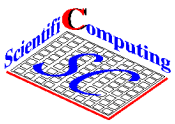
Institut für Wissenschaftliches Rechnen

Prof. Hermann G. Matthies, Ph.D.



der TU Braunschweig

Jahresbericht 2012

Institut für Wissenschaftliches Rechnen der TU Braunschweig

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1 Vorwort

Dear Reader,

the past year has been unprecedented in the number of theses completed by members of the Institute. First Dr. Josef Schüle completed his habilitation, and the corresponding thesis treating parallel computation on GPUs has been published as a monograph. A total of four doctoral theses were completed during the year, starting with Dr. Elmar Zander, who worked on low-rank tuncations combined with iterative solution schemes for stochastic partial differential equations (SPDEs). He was followed a short while later by Dr. Oliver Pajonk, who used the methods for SPDEs to derive spectral Bayesian updates for the purpose of parameter identification. In the autumn there were two thesis defenses in one week: one by Dr. Martin Krosche on a software component framework and greedy low-rank methods for SPDEs, and one by Dr. Bojana Rosić on stochastic plasticity and corresponding variational inequalities. I am very happy to report on these tidings, and to add my best wishes for the canditates' further careers. These theses reflect also very much the scientific work performed at the Institute, and at the same time set the basis for future projects. These continue to be broadly the work on efficient numerical methods for coupled and stochastic problems, as well as the use of these techniques for the identification of parameters and other system properties. The following pages will give more detail, and I hope the interested reader will glean the essential ideas and also find further pointers in the case of deeper interest.

Sincerely Yours

Hermann G. Matthies

2 Forschung

2.1 An Artifact Object Model

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In scientific computing several domains of research have to work closely together to solve challenging problems. In this demanding field the challenge of solving complex computational problems is inherent and the reason why scientists have to use state-of-the-art technology and methods from many scientific fields. In the development of interdisciplinary numerical simulations each participating scientist is a specialist in a certain field of expertise. This makes it necessary to split the responsibilities for parts of a scientific software-system. More than in other software development areas it is important to achieve a separation of concerns (SoC) [2, 4]. Therefore, core parts of scientific software need to be developed by domain experts, who often follow a pragmatic view of software-engineering [3].

On the other hand, software for simulating complex phenomena has to be carefully designed to provide high performance. Often, besides the right numerical method, profound special knowledge about hardware and software components has to be applied, which increases development costs and places additional challenges to the domain experts. A meaningful separation of system-related and domain-specific concerns is often hindered by technical reasons such as a strong coupling between these concerns. This strong coupling is induced by a gap in the scale of both concerns. While technical concerns are generally focused on implementation details, domain-specific concerns are orders of magnitude coarser, and current component models do not provide a solution to fill this gap. While classical component based software engineering puts its focus on the decomposition of functional units of similar scale, very fine-grained components are not in the scope. The decomposition of artifacts of much differing scales is a matter of the building environment of software.

The goal of build-systems is to provide means of translating sets of input files into sets of output files, hence it is common practice to provide build-systems as parts of software source-codes. In a component based approach where each component is understood as a standalone software system [6], the approach runs into a dilemma: on the one hand, a component based application is understood as standalone software, which in turn provides a build-system, and on the other hand its components are

standalone as well and therefore require their own build-system. In this situation, the build-system motivates developers to either

- (1) group components to coarse-grained libraries by defining a common build-system, or
- (2) to maintain a large set of independent build-systems.

The grouping (1) results in a relatively small build-system and therefore less development overhead for the built, but hampers the flexibility to reuse components separately, and motivates ad hoc reuse patterns within the library, which contradicts a primary goal of component based development [1], namely to exclusively allow systematic reuse. The second case (2) on the other hand indeed results in standalone, separable components, but the overhead to write the individual build-systems increases, and component-composition requires the composition of build-systems, which is a non-trivial task. This condition is often resolved by defining build-systems of composites as a recursive process, which successively runs the build of all of its components independently. Peter Miller discusses in [5] some issues which *recursive makefiles* induce in build-systems. The most essential one is an incomplete dependency relation. This issue is not unique to *makefiles* and emerges from the incomplete connection of the dependency- graphs, which is partitioned artificially and results in a broken transitivity of dependencies.

We propose an *Artifact Object Model* (AOM) to describe the build-system of a code-artifact in a local, compact, and declarative way. The model can be used to define the build-process for individual components and additionally allow components to be coupled by using a set of coupling operators.

This work provides an approach for a build-level composition of scientific software artifacts. The approach is made explicitly in the context of scientific computing, and integrates solutions for specific problems in this domain including

Grid computing to make composed applications portable for the Grid, and

Separation of Concerns our proposed domain-specific language provides an interface between the domain of build-systems and the development of softwaren which is commonly performed by experts in fields not concerned with software-engineering.

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2.2 Uncertainty Quantification in the Preliminary Aircraft Design

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During the design process of an aircraft uncertainty is present at many places [10, 11]. A deterministic reference model of a CESTOL (cruise efficient short take-off and landing) aircraft design in the preliminary design phase is analysed with respect to its robustness towards uncertainties. For this purpose a stochastic description is introduced for parameters of the reference model. In this manner, the deterministic reference model becomes a probabilistic one.

Section 2.2.1 outlines the robustness analysis of the aircraft configuration and focuses on a surrogate model representation of the probabilistic model. Further on, Section 2.2.2 investigates the sensitivity of the flight dynamics on the presence of structural or parameteric uncertainty coming from the description of aerodynamic forces, geometric and boundary conditions, model uncertainties etc.

Financial support has been provided by the DFG (Deutsche Forschungsgemeinschaft) in the framework of the SFB (Sonderforschungsbereich) 880.

2.2.1 Robustness Analysis of the Aircraft Configuration

The reference aircraft design is shown in Figure 1. Fourteen configuration parameters — which mostly affect the aircraft design — are described by uniformly distributed stochastic variables which are mutually independent.

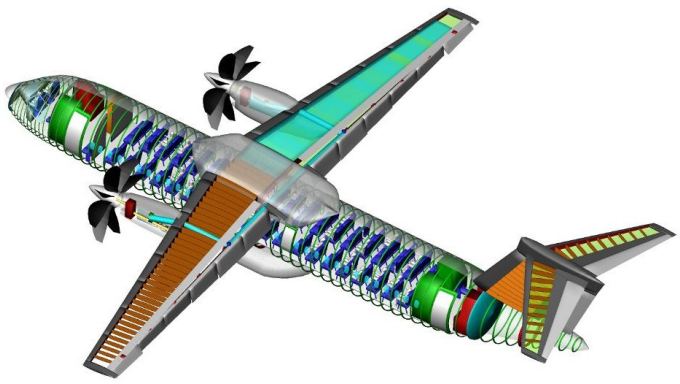
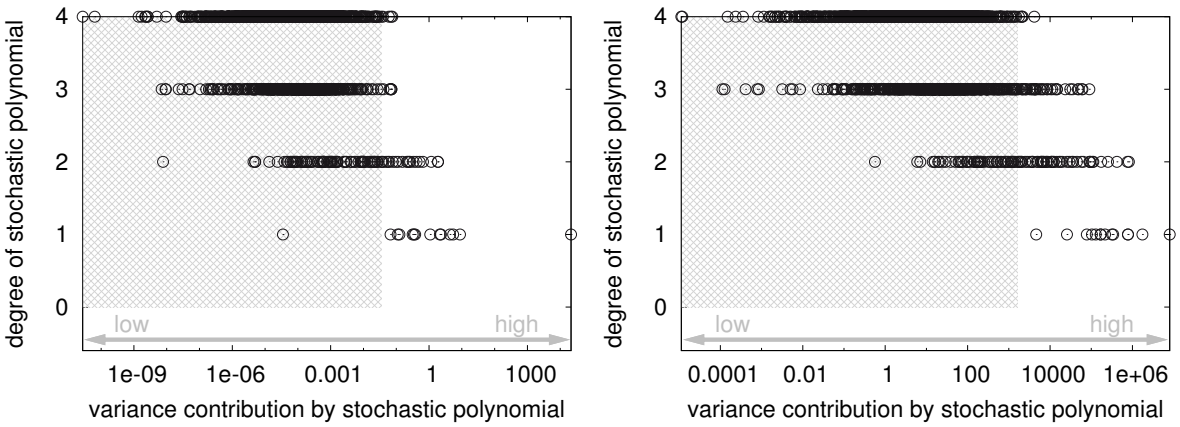


Figure 1: Reference aircraft design in the SFB 880 (this picture is kindly provided by Wolfgang Heinze, IFL, TU Braunschweig).

