not require parameter standardization, as each parameter change is compared only with changes of the same parameter. In contrast, the original MORE method requires standardization of parameters as the individual parameter changes are summed to form a single value, in order to determine the minimum combined change to reach rank-equivalence. The removal of parameter standardization alleviates an additional source of variation that is present within the original MORE sensitivity analysis.

The extension to the MORE method is investigated using a case study of an integrated catchment model of the Namoi Catchment in northern New South Wales, Australia. The results are compared with those obtained using the standard MORE method, as well as the FAST [2][3] and Sobol' [4] methods of sensitivity analysis. For this case study the nondominated sorting Genetic Algorithm, NSGA-II [5], to obtain the non-dominated parameter vectors on the rank-equivalence boundary. NSGA-II incorporates elitism, allowing the best solutions from both the parent and daughter pools of chromosomes to be retained, as well as incorporating a crowding distance calculation, to ensure that solutions are spread out along the pareto front, rather than converging to a single solution. From this investigation, the extension to the MORE method proposed in this paper shows promise in supplementing the results provided by the MORE method and providing more extensive information on the sensitivity of a decision to changes in model parameters.

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SENSITIVITY ANALYSIS APPLIED TO A COMPLEX CROP MODEL FOR DURUM WHEAT IN THE MEDITERRANEAN

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Complex mechanistic models for crop growth have been widely used to assess the sustainability of agricultural systems and the risk and impact of climatic change. Usually, these models are calibrated for site specific data, and may not apply in other circumstances due to the implicit empiricism. We carried out a global sensitivity analysis (SA) to rank the parameters of the STAMINA crop model in terms of their importance. STAMINA is a generic but complex cropping system model, which simulates agro-meteorology, hydrology, crop development and photosynthesis in hilly terrain [1] [2]. As model sensitivity depends on parameter variation and the environment [3] we were interested in the relative effects of the environmental drivers (soil and climate), when applying the SA to the rain-fed production of *Triticum durum* (Durum wheat, DW) in the Southern Mediterranean. Our main objective here was to analyze the effect of the environment, namely the effect of water availability (storage in the soil; rainfall) and differences in the *a priori* parameter distribution.

Materials and methods

The model sensitivity was determined for DW, (1) on a silty clay-loam in Volturino (Apulia Region, Italy), and (2) on a drought-prone sandy soil in Nabeul (Tunisia). The analysis used single event data (Italy, 2002-03; Tunisia, 1990/91) for separately calibrated parameter sets. We applied the Morris method [4], which is parsimonious in terms of number of model runs required and suitable for the STAMINA model due to the large number of parameters and complexity. The STAMINA software implements the WARMSIMLAB library analyzing the sensitivity of crop parameters and other inputs. For the Italian site, a maximum of 57 crop parameters were selected, characterised by mean values and standard deviation according to calibration, assuming a normal distribution. For the Tunisian site we reduced the number of parameters to 32. A maximum of 464 simulations were executed as a result of 8 trajectories and 4 levels. μ^* and σ are the mean and standard deviation of the change in yield per change of parameter.

Results

In Volturino, 5 out of 57 parameters were not important for yield formation, in Nabeul 3 out of 32 crop parameters were irrelevant. For both sites, the range of μ^* and σ spanned over several orders of magnitude and we display the results on a log-log scale. Parameters were grouped according to their role in the crop simulation: establishment, development, photosynthesis, partitioning, water stress and senescence. In Volturino, parameters which determine flowering date (T_{base}, GDD), leaf area increase (T_{base}, LAI0) and early allocation to the shoot were highly sensitive. Parameters for establishment ranked very highly overall, directly or indirectly (**Figure 1a**). In Nabeul, among the top 15 ranks of sensitivity, four parameters were related to early growth (**Figure 1b**), four to plant development, and two each to photosynthesis and senescence (start, rate of wilting). Management (e.g. sowing date) can play a crucial role in mitigating the establishment characteristics of crops.