A distributed component-based Monte Carlo (MC) simulation with 12,191 samples was performed on a Linux-cluster. An aircraft sample

was simulated by PrADO (Preliminary Aircraft Design and Optimisation program) [3, 9] which was ported from Windows to Linux before. The expectation of the runtime for the simulation of a single sample was 4.203 h. Expectations, standard deviations, distribution functions and correlations were considered which identified the reference model of the aircraft to be robust.

A surrogate model for the probabilistic model is represented by a truncated polynomial chaos (PC) expansion. It was computed for different maximum polynomial degrees through a regression approach [1] on the basis of the MC samples. It came out that next to the linear terms at least quadratic terms are required for the PC representation to reach the same quality for the statistics than the pure MC simulation provided. Furthermore, the surrogate model required far less samples for its construction to reach that quality.



(a) (b)

Figure 2: Each circle in the plots identifies the variance contribution and the degree of a stochastic polynomial which belongs to a truncated PCE up to fourth polynomial degree representing the surrogate model. Figure (a) focuses on the mass of the fuselage, Figure (b) focuses on the static thrust of the engine.

However, most of the PC terms are negligible that means they do not have a large impact in describing the probabilistic model. That is demonstrated in Figures 2(a) and (b). In both figures the PC representation up to fourth polynomial degree with 3060 stochastic polynomials is considered; the degree of a stochastic polynomial is plotted over its contribution to the variance (in absolute values) provided by the PC representation. For the mass of the fuselage 44 polynomials are enough to reach 99.99% of the variance, see Figure 2(a); the hatched area in the plot identify the polynomials which contribute the remaining 0.01% of the variance. Analogously, for the static thrust of the engine 106 polynomials are enough to reach 99% of the variance, see Figure 2(b).

2.2.2 Uncertainty Quantification of the Basic Aircraft Model

This section is concerned with the uncertainty quantification of the basic aircraft model (BACM) used to simulate the flight dynamics [2, 7]. Mathematically speaking the considered model is represented by a system of first order differential equations with initial conditions:

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{\kappa}, t), \quad \boldsymbol{x}(0) = \boldsymbol{x}_0, \tag{1}$$

where $\boldsymbol{\kappa}$ is a vector of input parameters related to the aerodynamics and the structure of the aircraft. The initial conditions $\boldsymbol{x}_0$ and input parameters $\boldsymbol{\kappa}$ are modelled as random variables and processes whose probability distributions are chosen according to the maximum entropy principle and available experimental data. Initially the prescribed uncertainties (the maximal and minimal percentages) are taken to be normally (3σ region) or uniformly distributed. For an initial computation this assumption is not of very high importance as in a future work the parameter descriptions will be improved in a Bayesian identification setting using existing measurement data [6, 8]. According to the first available data the input parameters are described such that the mean values are chosen to be the default BACM values and the standard deviations are prescribed by the calculated errors between the measurements and DATCOM analysis software. Thus, the modelled uncertainty does not truly come from the parameters, but from the modelling error accompanied by measurement noise.

The presence of uncertainty allows a reformulation of the initial deterministic problem to a ordinary differential equation with random coefficients whose solution is computed numerically with the help of algorithms for time and stochastic integration. Embedding the original BACM explicit time integration in the stochastic algorithm, the numerical solution of the system of random differential equations is computed in a purely non-intrusive manner via the direct integration [4] and stochastic collocation approaches [5].

The sensitivity of the system behaviour in clean cruise configuration on the input uncertainty at the end of the time interval ($t = 50$ [s]) is investigated with the help of a MC simulation with $20,000$ samples. The results in Table 1 show that the uncertainties in lift coefficients have the highest impact on the output uncertainty. The most sensitive quantity is the pitch rate q [deg/s], whose coefficient of variation is 12%. The true air speed V_{TAS}[kt] and height h [ft] are less sensitive as the uncertainty in the output is around 1% and 2%. However, the statistics of the system behaviour at some specific time are not enough to investigate the sensitivity. Therefore the mean system paths together with $\pm\sigma$ regions (the blue areas) are plotted in Figure 3 for the observed time interval

Table 1: The coefficient of variation of the output response at $t = 50$ [s] on the uncertainty in input parameter C_{A0} only, C_α only, C_{W0} only and all parameters together.

Output	C_{A0}	C_α	C_{W0}	all
α	2.4e-04	3.2e-04	1e-13	4.2e-04
V_{TAS}	0.01	0.01	1e-14	0.01
h	0.01	0.02	1e-13	0.02
q	0.06	0.10	1e-14	0.12

$[0, 50]$. According to these plots the system path has the highest uncertainty when the maximal or minimal values ($t = 40$ [s]) of the response are achieved as expected. However, one should have in mind that these solutions are not representing the natural uncertainty in the system but only consequences of the modelling error.

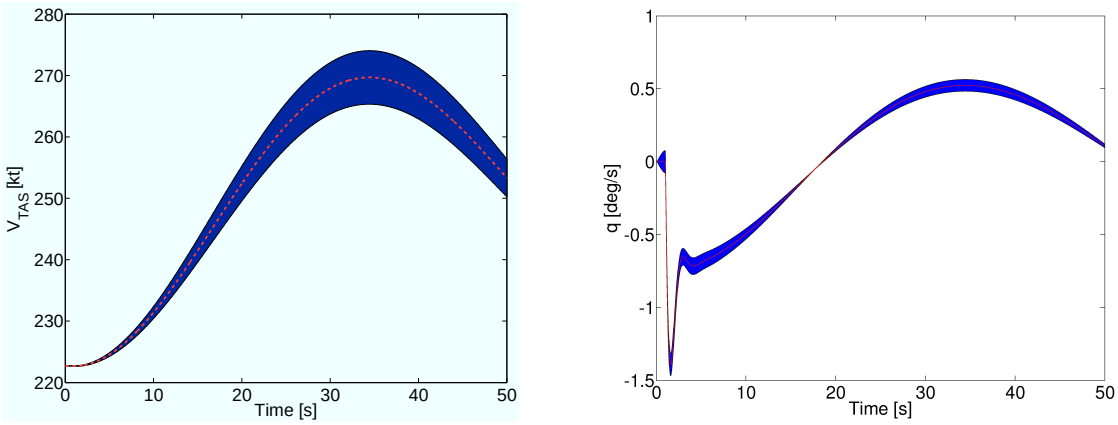


Figure 3: The mean value of the true air speed V_{TAS} and pitch rate q and the region of their $\pm\sigma$ uncertainty

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2.3 Solving a Probabilistic Model of a Composite Laminate

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Modelling and simulating the uncertain characteristics of a composite laminate is challenging [8, 7, 1]. A loaded three-dimensional composite laminate with a linear constitutive law and a partially uncertain and fully anisotropic material is considered here. The corresponding mathematical system is discretised by the stochastic Galerkin method [6]. A low-rank representation of the solution is approximated here adaptively by a greedy algorithm [5].

The description of the composite material is shortly explained in Section 2.3.1 while the main focus is on the simulation presented in Section 2.3.2. Finally, the distributed generic component-based software realisation of the simulation is briefly explained in Section 2.3.3.

Financial support has been provided by the European Community's Seventh Framework Program FP7/2007–2013 under Grant Agreement n° 213371 in the project "More Affordable Aircraft through eXtended, Integrated and Mature nUmerical Sizing" (MAAXIMUS).

2.3.1 A Stochastic Model of the Composite Material

A stochastic model of the composite material was derived from photographic images of a test specimen which was not externally loaded, see our publication [2]. Figure 4 shows some samples of Young's modulus corresponding to a computed stochastic layer of the composite material. A truncated Karhunen-Loève expansion (KLE) of the stochastic model was determined on the basis of a PC representation up to second polynomial degree and used for the material description of the simulated composite laminate, see Section 2.3.2.

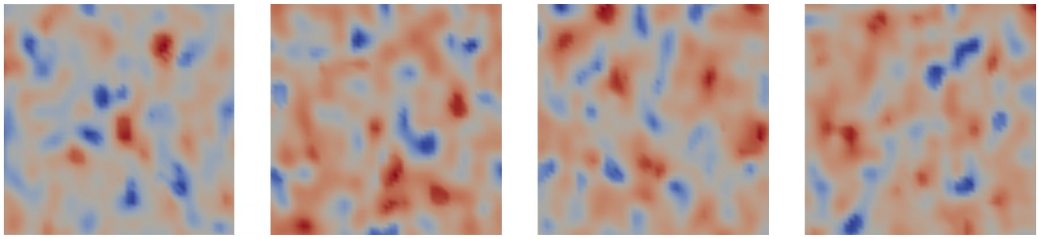

Figure 4: Four samples of Young's modulus which belong to a stochastic layer of a composite material.

2.3.2 The Simulation of the Composite Laminate

The model of a composite laminate with a linear constitutive law consists of fifteen layers, see Figure 5. The anisotropic material description of one layer is considered to be uncertain and represented by a truncated KLE. The composite laminate is fixed on one side and loaded by an external force on the other side. It is discretised by the finite element method in the spatial domain. The discretised model consists of $78,612$ spatial degrees of freedom.

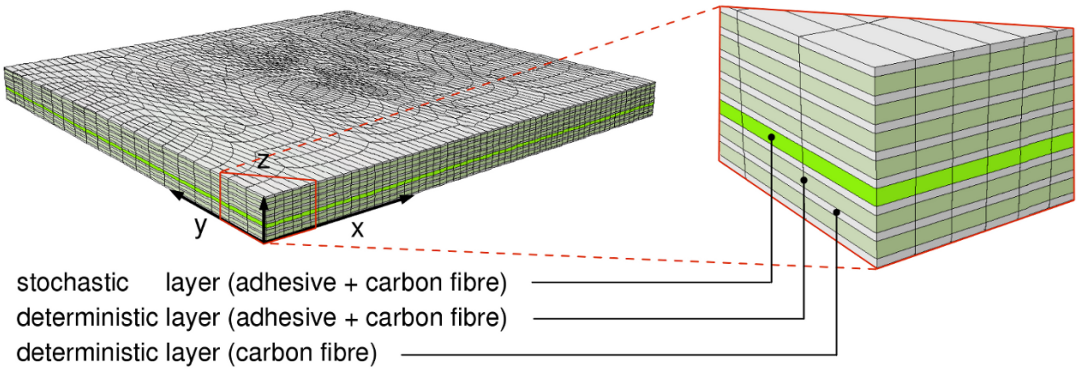

Figure 5: The model of the simulated composite laminate.

The basic VLR-SR1U scheme introduced in [5] is applied to approximate a low-rank representation of the solution in a linear stochastic solution space spanned by 601 polynomials. The number of polyomials indicates the full rank of the solution. The scheme performs successive rank-one updates in a greedy manner, and tries to provide a low-rank approximation which minimises the expectation of the total potential energy in comparison with all other approximations of the same rank. However, the low-rank approximation is usually suboptimal. The VLR-OPT scheme also introduced in [5] can be applied in different ways to optimise a given low-rank approximation.

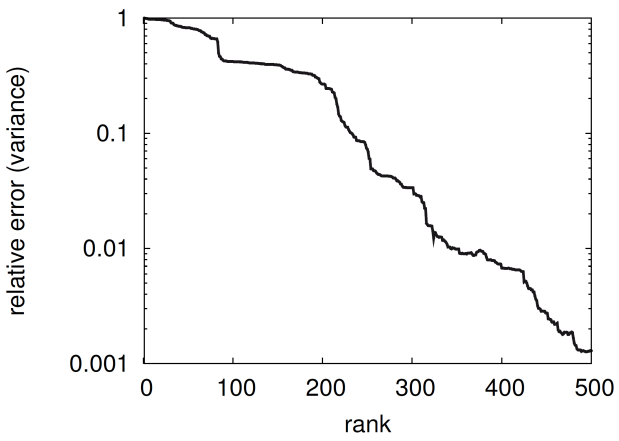

Figure 6: The convergence of the 2-norm of the spatial point variance of the solution computed by the basic VLR-SR1U scheme.

Figure 6 shows the convergence of the successively updated low-rank approximation of the solution of the composite laminate model. The 2-norm of the spatial point variance falls below a relative error of 0.1 not before rank 220 is reached. This rank is more than one-third of the full rank. That indicates a slow convergence. Because the computed low-rank approximations are suboptimal some selected approximations were optimised by the VLR-OPT scheme to get an idea about the accuracy of a suboptimal approximation. It came out that only slight improvements could be gained by an optimisation. As a consequence, one can conclude that an accurate approximation of the solution in the considered solution space requires a comparatively high rank.

2.3.3 Distributed Generic Component-Based Software Approach

The component-based software framework introduced in our publications [3, 4] was used to simulate the composite laminate. A software component is a software unit which is specified by its (component) interface. The framework is distributed because single components may be located and executed on a remote machine. It is generic because the component interfaces contain generic type declarations. Individual application-specific semantics — e.g. the laminate composite — is introduced to the framework not before runtime. At runtime this semantics is brought through a concrete implementation of a specific component, the deterministic simulator component. This component administrates the deterministic model of the individual application. The corresponding component interface represents only general conceptions, no individual ones. All these features have led to a flexible framework which is configurable at runtime.

The mentioned software framework uses the CTL (Component Template Library) [10], an in-house developed library to realise distributed generic software systems. The implementation of the deterministic simulator component used in the context of the composite laminate is the C++ finite element code ParaFEP (Parallel Finite Element Program) [9].

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2.4 Kriging and spatial design accelerated by orders of magnitude: combining low-rank covariance approximations with FFT-techniques

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This is a joint work with Prof. W. Nowak from the University of Stuttgart.
Computational power poses heavy limitations to the achievable problem size for Kriging. In separate research lines, Kriging algorithms based on FFT, the separability of certain covariance functions and low-rank representations of covariance functions have been investigated, all three leading to drastic speedup factors [2]. There we developed new algorithms for large-scale Kriging problems (including the estimation of variance and measures for the optimality of sampling patterns), combining low-rank tensor approximations with existing fast methods based on the FFT. The starting point is the dual formulation of Kriging, not working with any local neighborhoods. The computational complexity is as low as $\mathcal{O}(k_q m d L^* \log L^*)$, where $k_q \geq 1$ is the rank of the tensor product approximation for the covariance function, m is the number of measurement values, d is the physical dimensionality of the problem (e.g., $d = 2, 3, 4$) and $L^* = \max(n_i)$ is the number of points along the single longest edge of the estimation grid with $n = \prod_{i=1}^{d} n_i$ nodes. The presented numerical techniques have memory requirements as low as $\mathcal{O}\left([k_q + m]dL\right)$, where $L = \sum_{i=1}^{d} n_i$ is the total length of the grid edges. The resulting methods outperform previous methods by orders of magnitude, and the speedup and memory efficiency will increase even more with increasing dimensionality of the problem.

For separable (factorized) covariance functions, the results are exact, and non-separable covariance functions can be approximated well through sums of separable components. Only outputting the final estimate as explicit map causes computational costs of $\mathcal{O}(n)$, where n is the number of estimation points. In illustrative numerical test cases, we achieve speedup factors up to 10^8 (eight orders of magnitude), and we can treat problem sizes of up to 15 trillion and two quadrillion estimation points for Kriging and spatial design, respectively, within seconds on a contemporary desktop computer. The fundamental assumptions are second-order stationarity, estimation on a regular equispaced grid, the measurement data must fall onto a subset of the estimation grid, and the covariance function must be either separable, or must be approximated by low-rank tensor product sums.