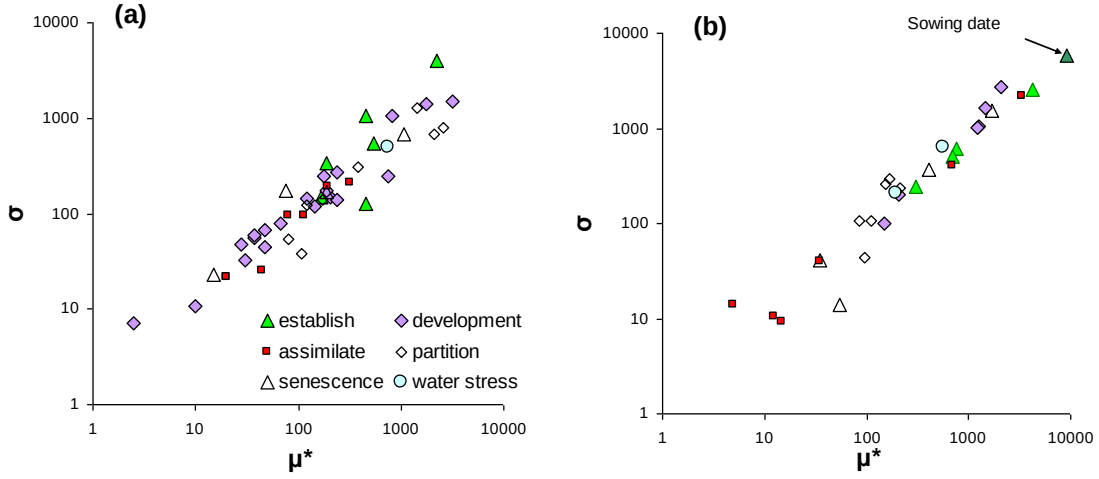

Figure 9 Graphical display of Morris sensitivity measures (μ^*, σ) for crop model input parameters applied to durum wheat experiments in (a) Italy (Volturino, 2003), and (b) Tunisia (Nabeul; 1991)

The parameters on which CO_2 assimilation depends were highly important in Nabeul (μ* >3000 for assimilation rate at light saturation, ~700 for initial light use efficiency), much less in Volturino (320). Both analyses revealed that the parameters for the temperature response curve of photosynthesis were less important. The water stress parameters ranked similar sensitivity (9 at Volturino; 12 at Nabeul), stomatal resistance ranked 18 at Nabeul.

Averaging the parameter groups the overall ranking (**Table 1**) according to mean sensitivity (μ*) show that parameters describing early establishment (initial LAI, temperature factor for GLAI) had the greatest impact on yield of DW grown on a sandy soil in Tunisia, Overall, parameters related to crop establishment played a key role in the Mediterranean environment but in Volturino these parameters were less important than at Nabeul, possibly due to difference in soil. The sensitivity to parameters of dry matter partition is more important at Volturino than at Nabeul, however, some of these parameters were related to early leaf development.

Table 2: Ranking of parameter groups according to mean Morris sensitivity (μ*) in relevance for yield formation of Durum wheat (DW) in Tunisia and Italy

	Italy, Silty Clay Loam		**Tunisia, Loamy Sand**	
Group	***Average μ****	***Average σ***	**Average μ***	**Average σ**
Establishment	677	1035	1501	979
Development	408	292	1063	1121
Photosynthesis	113	95	591	380
Water stress	755	488	380	415
Senescence	336	264	362	326
Partitioning	873	425	138	175

Discussion

The SA for our crop growth model emphasises the importance of early establishment for DW, which confirms other findings in the Mediterranean for wheat [5] and other crops [6]. It further highlights the importance of correctly simulating photosynthesis and crop development, however. The individual and the overall ranking of the parameter sensitivity can be different depending on the environment. At both sites, the time span of grain filling is critically determined by flowering date and the speed of maturation. The latter is determined by the onset of senescence and the senescence rate, in which the results of the SA agree very well for both environments, confirming that the duration of the late growth stages is important in Mediterranean conditions [7] either by management or variety selection. It is surprising that in both environments (soil in Volturino holds more water) the sensitivity to changes in the water stress parameter was similar.

Further work will be presented that uses the same parameter sets in different environments and alters the soil and weather inputs within the range of variation typical for the region. More analysis is also needed on the artefacts possible in the SA related to (a) the variation of the parameters that are too small in relation to the mean value; or (b) parameters that are missed out because of *a priori* neglecting of a process.. Finally, parameter selection should avoid the model becoming over-parameterised and in the SA some parameters could be omitted as they are complementary, intimately linked, like phenology and partitioning, or sequential (growth stages).

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UNCERTAINTY AND SENSITIVITY ANALYSIS FOR PEDOTRANSFER FUNCTIONS

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The characterization of the soil hydraulic properties results indispensable in numerous hydrological applications and in the studies of many practical problems requiring a large spatial scale. It isn't possible to perform always direct measurements of the soil hydraulic properties, because they are cost and time consuming and highly variable spatially and temporally [1]. Consequently, for their estimate the pedotransfer functions (PTFs) are often used; these utilize basic information that are translated easily in the simulation model [2]. However, the PTFs models provide predictions, influenced by uncertainties, which originate in the input variables (measurement errors, etc.) and in the simulation model. Many authors analyzed PTFs uncertainty and evaluated the effect on the output, using different methods [3] [4] [5] [6]. Minasny et. al. [7] showed that the PTFs model uncertainty, often produced by internal parameters and by utilized database, is usually small in comparison to the input variables, which influence the output expectations by a propagation of the initial error. In this study the Monte Carlo (MC) method was utilized, by assuming the probability distribution of each input variable and by estimating that of the output variables. N. 30 undisturbed soil samplings were taken on the alluvial area of 800 m^2 (40 m x 20m), with a slope of 6 %, in the Turbolo basin, in Calabria (Italy). These samplings, with a diameter of 5.1 cm and height of 5.6 cm, were analyzed in the laboratory by using gravimetric method, where the values of the pressure head were fixed (pF = 0.00; 0.50; 1.00; 1.50; 2.00; 2.30; 2.80; 3.40; 4.20) and the corresponding values of θ were determined. By the RETC code [8], for each sample, or rather for each location, assigned $m = 1 - \frac{1}{n}$, the following parameters of unsaturated soil was obtained: saturated water content (θ_s), residual water content (θ_r), scaling parameter (α), shape factor (n) and pressure head (h). These parameters are in the PTF of Van Genucten model, which represents the retention curve:

$$\vartheta(h) = \left[(\vartheta_s - \vartheta_r) \left(\frac{1}{1 + (\alpha \cdot h)^n} \right)^m \right] + \vartheta_r \qquad (1)$$

Given θ_r = 0 and assuming for the other input parameters a normal distribution, on the basis of the statistical tests (Pearson, Shapiro-Wilk, Kolmogorov-Smirnov) for a confidence level of 95%, the corresponding main statistical parameters are reported in the following Tab. 1:

Tab. 1: Main statistical parameters of the input variables of Eq. (1).

Parameters	θ_s	H	α	N
Mean	0.357446071	1.966667	0.334489286	3.57264142857143
Median	0.35471	2	0.323255	3.729735
Standard Deviation	0.028203783	1.370219	0.057598041	0.722674
Variance	0.000795453	1.8775	0.003317534	0.522258
Coefficient of Variation	0.078903605	0.696722	0.172196969	0.20228
Skewness	0.171869081	0.183251	3.868204791	-1.13398

Successively, the uncertainty analysis (UA) and the sensitivity analysis (SA) were carried out on the model, by using following methods: FAST, Random, Latin Hypercube, Sobol, Morris [9]. The FAST method performs the SA, by estimating the sensitivity indexes like main effects (or first order indexes) and total order indexes, as shown in Tab. 2.

Tab. 2: FAST sensitivity indexes.

	$\vartheta(h)$	
	Fast first order indexes	**Fast total order Indexes**
θ_s	0.0644	0.090503
α	0.0726	0.125671
n	0.0015	0.033100
h	0.8016	0.880219

In Tab. 3, the SA results are reported for Random and Latin Hypercube methods; the ranks of the sensitivity indexes are shown in this table, according to Pearson, Spearman, Partial Correlation Coefficient, Partial Rank

Correlation Coefficient, Standardised Regression Coefficient, Standardised Rank Regression Coefficient, Smirnov.

Tab. 3: SA for Random (R) and Latin Hypercube (LH) methods (confidence level of 95%).

	PEAR		SPEA		PCC		PRCC		SRC		SRRC		Smirnov	
	R	L H	R	L H	R	L H	R	L H	R	L H	R	L H	R	L H
θ_s	3	3	2	3	3	3	2	3	3	3	2	2	1	1
α	2	2	3	2	2	2	3	2	2	2	3	3	3	3
n	4	4	4	4	4	4	4	4	4	4	4	4	4	4
h	1	1	1	1	1	1	1	1	1	1	1	1	1	2

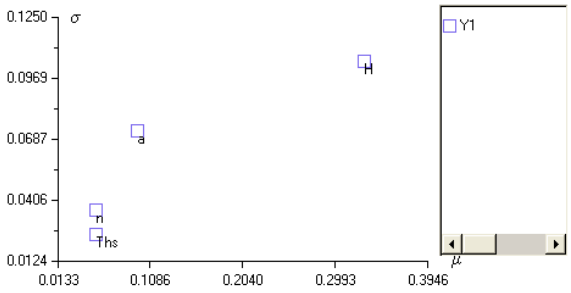
Also SOBOL method is used and the results are shown in Tab. 4.

Tab. 4: Sensitivity indexes of first and total order for the SOBOL method.

	First order indexes	Total order indexes
	$\vartheta(h)$	$\vartheta(h)$
θ_s	0.093091	0.067229
α	0.066166	0.174351
n	-0.00335	0.02697
h	0.890363	0.994241

Finally, in Fig. 1and in Tab. 5 results of Morris method are reported:

Fig. 1: Trend μ - σ for Morris.



Tab. 5: Morris indexes.

	$\vartheta(h)$	
	μ	σ
θ_s	0.0533	0.0252
α	0.0967	0.0727
N	0.0533	0.0364
H	0.3301	0.1052

This analysis was carried out by the SIMLAB 2.2 code [10]. The obtained results shown altogether for the PTF model (1) a not monotonic behaviour; moreover, referring to the considered model, only the pressure head h results clearly sensitive for the water content θ.

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LOCAL SENSITIVITY ANALYSIS FOR BAYESIAN MIXTURE MODELS

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The analysis of finite mixture models is recently playing an important role in theoretical as well as in applied statistics (see, for example, Mclachlan and Peel [1] and Böhning and Seidel [2]). Mixture models are excellent tools that can be used to describe complex systems over a wide range of applications in many fields of knowledge. Since the advent of Markov Chain Monte Carlo (MCMC) methods, many advances have been achieved for the Bayesian analysis of finite mixture models.