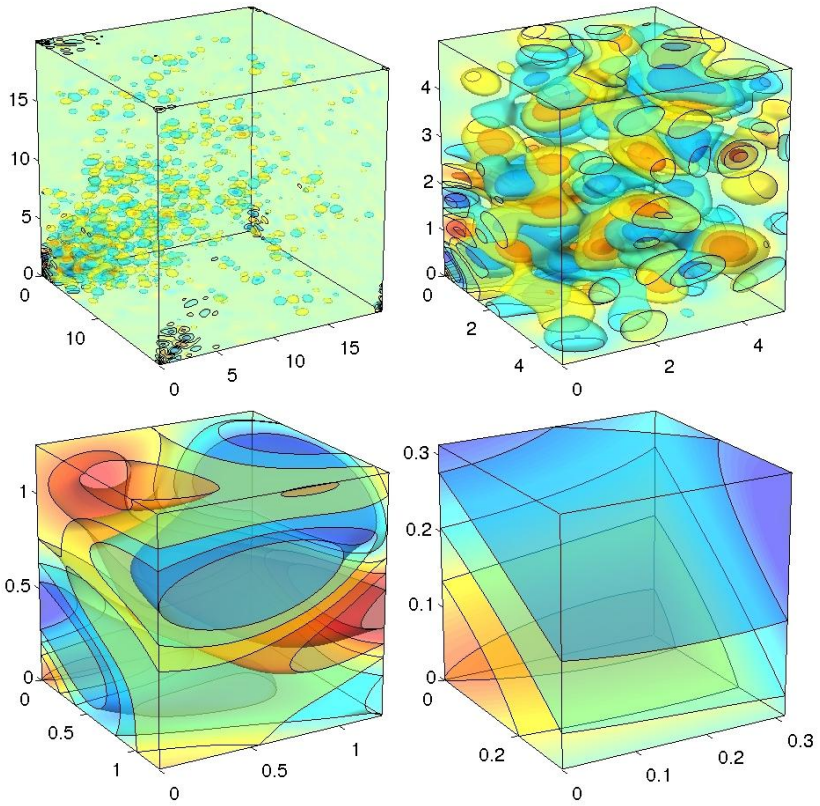

Figure 7: Three-dimensional Kriging results on a grid of $25,000 \times 25,000 \times 25,000$ (totaling approximately 15 trillion) estimation points in a $20m \times 20m \times 20m$ domain. The top left figure shows the entire domain at a sampling rate of 1:64 per direction, and then a series of zooms into the respective lower left back corner with zoom factors (sampling rates) of 4 (1:16), 16 (1:4), 64 (1:1) for the top right, bottom left and bottom right plots, respectively. Color scale: standardized (unit variance), adjusted to show the 95% confidence interval.

We perform FFT/Kronecker Kriging without final evaluation of the Kronecker product. Only in post-processing, we extract the full data-format estimate as demanded by the user. This can be used for interactive visualization, as insinuated in Fig. 7. It shows how a user first looks at the entire volume in coarse resolution (1:64), and then zooms into a small region of special interest in several steps of increasing resolution. The computing time for this example was 18 seconds. The entire field, in explicit form, would require about 120 TeraBytes of memory at double precision (eight Bytes per value). On our test computer, we were able to hold only one sixteenth of the field per dimension in the working memory (15GB) at a time.

Overall, the approaches developed in this work were able to perform on a contemporary computer with 16GB RAM:

- two-dimensional Kriging problems with approximately 270 million estimation points and 100 measurement data values in a quarter of a second,
- to compute the estimation variance for the same problem in less

than one minute,

- to evaluate the spatial average of the estimation variance (the A-criterion of geostatistical optimal design) for about 2 trillion estimation points in less than half a minute,
- to compute a quadratic form with the conditional covariance matrix (the C-criterion of geostatistical optimal design) for more than 2 quadrillion estimation points also in less than half a minute, and
- solve a three-dimensional Kriging problem with 15 trillion estimation points and 4000 measurement data values in less than 20 seconds.

All the above results were obtained with an exact rank-1 representation of the Gaussian covariance function, and computing times will grow linearly with k_q when using rank-k_q approximations for non-separable covariance functions. While the test cases for illustration were set up as two- and three-dimensional, application to more dimensions is straightforward. This includes, among other applications, space-time Kriging. We have also assumed that the measurement data fall onto an irregular grid, but yet coincide with points on the fine regular grid of estimation points. In some practical applications such as space-time Kriging, even the data may fall onto tensor grids, and further speedups will be possible [1]. Also, the simple and repeated FFT-based computations performed within our method are easily accessible to further speedup by exploiting the immensely fast FFT capabilities of graphics cards.

We have assumed that the covariance function is already known. Maximum likelihood covariance parameter estimation involves evaluating the determinant and inverse of covariance matrices. In both matrix operations, the matrix formats used in our work are very helpful, and in the future we may look at corresponding extensions of our work.

This research has been funded by the joint DFG project “Effective approaches and solution techniques for conditioning, robust design and control in the subsurface” (DFG NO 805/3−1 and DFG MA 2236/16−1).

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2.5 Approximation of the stochastic Galerkin matrix in low-rank canonical tensor format

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This is a joint work with group of Prof. W. Hackbusch from the Max-Planck Institute for Mathematics in the Sciences in Leipzig. In this work we describe an efficient approximation of the stochastic Galerkin matrix which stems from a stationary diffusion equation [1, 5]. The uncertain permeability coefficient is assumed to be a log-normal random field with given covariance and mean functions. The approximation is first done in the canonical tensor format, and then compared numerically with the tensor train and hierarchical tensor formats. It will be shown that under additional assumptions the approximation error depends only on the smoothness of the covariance function, and does not depend either on the number of random variables, nor on the degree of the multivariate Hermite polynomials.

The particular problem considered here is formally a stationary diffusion equation described by an uncertain conductivity parameter. Let $D \subset \mathbb{R}^d$ be a compact domain and $(\Omega, \mathcal{A}, \mathbb{P})$ a probability space. The diffusion problem is given by

$$\begin{aligned} -\mathrm{div}(\kappa(\omega,x)\nabla u(\omega,x)) &= f(\omega,x) && \text{for all } x \in \mathring{D} \\ u(\omega,x) &= 0 && \text{for all } x \in \partial D \text{ a.s. in } \omega \in \Omega, \end{aligned} \tag{2}$$

where the conductivity κ and the source term f are random fields over $\Omega \times D$. For the weak formulation of (2) see [2].

In order to solve (2) numerically, one has to perform its full discretisation, in both the deterministic and stochastic spaces. The method of choice is the stochastic Galerkin discretisation, see e.g. [2]. We assume that there exists a Gaussian random field γ such that $\kappa = \exp\gamma$, and $\kappa(\cdot,x) \in L^2(\Omega)$ holds for almost every $x \in D$. The mean function $m_\kappa(x) := \mathbb{E}(\kappa(\cdot,x))$ and the covariance function $\Gamma_\kappa(x,y) := \mathrm{cov}(\kappa(\cdot,x),\kappa(\cdot,y))$ are given as continuous functions.

Let $\mathcal{C}_\kappa$ and $\mathcal{C}_\gamma$ be the integral operators on $L^2(D)$ with kernels Γ_κ and Γ_γ respectively. Since the kernels are continuous and the domain D is compact, these operators are Hilbert-Schmidt operators. Hence there exists an orthonormal basis $\kappa_1, \kappa_2, \ldots \in L^2(D)$ of eigenfunctions and a sequence of associated eigenvalues $\lambda_1 \geq \lambda_2 \geq \ldots \geq 0$ of $\mathcal{C}_\kappa$ such that $\mathcal{C}_\kappa \kappa_l = \lambda_l \kappa_l$ for all $l \in \mathbb{N}$.

Accordingly, let $\gamma_1, \gamma_2, \ldots \in L^2(D)$ denote the orthonormal basis of eigenfunctions and $\lambda'_1 \geq \lambda'_2 \geq \ldots \geq 0$ the corresponding eigenvalues

of $\mathcal{C}_\gamma$. The functions $\theta_k(\omega) = \frac{1}{\lambda'_k}\int_D(\gamma(\omega,x) - m_\gamma(x))\gamma_k(x)dx$ for those $k \in \mathbb{N}$, where $\lambda'_k > 0$ are jointly normally distributed and orthonormal (uncorrelated, here even independent) random variables in $L^2(\Omega)$. Here $m_\gamma(x)$ denotes the mean value of $\gamma(\omega, x)$. We shall write $\boldsymbol{\theta}$ as a short hand for the sequence consisting of these $\theta_1, \theta_2, \ldots$.

Let $(\mathbb{N}_0)_c^{\mathbb{N}} := \{(\alpha_1, \alpha_2, \ldots) \in (\mathbb{N}_0)^{\mathbb{N}} \,|\, \exists K \in \mathbb{N}\ \forall k \geq K\ :\ \alpha_k = 0\}$ be the set of sequences in $\mathbb{N}_0$ with only finitely many nonzero elements. For $\boldsymbol{\iota} \in (\mathbb{N}_0)_c^{\mathbb{N}}$ we set $H_{\boldsymbol{\iota}}(\boldsymbol{x}) = \prod_{k=1}^{\infty} h_{\iota_k}(x_k)$ for $\boldsymbol{x} \in \mathbb{R}^{\mathbb{N}}$, where h_ι denotes the ι-th Hermite polynomial. The random variable $\kappa(\cdot, x) = \exp\gamma(\cdot, x) - m_\kappa(x)$ has the following expansion coefficients

$$\mathbb{E}(\tilde{\kappa}(\cdot,x)\tfrac{1}{\sqrt{\boldsymbol{\iota}!}}H_{\boldsymbol{\iota}}(\boldsymbol{\theta})) = m_\kappa(x)\cdot\prod_{k=1}^{\infty}\frac{\left[\sqrt{\lambda'_k}\gamma_k(x)\right]^{\iota_k}}{\sqrt{\iota_k!}},$$

(see for example [3, p. 71] or [4, p. 16]). At $x \in D$, and in the orthonormal basis $\left\{\frac{1}{\sqrt{\boldsymbol{\iota}!}}H_{\boldsymbol{\iota}}(\boldsymbol{\theta})\otimes\kappa_\ell \,|\, \boldsymbol{\iota} \in (\mathbb{N}_0)_c^{\mathbb{N}}, \ell \in \mathbb{N}\right\}$ it has the Fourier coefficients

$$\begin{aligned}\xi_\ell^{(\boldsymbol{\iota})} &= \frac{1}{\sqrt{\boldsymbol{\iota}!}}\int_D \kappa_\ell(x)\cdot\mathbb{E}(\tilde{\kappa}(\cdot,x)H_{\boldsymbol{\iota}}(\boldsymbol{\theta}))dx = \\ &= \int_D \kappa_\ell(x)\cdot m_\kappa(x)\cdot\prod_{k=1}^{\infty}\frac{\left[\sqrt{\lambda'_k}\gamma_k(x)\right]^{\iota_k}}{\sqrt{\iota_k!}}dx - \int_D \kappa_\ell(x)m_\kappa(x)dx\cdot\delta_{0\boldsymbol{\iota}},\end{aligned} \tag{3}$$

where $\delta_{\boldsymbol{\iota}0} = \delta_{\iota_1 0}\cdot\delta_{\iota_2 0}\cdots$ is the product of the usual Kronecker deltas.

Let $V_N \subseteq H_0^1(D)$ be an N-dimensional subspace with basis $\{\phi_1, \ldots, \phi_N\} \subset V_N$. The subspace in $L^2(\Omega)$ will be chosen accordingly to a given number of stochastic variables $K \in \mathbb{N}$ and the maximal degrees of the multivariate Hermite polynomials $\boldsymbol{p} = (p_1, \ldots, p_K) \in \mathbb{N}^K$. The subset $\mathcal{J}_{\boldsymbol{p}} \subseteq (\mathbb{N})_c^{\mathbb{N}}$ consists of all sequences $\boldsymbol{\alpha} \in (\mathbb{N}_0)_c^{\mathbb{N}}$ such that $0 \leq \alpha_k \leq p_k$ for all $k = 1, \ldots, K$ and $\alpha_k = 0$ for all $k > K$. Let $S_{\mathcal{J}_{\boldsymbol{p}}} \subseteq L^2(\Omega)$ be the subspace spanned by the $\{H_{\boldsymbol{\alpha}}(\boldsymbol{\theta}) \,|\, \boldsymbol{\alpha} \in \mathcal{J}_{\boldsymbol{p}}\}$.

The bilinear form a applied to these basis elements of $S_{\mathcal{J}_{\boldsymbol{p}}}\otimes V_N$ yields (see also [2])

$$\begin{aligned}\mathsf{a}(H_{\boldsymbol{\alpha}}(\boldsymbol{\theta})\otimes\phi_i, H_{\boldsymbol{\beta}}(\boldsymbol{\theta})\otimes\phi_j) &= \int_D m_\kappa(x)\nabla\phi_i(x)\cdot\nabla\phi_j(x)dx\cdot\delta_{\boldsymbol{\alpha}\boldsymbol{\beta}} \\ &+ \sum_{\ell=1}^{\infty}\sum_{\boldsymbol{\iota}\in(\mathbb{N})_c^{\mathbb{N}}}\xi_\ell^{(\boldsymbol{\iota})}\cdot\mathbb{E}(H_{\boldsymbol{\iota}}(\boldsymbol{\theta})H_{\boldsymbol{\alpha}}(\boldsymbol{\theta})H_{\boldsymbol{\beta}}(\boldsymbol{\theta}))\cdot\int_D\kappa_\ell(x)\nabla\phi_i(x)\cdot\nabla\phi_j(x)dx \\ &= (\boldsymbol{K}_0)_{ij}\cdot(\boldsymbol{\Delta_0})_{\boldsymbol{\alpha}\boldsymbol{\beta}} + \sum_{\ell=1}^{\infty}(\boldsymbol{K}_\ell)_{ij}\sum_{\boldsymbol{\iota}\in(\mathbb{N}_0)_c^{\mathbb{N}}}\xi_\ell^{(\boldsymbol{\iota})}\cdot(\boldsymbol{\Delta}_{\boldsymbol{\iota}})_{\boldsymbol{\alpha}\boldsymbol{\beta}},\end{aligned}$$

wherein $(\boldsymbol{\Delta}_{\boldsymbol{\iota}})_{\boldsymbol{\alpha}\boldsymbol{\beta}} = \mathbb{E}(H_{\boldsymbol{\iota}}(\theta)H_{\boldsymbol{\alpha}}(\theta)H_{\boldsymbol{\beta}}(\theta)) = \prod_{k=1}^{\infty}\mathbb{E}(h_{\iota_k}(\theta_k)h_{\alpha_k}(\theta_k)h_{\beta_k}(\theta_k))$, $(\boldsymbol{K}_\ell)_{ij} = \int_D\kappa_\ell(x)\nabla\phi_i(x)\cdot\nabla\phi_j(x)dx$, $\kappa_0(x) := m_\kappa(x)$.

By definition of $(\boldsymbol{\Delta}_{\boldsymbol{\iota}})_{\boldsymbol{\alpha\beta}}$ we have $\boldsymbol{\Delta}_{\boldsymbol{\iota}} = \bigotimes_{k=1}^{K} \boldsymbol{\Delta}_{\iota_k}$ and thus, finally, the stiffness matrix $\mathbf{K}$ can be written as

$$\mathbf{K} = \boldsymbol{\Delta}_{\mathbf{0}} \otimes \boldsymbol{K}_0 + \sum_{\ell=1}^{\infty} \sum_{\boldsymbol{\iota} \in \mathcal{J}_{2\boldsymbol{p}}} \xi_{\ell}^{(\boldsymbol{\iota})} \cdot \left(\bigotimes_{k=1}^{K} \boldsymbol{\Delta}_{\iota_k} \right) \otimes \boldsymbol{K}_{\ell} \in \mathcal{T} := \left(\bigotimes_{k=1}^{K} \mathbb{R}^{p_k \times p_k} \right) \otimes \mathbb{R}^{N \times N}. \tag{4}$$

As a further step of discretisation we truncate the series in ℓ in (4) to $M \in \mathbb{N}$ terms. The error measured in the Frobenius norm is bounded by some constant times $\sum_{\ell=M+1}^{\infty} \lambda_{\ell}$, which tends to zero for $M \to \infty$. In the following we shall simply write $\mathbf{K}$ for the truncated series and $\boldsymbol{\xi}$ for the tensor consisting of all coefficients $\xi_{\ell}^{(\boldsymbol{\iota})}$, where $\boldsymbol{\xi} \in \left(\bigotimes_{k=1}^{K} \mathbb{R}^{p_k} \right) \otimes \mathbb{R}^{M}$.

The number of entries in the stiffness matrix $\mathbf{K}$ depends exponentially on the number K of random variables $\theta_1, \ldots, \theta_K$ used for the stochastic Galerkin discretisation. However, in order to minimise the error of this discretisation it is important to choose the finite dimensional space $S_{\mathcal{J}_{\boldsymbol{p}}} \otimes V_N \subseteq L^2(\Omega) \otimes H_0^1(D)$ as large as possible.