Inference of a probability distribution for lifetime data is necessary in any reliability analysis. Often this inference is complicated by the presence of multiple failure modes and variations in manufacturing that may create a heterogeneous component population. In these cases, standard distributions are inadequate. Mixture models provide additional modeling flexibility and have the physical interpretation of representing failures from a heterogeneous population. Titterington et al [3] give detailed references about mixtures for lifetime data.

In spite of the modeling advantages, the practical implementation of finite mixture models sometimes introduces additional complexity because they often have many parameters and the calculations become difficult. Rufo et al [4] provided a general approach to address Bayesian analysis of finite mixture models of distributions from natural exponential families with quadratic variance function (NEF-QVF). Note that the families in this class are normal, gamma, hyperbolic-secant, Poisson, binomial and negative-binomial. This general approach solves the prior distribution choice and the unidentifiability problems in this kind of mixtures. However, a sensitivity analysis on the choice of the parameters in the prior distribution is needed. Most sensitivity analysis are informal ones and are based on changing the values in the prior parameters and observe how the output changes. This needs re-running the sampling algorithm for several parameter values with the corresponding computational cost. In this context, formal sensitivity analysis is a difficult task demanded by several authors. Pérez et al [5] proposed a computationally low-cost method to estimate local sensitivities in Bayesian models. This method is based on importance sampling and it requires to compute prior derivatives. It can be applied (but not only) to complex Bayesian models that need to be solved by MCMC methods, and it allows to estimate the sensitivity measures and their errors with no additional random sampling.

In this work, a formal sensitivity analysis for the parameter values of the prior distribution in finite mixtures of distributions from NEF-QVF is described and applied. The derivatives that are needed to apply the method are obtained for all the distributions in this family class. This fact allows a direct implementation, and, therefore, the applicability to mixtures of lifetime distributions. The sensitivities are evaluated and give us information about a proper choice of the prior parameter values. This method can be applied in many applications arising in reliability contexts.

Acknowledgement: This research has been partially supported by *Ministerio de Educación y Ciencia*, Spain (Project TSI2004-06801-C04-03).

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EXTENSION OF LATIN HYPERCUBE SAMPLES WITH CORRELATED VARIABLES

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Latin Hypercube Sampling (LHS) [1] is widely used as sampling based method for probabilistic calculations in support of both uncertainty analyses and sensitivity analyses ([2], [3]). This method has some clear advantages over classical random sampling (RS) that derive from its efficient stratification properties. However, LHS is not perfect. One of its limitations is that it is not possible to extend the size of an initial sample by simply adding new simulations, as this will lead to a loss of the efficient stratification associated with LHS. We describe a new method to extend the size of an LHS to n (>=2) times its original size while preserving both the LHS structure and any induced correlations between the input parameters. This method involves introducing a refined grid for the original sample (Figure 1) and then filling in empty rows and columns with new data in a way that conserves both the LHS structure and any induced correlations (Figure 2). An estimate of the bounds of the resulting correlation between two variables is derived for n=2. This result shows that the final correlation gets closer to the average of the correlations from the original sample and the new sample used in the infilling of the empty rows and columns indicated above as the sample size increase.