The main purpose of this article is to approximate the coefficients tensor $\boldsymbol{\xi}$ in (4) by a tensor $\boldsymbol{\eta} \in \left(\bigotimes_{k=1}^{K} \mathbb{R}^{p_k} \right) \otimes \mathbb{R}^{M}$ represented in the canonical tensor format. If $\boldsymbol{\eta}$ is given by $\eta_{\ell}^{(\boldsymbol{\iota})} = \sum_{j=1}^{R} \prod_{k=1}^{K} (\eta_{jk})_{\iota_k} \cdot (\eta_j)_{\ell}$, we have

$$\begin{aligned} \hat{\mathbf{K}} &= \boldsymbol{\Delta}_0 \otimes \boldsymbol{K}_0 + \sum_{\ell=1}^{M} \sum_{\boldsymbol{\iota} \in \mathcal{J}_{2\boldsymbol{p}}} \left[\sum_{j=1}^{R} \prod_{k=1}^{K} (\eta_{jk})_{\iota_k} (\eta_j)_{\ell} \right] \left(\bigotimes_{k=1}^{K} \boldsymbol{\Delta}_{\iota_k} \right) \otimes \boldsymbol{K}_{\ell} \\ &= \boldsymbol{\Delta}_0 \otimes \boldsymbol{K}_0 + \sum_{j=1}^{R} \left(\bigotimes_{k=1}^{K} \left[\sum_{\iota_k=0}^{2p_k} (\eta_{jk})_{\iota_k} \boldsymbol{\Delta}_{\iota_k} \right] \right) \otimes \left[\sum_{\ell=1}^{M} (\eta_j)_{\ell} \boldsymbol{K}_{\ell} \right]. \end{aligned}$$

Obviously, the representation of $\boldsymbol{\eta}$ in the canonical tensor format leads us to a representation of $\hat{\mathbf{K}}$ in the canonical tensor format in $\left(\bigotimes_{k=1}^{K} \mathbb{R}^{p_k \times p_k} \right) \otimes \mathbb{R}^{N \times N}$, whose rank is bounded by the representation rank R of $\boldsymbol{\eta}$.

The main advantage of the canonical tensor representation is the linear scaling in K of further numerical operations like matrix-vector multiplication, computation of the maximum (minimum) value and level-sets of the tensor, see e.g. [2] for more details. Since one is usually interested in a solution u of (2) it is important to estimate the error between the exact solution u and the solution $\hat{u}$ which stems from (2) if we replace the conductivity Fourier coefficient tensor $\boldsymbol{\xi}$ by $\boldsymbol{\eta}$.

2.5.1 Low rank approximation of $\boldsymbol{\xi}$

The most obvious way to approximate the coefficient tensor $\boldsymbol{\xi}$ from (3) is to apply a quadrature rule to the integral. Since the integrand of $\boldsymbol{\xi}$ already separates we immediately obtain an approximation of $\boldsymbol{\xi}$ in the canonical tensor format. Theorem 3.1 from [1] reveals that the error

introduced by this approximation does not depend on the number of random variables K nor on the maximal degrees of the multivariate Hermite polynomials $\boldsymbol{p}$. Nevertheless it depends on the analytical properties of the covariance function Γ_κ and the eigenvalues of the covariance operator $\mathcal{C}_\kappa$ and the quality of the used quadrature and its error estimation [1]. For numerical results see also [1].

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2.6 Hierarchical Ordering of Simulation Interfaces by Inheritance

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The Component Template Library (CTL) is a C++ template library, which uses template meta-programming to hide as much as possible technical details from the programmer. It has been successfully applied in computational applications like multi-physics simulation [1, 2, 7, 10, 9], multi-scale simulation [8, 5], stochastic finite element analysis [4, 3] and optimisation [6].
Since version 1.3 the CTL allows an interface to extend other interfaces. This enables one to organise the different facilities of different simulation codes in a hierarchy of interfaces. If a code implements an interface it automatically implements all interfaces directly or indirectly extended. Therefore this ordering can be used to optimise the interchangeability of simulation codes, e.g. in multi-physical simulation.

Example: Dirichlet-Neumann coupling Any useful simulation code should at least implement an interface stationarySimulationCI like:

```
interface stationarySimulationCI
{
 stationarySimulationCI (const string /*input-file*/);
 void solve();
 void get_state(array<real8>/*state*/) const;
};
```

Using (for a stationary problem) Gauss-Seidel- or Jacobi-type solution schemes each Neumann controlled part of a coupled simulation needs at least to implement the interface:

```
interface stationaryNeumannCI: extends stationarySimulationCI
{
 void set_load(const array<real8> /*load*/);
};
```

In this case the part controlled by Dirichlet-conditions needs at least to implement an interface stationaryDirichletCI like:

```
interface stationaryDirichletCI: extends stationarySimulationCI
{
 void set_state(const array<real8> /*state*/);
};
```

An instationary coupling solved by a Gauss-Seidel- or Jacobi-type scheme will be supported now by defining and implementing the interfaces:

```
interface simulationCI: extends stationarySimulationCI
{
 void time_step(const real8 /*delta_t*/);
};
interface NeumannCI: extends stationaryNeumannCI,
                     extends simulationCI
{};
interface DirichletCI: extends stationaryDirichletCI,
                       extends simulationCI
{};
```

This simple example shows the advantage. Not only some lines of code in the definitions of the interfaces for non-stationary simulations are saved. More important is that the components implementing the non-stationary case can also be used in the stationary case, i.e. the mechanism of inheritance is transmitted to software-components.
Particularly with regard to multi-physics and multi-scale simulations with a growing number of codes incorporated, the hierarchical ordering of simulation codes, defined by inheritance of the interfaces they implement, becomes interesting because this ordering defines exactly the interchangeability of codes given by the functionality they offer.

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2.7 A Polynomial-Chaos-based Square-Root-Filter for non-Gaussian Bayesian Estimation

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The problem of updating the knowledge of an uncertain quantity in a sequential way from noisy and incomplete data is considered. This is a so-called inverse problem of identification. The goal is to regularise the ill-posed inverse problem by a Bayesian method, which uses a priori knowledge as additional information to the given set of data. For an introduction into the topic, e.g. see [16].

Well established methods for computing Bayesian estimates can be coarsely grouped into two classes: so-called "Bayes linear" [5] methods, which update functionals of the random variables (the simplest of which are the Kalman-type methods), and updates based on Bayes's formula itself. The latter ones are usually implemented as sequential Monte Carlo (SMC) methods—also called particle filters (e.g. [6])—or Markov chain Monte Carlo methods (MCMC) (e.g. [7]). However, due to the large number of samples required to obtain satisfying results they are computationally quite demanding and hence not very practical. Methods like the Gaussian sum filter [1] are trying to approximate Bayes's formula. But they, too, tend to have a quite large computational overhead [8].

On the other hand, methods like the extended Kalman filter run into closure problems for non-linear models [3]. Additionally, they are not suitable for high dimensions. Approaching these two problems, the class of Monte Carlo based Kalman-type filters has become quite popular over the last years. The fact that for constant variance the asymptotic rate of convergence of Monte Carlo methods does not depend on the dimension of the sampled space makes these methods applicable to very high dimensional problems, which appear for example in weather forecasting, oceanography, and geophysics. Additionally, these methods naturally allow for non-linear forward models and thus avoid the possibly severe truncation errors coming from linearisation, as they appear for example in the extended Kalman filter. Specific implementations of this kind of filter are based on the Potter filter [15], a numerically superior implementation of the original Kalman filter.

The main idea of this work [13] is to perform a Bayesian update without sampling, but in a direct, purely algebraic way by employing a polynomial chaos expansion (PCE) representation of the involved random variables. The specific implementation is similar to ensemble square root filters [4]; its main advantage over previous work [12] is that the

PCE-basis does not need to be extended with additional random variables. Here we use Wiener's polynomial chaos, but any other orthonormal basis would do. The method has been developed as a sequel of ideas presented in [11, 9]. A similar idea has independently appeared in a simpler form in [2] in another context, where it is developed as a combination of polynomial chaos and extended Kalman filter theory. Related approaches include [14] who combine polynomial chaos theory with maximum likelihood estimation. There, the resulting optimisation problem is solved by gradient descent or a random search algorithm. [10] use generalised PCE methods for the forward problem and combine it with a sampling-based ensemble square root filter to efficiently obtain sequentially updated PCE coefficiensts. In contrast, we propose a method which does not need any sampling. It is a minimum variance estimator entirely based on white noise analysis or PCE as introduced by [17]. This kind of estimator is obtained by a simple orthogonal projection of an abstract estimation formula onto a polynomial chaos basis. In the special case when the problem is linear and employs Gaussian random variables the method reduces to the Kalman filter, and in fact the Kalman filter relations are the low-order part of the method. The proposed method, which is an alternative way of computing a linear Bayesian estimator, allows for updates of non-Gaussian quantities (e.g. state vectors), and also for non-Gaussian measurement noise.

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2.8 Galerkin methods for the stochastic Navier-Stokes equations

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In this project the incompressible Navier–Stokes equations are considered with uncertainties, i. e. we assume that the Reynolds number, the boundary conditions and the right-hand side are not known exactly. The numerical solution is determined with stochastic Galerkin methods and a low-rank approximation. Therefore not only the input and the output quantities are represented. The aim of this project is to used this data format in the whole computing process.

Starting point of our considerations are time dependent incompressible Navier–Stokes equations which are given in dimensionaless form by

$$\begin{aligned} \dot{u} - \tfrac{1}{Re}\Delta u + (u\cdot\nabla)u + \nabla p &= f(t,x_1,x_2,x_3,\omega) && \text{in } [0,T]\times\mathcal{G}, \\ \nabla\cdot u &= 0 && \text{in } [0,T]\times\mathcal{G}. \end{aligned} \tag{5}$$

Here, $x = (x_1,x_2,x_3)^\top \in \mathcal{G} \subseteq \mathbb{R}^3$, and ω is an elementary event of a realisation in a random space $(\Omega,\mathcal{A},\mathbb{P})$ of random events. Moreover we need boundary and initial conditions for obtaining a unique solution of (5). Uncertain my the right-hand side $f(t,x,\omega)$, the coefficients or the boundary conditions.

The stochastic solution $u(t,x,\omega)$ can be represented with the help of the isomorphies $L_2([0,T]\times\mathcal{G}\times\Omega) = L_2([0,T]\times\mathcal{G})\otimes L_2(\Omega)$ and $(\Omega,\mathcal{A},\mathbb{P}) = \Pi_{j=1}^{\infty}(\Omega_j,\mathcal{A}_j,\mathbb{P})$. For the numerical approximation we need only finitely many random spaces $(\Omega_j,\mathcal{A}_j,\mathbb{P})$. For the representation of the solution not only the separation of deterministic and stochastic part are used. Moreover the solution is considered in a low-rank approximation where a further separation of the stochastic parts with the isomorphie

$$L_2\left([0,T]\times\mathcal{G}\times\prod_{j=1}^{M}\Omega_j\right) = L_2([0,T]\times\mathcal{G})\otimes\left(\bigotimes_{j=1}^{M}L_2(\Omega_j,\mathcal{A}_j,\mathbb{P})\right)$$

is used. A discretisation in the deterministic and in stochastic domain with Finite Elements or Volumes and a stochastic Bubnov-Galerkin method least to a differential algebraic equation of the form

$$M\dot{\mathbf{v}} + N(\mathbf{v},\mathbf{v}) + K\mathbf{v} + B\mathbf{p} = \mathbf{g}, \text{ und } B^T\mathbf{v} = 0.$$

The bilinear operator $N(\cdot,\cdot)$ is obtained from the nonlinear convection, K is the matrix which belongs to the diffusive part, and B is the discretised gradient. Moreover $\mathbf{v}$ and $\mathbf{p}$ are vectors for the discrete velocity

v and for the discrete pressure p. If these terms are expanded in a PCE, i. e. with

$$\begin{aligned}\mathbf{v}(\theta(\omega)) &= \sum_{\alpha\in\mathcal{J}_M} \mathbf{v}^{(\alpha)} H_\alpha(\theta(\omega)), \quad \mathbf{p}(\theta(\omega)) = \sum_{\beta\in\mathcal{J}_M} \mathbf{p}^{(\beta)} H_\beta(\theta(\omega)),\\ \mathbf{g}(\theta(\omega)) &= \sum_{\gamma\in\mathcal{J}_M} \mathbf{g}^{(\gamma)} H_\gamma(\theta(\omega)),\end{aligned}$$

we obtain an explicite PCE representation of the nonlinear instationary incompressible Navier–Stokes equations, which can be written as

$$\begin{aligned} M\dot{\mathbf{v}} + N(\mathbf{v},\mathbf{v}) + (I\otimes K)\mathbf{v} + (I\otimes B)\mathbf{p} &= \mathbf{g},\\ \text{und } (I\otimes B^T)\mathbf{v} &= 0.\end{aligned}$$

This is a pure deterministic DAE of high dimension. Therefore the stochastic quantities are representation in a low-rank representation.

2.9 An analysis of the Prothero-Robinson example for constructing new DIRK and ROW methods

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2.9.1 Introduction

One possibility to solve stiff ODEs like the example of Prothero and Robinson [3] or differential algebraic equations are Runge-Kutta methods [1, 6]. The theoretical convergence order may not be achieved [1, 6], in this case, i. e. the so-called order reduction phenomenom can be observed. In the last years a lot of papers are published considering this phenomenom [5].

In this project the example of Prothero and Robinson is applied on diagonally implicit Runge–Kutta methods (DIRK methods) and on Rosenbrock–Wanner methods (ROW methods) since the local error is analysed. It can be shown that a DIRK or ROW method should satisfy some further order conditions to reduce the order reduction.

2.9.2 New order conditions

Consider an ODE of the form $\dot{\mathbf{u}} = \mathbf{F}(t, \mathbf{u})$ with the initial condition $\mathbf{u}(0) = \mathbf{u}_0$. A Rosenbrock–Wanner–method (ROW–method) with s internal stages is given by the formulas

$$\mathbf{k}_i = \mathbf{F}\left(t_m + \alpha_i \tau_m, \tilde{\mathbf{U}}_i\right) + \tau_m J \sum_{j=1}^{i} \gamma_{ij} \mathbf{k}_j + \tau_m \gamma_i \dot{\mathbf{F}}(t_m, \mathbf{u}_m), \tag{6}$$

$$\tilde{\mathbf{U}}_i = \mathbf{u}_m + \tau_m \sum_{j=1}^{i-1} a_{ij} \mathbf{k}_j, \quad i = 1, \ldots, s,$$

$$\mathbf{u}_{m+1} = \mathbf{u}_m + \tau_m \sum_{i=1}^{s} b_i \mathbf{k}_i, \tag{7}$$

where $J := \partial_{\mathbf{u}} \mathbf{F}(t_m, \mathbf{u}_m)$, α_{ij}, γ_{ij}, b_i are the parameters of the method,

$$\alpha_i := \sum_{j=1}^{i-1} \alpha_{ij}, \quad \gamma_i := \sum_{j=1}^{i-1} \gamma_{ij}, \quad \gamma := \gamma_{ii} > 0, \ i = 1, \ldots, s.$$

If we apply the ROW method on the example of Prothero and Robinson and use a Taylor expansion we get a representation of the local error

$$\begin{aligned}\delta_\tau(t_{m+1}) = &\sum_{k=2}^{p-1}\left[\mathbf{b}^\top B^{-1}\alpha^k - 1\right]\varphi_m^{(k)}\frac{\tau^k}{k!} + \mathcal{O}(\tau^{p+1}) \\ &+ \sum_{k=2}^{p+1}\mathbf{b}^\top\sum_{l=1}^{k-2}\left\{B^{-l-1}\left[\alpha^{k-l} + \gamma\delta_{k-l,1}\right]\frac{1}{(k-l)}\right. \\ &\left. - B^{-l}\left[\alpha^{k-l-1} + \gamma\delta_{k-l-1,1}\right]\right\}\cdot\varphi_m^{(k-l)}\frac{\tau^{k-l}}{(k-l-1)!z^l},\end{aligned}$$

where $B = (\beta_{ij})_{i,j=1}^s$, $\mathbf{b} = (b_1,\ldots,b_s)^\top$, $\alpha = (\alpha_1,\ldots,\alpha_s)^\top$, and $\gamma = (\gamma_1,\ldots,\gamma_s)^\top$. Finally we get the new order conditions

$$\mathbf{b}^\top B^{-1}\alpha^k = 1, \quad k = 2,\ldots,p, \tag{8}$$

$$\mathbf{b}^\top B^{-(l+1)}\frac{1}{k-l}\alpha^{k-l} = \mathbf{b}^\top B^{-l}\left[\alpha^{k-l-1} + \gamma\delta_{k-l-1,1}\right], \tag{9}$$

for $l = 1,\ldots,k-2$ and $k = 1,\ldots,p+1$. Note, that order conditions derived by Lubich and Ostermann in [2] are special cases of our new order conditions.