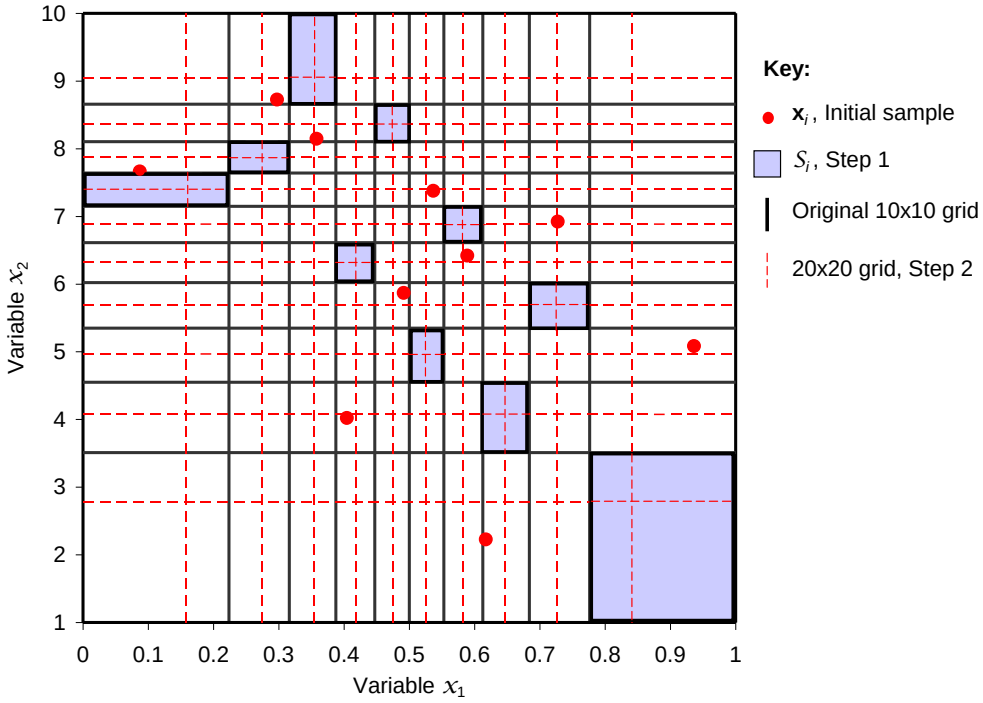

Figure 10: refinement of original grid and selection of an area for extended LHS, respecting correlation

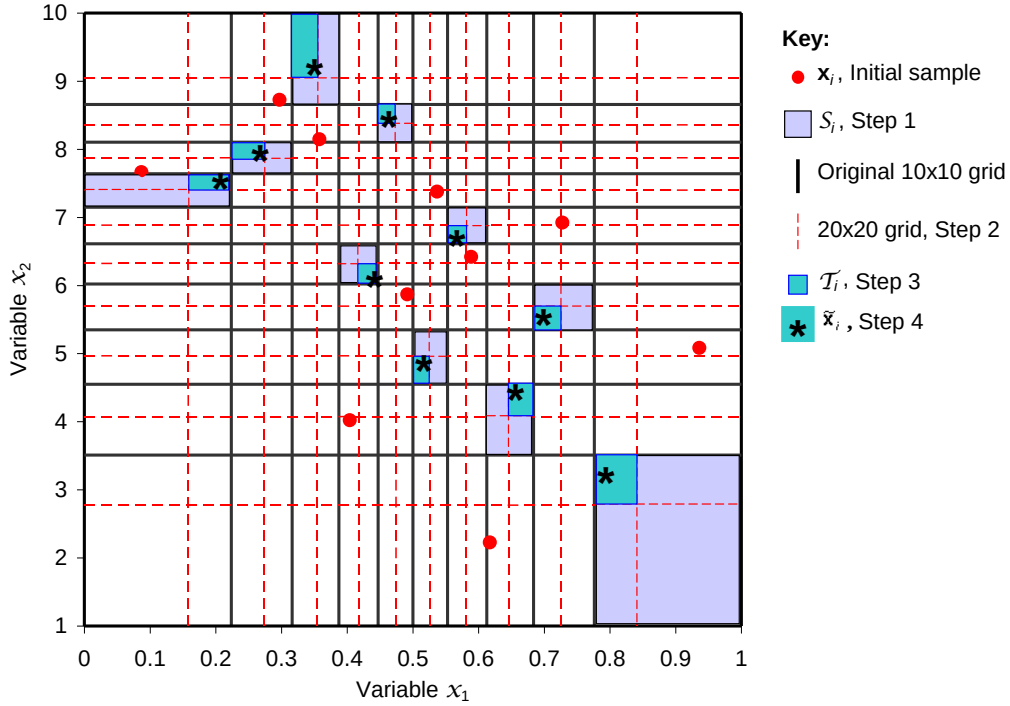

Figure 2: Random selection of points in authorized area for extended LHS

Acknowledgement:

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PARAMETRIC SENSITIVITY ANALYSIS OF NONLINEAR MULTIPARMETER REGRESSION MODEL SYSTEMS

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Parametric sensitivity analysis is applied here in the context of nonlinear regression parameter estimation in multi-response models. The predictions from these models are subject to uncertainties propagated from the estimated parameters using available experimental data. When the uncertainties associated with these estimates are unacceptably large, an alternative purpose of the experimental effort could be to reduce some or all of the parameter uncertainties that propagate into the model predictions. This situation motivates the parametric sensitivity analysis in regression parameter estimation.

The conventional approach for summarizing parametric sensitivity of the predicted responses is through the use of the first-order derivatives of the predicted response(s) with respect to each parameter. These sensitivity coefficients can be termed as "marginal" sensitivities because they focus on individual parameters only. While they provide helpful insight into the estimation characteristics, they can be misleading when correlations among parameters exist.

Sulieman et al. (Technometrics 43 (4), 2001) developed a new parametric sensitivity measure based on profiling algorithm used to assess parameter nonlinearities in regression models and to construct likelihood intervals for the individual parameters. They applied the measure to single-response nonlinear models and later extended the approach to assess parameter sensitivities in multi-response regression models. The profile-based sensitivity coefficient can be defined as the total derivative of the model response predicted function with respect to a parameter of interest, with the remaining parameters held at their conditional estimates. Consequently and in contrast with marginal sensitivity coefficient, the profile-based sensitivity measure accounts for both correlation structure among the parameters and model nonlinearity. It also provides sensitivity information over wide range of parameter uncertainties.

In this paper, an overview of profile-based sensitivity measure for multi-response regression models and some related computational aspects are given. The new sensitivity approach is applied to regression models described by systems of Ordinary Differential Equations using Box-Draper determinant criterion for parameter estimation. Application of the approach is illustrated using a model formulated by the Dow Chemical Company to describe the kinetics of an isothermal batch reactor system. The following formulation of the model was studied by Biegler and Tjoa (1991) and is used here.

$$\frac{dy_1}{dt} = \quad k_2 y_1 y_2 A$$

$$\frac{dy_2}{dt} = \quad k_1 y_2 (x_2 + 2x_3 \quad x_4 \quad 2y_1 + y_2 \quad y_3) \quad k_2 y_1 y_2 A + k_{\ 1}\beta_1 (\ x_3 + x_4 + y_1 \quad y_2) A$$

$$\frac{dy_3}{dt} = k_1 (x_3 \quad y_1 \quad y_3)(x_2 + 2x_3 \quad x_4 \quad 2y_1 + y_2 \quad y_3) + k_2 y_1 y_2 A \quad \frac{1}{2} k_{\ 1}\beta_2 y_3 A$$

Where

$$k_i = k_{i0} \exp\left(\frac{E_i}{R}\left(\frac{1}{x_i} \quad \frac{1}{T_0}\right)\right), i = \quad 1,1,2$$

$$A = \frac{2x_3 + x_4 + 2y_1 \quad y_2 + y_3}{y_1 + \beta(\ x_3 + x_4 + y_1 \quad y_2) + \beta_2 y_3}$$

$$\beta_1 = \frac{K_1}{K_2}, \beta_2 = \frac{K_3}{K_2}$$

The model includes eight parameters to be estimated using three sets of experimental data taken at

different settings and three response variables. A wide range of sensitivity behaviour is observed, including instances in which the traditional and profile-based sensitivity coefficients lead to different conclusions concerning the impact of a parameter of interest on the predicted responses from the model.

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SENSITIVITY RATIOS: EXACT RESULTS

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Recent numerical calculations on combustion and cell metabolism models suggest that ratios of sensitivities may show certain regularities and these relations might have deep meaning and consequences on the given chemical (combustion) or biological (cell cycle/metabolism) phenomena [1,3]. Here we give exact sufficient, necessary, and sufficient and necessary conditions for these regularities (local similarity, scaling relation, and global similarity) to hold. We also investigate the question, what happens if the conditions are only approximately fulfilled.

Consider the parameter dependent initial value problem

$$\mathbf{c}'(t,\mathbf{p}) = \mathbf{f}(\mathbf{c}(t,\mathbf{p}),\mathbf{p}), \quad \mathbf{c}(0,\mathbf{p}) = \mathbf{c_0},$$

with $N, P \in \mathbf{N}, \mathbf{f} \in C^2(\mathbf{R}^N \times \mathbf{R}^P, \mathbf{R}^N), \mathbf{c}_0 \in \mathbf{R}^N$. Let us suppose, for the sake of simplicity, that the complete solution to all initial value problems are defined on the whole real line, and let the derivative of the *i*th coordinate function with respect to the *k*th parameter be denoted by s_{ik}. These **sensitivities** are known to obey [2] the initial value problem

$$s_{ik}'(t,\mathbf{p}) = \sum_{n=1}^{N} \partial_n f_i(\mathbf{c}(t,\mathbf{p}),\mathbf{p}) s_{nk}(t,\mathbf{p}) + \partial_{N+k} f_i(c(t,\mathbf{p}),\mathbf{p}) \quad s_{ik}(0,\mathbf{p}) = 0.$$

Parameters p_k and p_m are said to be **locally similar** with respect to the state variables c_i and c_j with the similarity function $\lambda_{ij} : \mathbf{R} \times \mathbf{R}^P \to \mathbf{R}$, if for all $\mathbf{c}_0$ $\lambda_{ij} s_{jk} = s_{ik}$ and also $\lambda_{ij} s_{jm} = s_{im}$ holds. A **scaling relation** is said to hold with respect to the state variables c_i and c_j if for *i*,*j* and for all *k* and for all $\mathbf{c}_0$ $c_i' s_{jk} = c_j' s_{ik}$ is true. The parameters p_k and p_m are said to be **globally similar** with respect to the state variable with the similarity number μ_{ikm}, and they are **uniformly globally similar**, if the similarity number does not depend on *i*.

The necessary and sufficient condition for the scaling relation to hold is the existence of functions $\alpha, \beta : \mathbf{R}^N \to \mathbf{R}$ such that $\alpha(\mathbf{x}) f_i(\mathbf{x},\mathbf{p}) = \beta(\mathbf{x}) f_j(\mathbf{x},\mathbf{p})$ holds for all $\mathbf{x} \in \mathbf{R}^N$.

If $\alpha f_i = \beta f_j + \varepsilon$, then

$|c_i' s_{jk} - c_j' s_{ik}| \le K_{jk} \varepsilon_k$ with $\sup_{\mathbf{p}} \{|\varepsilon| + |\partial_{N=k} \varepsilon|\} \le \varepsilon_k$.

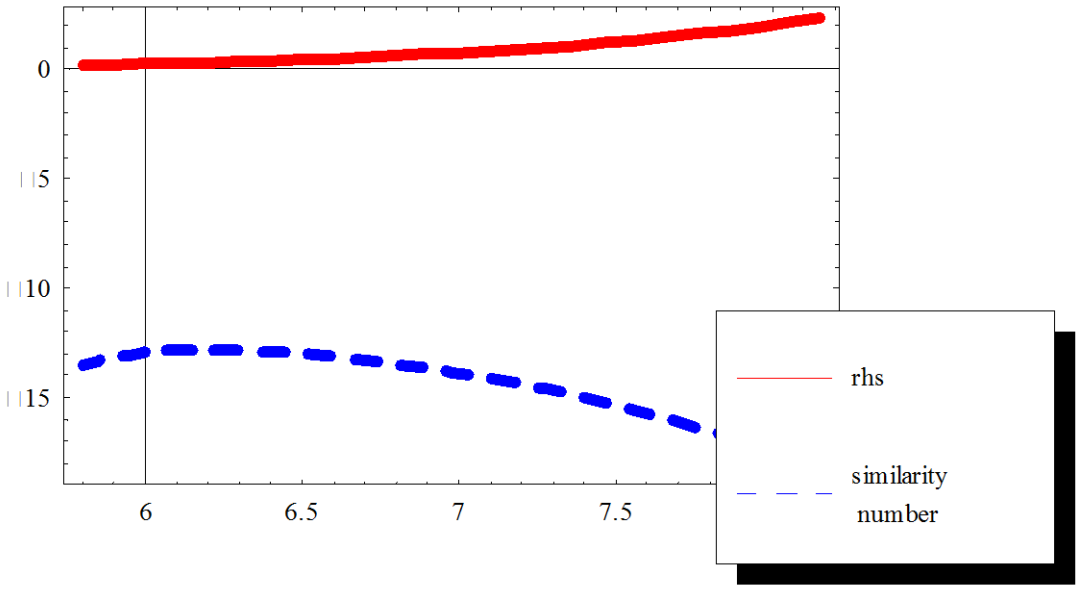
The necessary and sufficient condition for uniform global similarity of the parameters p_k and p_m with the similarity parameter $\bar{\mu}_{km}$ is that $\partial_{N+k}\mathbf{f}(\mathbf{x},\mathbf{p}) = \bar{\mu}_{km}\partial_{N+m}\mathbf{f}(\mathbf{x},\mathbf{p})$ holds for all $\mathbf{x} \in \mathbf{R}^N$. This also implies the explicit form of the right hand side: all of its coordinate functions do not depend on the parameters p_k and p_m separately, only on their linear combination $p_k \bar{\mu}_{km} + p_m$.

If the coordinate functions of the right hand side do not depend on the parameters p_k and p_m separately, only on their linear combination $p_k \bar{\mu}_{km} + p_m$ up to an additive error ε, then

$$\partial_{N+k}\mathbf{f}(\mathbf{x},\mathbf{p}) - \bar{\mu}_{km}\partial_{N+m}\mathbf{f}(\mathbf{x},\mathbf{p}) = \partial_{N+k}\varepsilon(\mathbf{x},\mathbf{p}) - \bar{\mu}_{km}\partial_{N+m}\varepsilon(\mathbf{x},\mathbf{p}).$$

If $\partial_{N+k}\mathbf{f}(\mathbf{x},\mathbf{p}) - \bar{\mu}_{km}\partial_{N+m}\mathbf{f}(\mathbf{x},\mathbf{p}) = \varepsilon(\mathbf{x},\mathbf{p})$, then $|\bar{\mu}_{km}\mathbf{s}_{.m}(t,\mathbf{p}) - s_{.k}(t,\mathbf{p})| \le \frac{\varepsilon(\mathbf{x})}{L} e^{Lt}$.

The figure shows in the case of the simple Volterra-Lotka model that approximate fulfilment of uniform global similarity implies approximate constancy of the right hand side.



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UNCERTAINTY ANALYSIS OF AN OZONE DEPOSITION MODEL

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Photochemical air pollutants, especially ozone, are the important chemical species that affects both vegetation and human health. Elevated ozone concentrations can be potentially damaging to agricultural and natural vegetation. Occasional extreme concentrations may cause visible injury to the vegetation while the long-term, growing- season averaged exposure can result in decreased productivity and crop yield. Air quality measures, based on Accumulated exposure Over a Threshold (AOT) such as AOT40 were therefore developed based on experiment in order to try to mitigate the damage. However, since ozone enters plants through the stomata, the response of vegetation to changes in the atmospheric ozone concentrations is more directly influenced by the stomatal ozone flux than its atmospheric concentration. Therefore, it has been suggested that the stomatal ozone flux is a more appropriate measure for ozone damage than the concentration based values. Stomatal flux of ozone is controlled by ozone concentration and by deposition velocity via parameterization of the canopy and stomatal conductances. Plant stomatal conductance plays an important role in most of all deposition models. In Jarvis model, multiplicative algorithm of stomatal conductance is applied. This type of model includes functions for the effects of photosynthetically active radiation, air temperature, soil water content, and other parameters on the stomatal conductance. The values of the model input parameters are very uncertain. Therefore, these parameters may give rise to uncertainties in simulation results. The nonlinear models can magnify the uncertainty of some parameters and damp it to each others. This means that models may overestimate or underestimate the stomatal ozone fluxes. Sensitivity analysis is an effective tool for the exploration of the relation between the output of mathematical models and the input data, which comprise the values of parameters as well as the initial conditions. To investigate the effects of the most important parameters on stomatal conductance of the ozone a Monte Carlo analysis has been performed. The large number of parameter sets is generated according to the probability density functions of these parameters. The model is simulated with each of these parameter sets, and the results are processed with statistical methods. Determination of the probability density functions of the model results from the joint probability density functions of the parameters from measurements will be presented. Estimation of the high spatial variability of the stomatal ozone fluxes over Central Europe under continental climate region will be also discussed. For this purpose a coupled Eulerian photochemical reaction-transport model and a detailed ozone dry deposition model (TREX; Transport EXchange Model) have been developed, and it has been coupled to ALADIN meso-scale limited area numerical weather prediction model. Hereby, estimation of the ozone deposition can be performed for a routine way.

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A SENSITIVITY ANALYSIS BASED HYBRID ALGORITHM FOR PARAMETER DETERMINATION IN STIFF BIOCHEMICAL PATHWAYS

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Sensitivity analysis is one of the most effective approaches for studying mathematical models of biochemical systems. One of the key issues in modern systems biology is the development of simulation parameters that may be used to build the models themselves. To build a quantitative, mathematically robust description of a biomedical pathway or network, both model structure and realistic kinetic parameter values are necessary [1-6]. We will present a recently developed sensitivity analysis based parameter estimation method designed for stiff biological systems. The parameter optimization method developed is a hybrid global/local optimization method and is based on a fast time-adaptive Rosenbrock sensitivity analysis integrator developed by our lab [7].

The basis for the optimization procedure is the stiff Rosenbrock integrator, which has been adapted for sensitivity analysis using a direct sensitivity approach. Automated sparse Jacobian and Hessian calculations of the coupled system (the original model equations and the sensitivity equations) have been implemented in the freely available systems biology *CellSim* [8]. To test this new integration method, both time-dependent concentration and parameter-based sensitivity coefficients are measured using several standard integration schemes. A key advantage of our scheme is the efficiency of calculating the sensitivity analysis. The method developed is shown to perform sensitivity analysis in a manner that is cost effective computationally with moderate accuracy and is furthermore *several orders of magnitude faster than standard integration techniques* [7].

In general, complex systems of biological reactions include hundreds of species involving large numbers of interactions, as well as parameter values that can span several orders of magnitude. For this reason, stiff integrators such as the Rosenbrock methods are a preferred method for solving biochemical systems and hold much promise in following the time evolution of the coupled system. The price of the Rosenbrock integrator, which has forestalled its use in systems biology, is the need to calculate the Hessian and the Jacobian terms of the original set of equations in an automated fashion. This task becomes more difficult as the scale of the biochemical systems becomes larger. We have developed a module that generates all the necessary terms automatically as well as analytically determine the appropriate matrix decompositions using the decomposition of the Jacobian of the original system equations. A custom sparse linear algebra package is used to increase the efficiency and reduce the computational overhead of each integration step.

Parameter estimation algorithms typically minimize a cost function over a parameter space and may be generally classified in two groups: those that use global and local estimation techniques. Local algorithms are computationally efficient, but stop at the first encountered local minimum and consequently not generally capable of finding the true global minimum. In contrast, global algorithms are able to search the parameter space beyond local minima, though they are in general significantly more computationally expensive.

We propose to build an approach that combines the best of each of these procedures: a sensitivity-based hybrid method that combines global algorithms. This hybrid approach tests several global optimization methods, including genetic algorithms (GA) [9-11], simulated annealing (SA) [12] with a series of local algorithms including conjugate gradient (CG), Broyden-Fletcher-Goldfarb-Shanno (BFGS) and the steepest decent method. The gradient information for the local integrators comes from our groups recently developed fast adaptive time step sensitivity analysis integration method [7] . A pure GA, a pure SA as well a full suite of sensitivity analysis based hybrid algorithms will be tested and compared. Three cases are chosen as benchmark: a) 36 parameters optimization of a nonlinear biochemical model [1], b) 20 parameters optimization of mechanism of irreversible inhibition of HIV protease [13], c) Complex mitogen-activated protein kinase (MAPK) pathway model of Bhalla and Iyengar [14]. All the procedures discussed will be made freely available to the scientific community under the GPL (Gnu Public License).

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