A similar calculation can be done for the DIRK–methods. In this case we obtain

$$\mathbf{b}^\top A^{-1}\mathbf{c}^k = 1, \quad k = 2,\ldots,p, \tag{10}$$

$$\mathbf{b}^\top A^{-(l+1)}\frac{1}{k-l}\mathbf{c}^{k-l} = \mathbf{b}^\top A^{-l}\mathbf{c}^{k-l-1}, \quad l = 1,\ldots,k-2, k = 1,\ldots,p+1. \tag{11}$$

Conditions (8) and (10) are automatically satisfied if the method is stiffly accurate. New second order methods satisfying these conditions can be found in [5]. In [4] a new third order method is derived.

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2.10 A stiffly accurate Rosenbrock-type method of order 2 applied to FE-analyses in finite strain viscoelasticity

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Since the works of [9] and [2] implicit finite elements based on material models defined by ordinary differential equations (ODEs) have been interpreted as a solution procedure using the method of vertical lines. The local equilibrium conditions (partial differential equations of elliptic type) are transferred into a weak form, which is solved using the finite element method. This is the spatial discretization step leading to a system of non-linear equations having the unknown nodal displacements as one set of unknowns. Additionally, the resulting equations depend on so-called internal variables. These variables have to be evaluated at the spatial quadrature points (commonly, these are Gauss-points), which are defined by ODEs or by differential-algebraic equations (DAEs) on Gauss-point level themselves. The evolution equations of the internal variables describe the hardening behavior of the material under consideration. These evolution equations depend on the internal variables and on the nodal displacements, so that a large coupled system of differential-algebraic equations results.

It is well-known that DAEs should be solved with implicit or linearly implicit time integration schemes, because if explicit methods are used, a stable numerical solution can only be obtained if the time step-size is sufficiently small [7, 3]. Implicit Runge–Kutta methods or Rosenbrock–Wanner methods (ROW-methods) seem to be a good choice to solve DAEs [7, 3]. It is well-known that Rosenbrock-type methods may exhibit order reduction if they are applied to large ODE systems resulting, e.g., from the semi-discretization in space of parabolic problems. Rosenbrock methods can decrease this order reduction if some additional conditions are fulfilled [6]. Moreover, many Rosenbrock solvers need the Jacobian and the time derivative of the right-hand side in each time-step. In [5], Lang compares Rosenbrock methods for several problems (PDEs, PDAEs of index 1 and of index 2), but all methods need an exact approximation of the Jacobian. The only exception is the order 2 method ROS2 from [8]. In this paper we propose a second order, stiffly accurate Rosenbrock method with 3 internal stages which need only an approximation of the Jacobian and the time derivative in the method, i. e. the time derivative of the right-hand side of the problem can be neglected. Unfortunately, W-methods using an approximation of the Jacobian have some disadvantages (see [5]), but if such methods are applied as usual,

i.e. the Jacobian is evaluated exactly, they are able to approximate the numerical solution very well (see [8]).

In particular, the new method is an attractive candidate for the numerical solution of the large ODE systems mentioned above. The numerical comparisons presented at the end of the paper illustrate the good qualities of the methods in both academic and more practical problems.

In this project the time discretization is realised by ROW-methods. The new method should be a seond order stiffly accurate ROW method which is stiffly accurate and is a so called W-method, i. e. the Jacobian need not be computed exactly. Such a method needs at least three internal stages. Therefore we have to take care about the order reduction. To reduce the order reduction we method should satisfied the order conditions given by Lubich and Ostermann [6]. A method satisfying all these condition is the method ROS2S (see Table 2) which is introduced in [4] This chemical reaction problem is called E5 and can be found in the

Table 2: Set of coefficients for ROS2S

γ	=	$2.9289321881345248e-01$			
α_{21}	=	$5.8578643762690495e-01$	γ_{21}	=	$-5.8578643762690495e-01$
α_{31}	=	$0.0000000000000000e+00$	γ_{31}	=	$3.5355339059327376e-01$
α_{32}	=	$1.0000000000000000e+00$	γ_{32}	=	$-6.4644660940672624e-01$
b_1	=	$3.5355339059327376e-01$	$\hat{b}_1$	=	$3.3333333333333333e-01$
b_2	=	$3.5355339059327376e-01$	$\hat{b}_2$	=	$3.3333333333333333e-01$
b_3	=	$2.9289321881345248e-01$	$\hat{b}_3$	=	$3.3333333333333333e-01$

collection by Enright, Hull, and Lindberg [1]. The equations are given by

$$\begin{aligned}
\dot{u}_1 &= -Au_1 - Bu_1u_3,\\
\dot{u}_2 &= Au_1 - MCu_2u_3,\\
\dot{u}_3 &= Au_1 - Bu_1u_3 - MCu_2u_3 + Cu_4,\\
\dot{u}_4 &= Bu_1u_3 - Cu_4
\end{aligned}$$

with the initial conditions $u_1(0) = 1,76 \times 10^{-3}$ and $u_i(0) = 0$, $i \in \{2,3,4\}$. Moreover we set as in [3] $A = 7,89 \times 10^{-10}$, $B = 1,1 \times 10^7$, $C = 1,13 \times 10^3$, and $M = 10^6$. The equations should be solved in the time interval $[0, 10^{13}]$. Note that the variables u_2, u_3, and u_4 satisfy the equation $u_2 - u_3 - u_4 = 0$. We compare only the methods ROS2, ROS2S, and ELLSIEPEN since the other methods (LIE, BE, and Scholz 4-5) have no embedded method. It can be observed from Figure 8 that ROS2S and ELLSIEPEN are more effective than ROS2. For further numerical results we refer to [4].

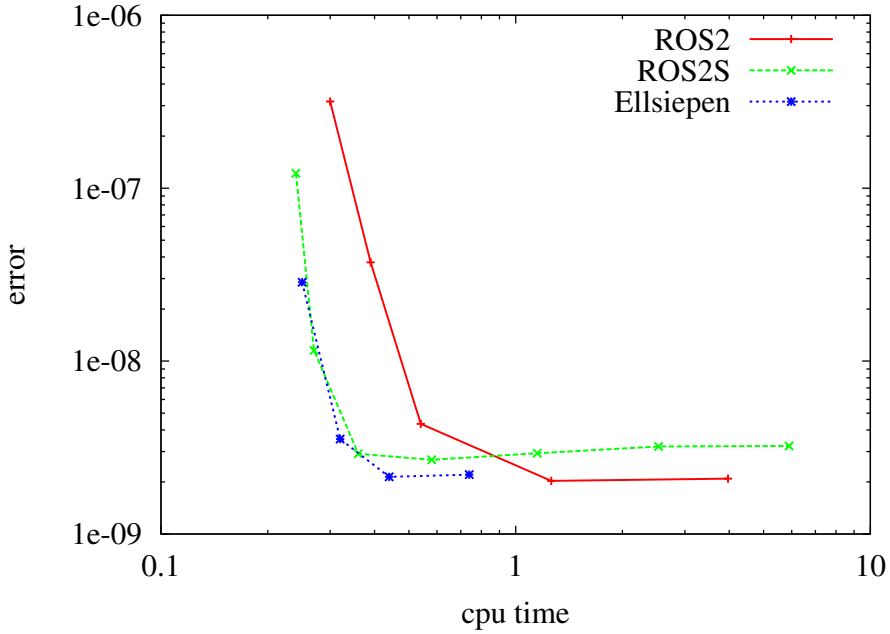

Figure 8: The solution of the problem E5

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2.11 Stochastic elastoplasticity

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Due to their widespread applications in industry, the descriptions of nonlinear elastic and elastoplastic phenomena have found an important place in the field of computational mechanics. Presently existing models rely on the assumption of complete knowledge of the system, i.e. one assumes that the material characteristics as well as the external loadings applied on the structure are entirely known. However, uncertainty is widely present, from the mathematical model which cannot perfectly match the data to the poorly known external loadings. Including both structural and parametric uncertainties into the model, this section provides an extended formulation of nonlinear phenomena in which existing uncertainties are modelled in a probabilistic manner.

The elastoplastic behaviour is described by a stochastic variational inequality due to presence of non-smooth evolution of internal variables. Basically, after the mathematical derivation as given in [3] the problem boils down to the equilibrium equation

$$A(\boldsymbol{u}(t)) + \boldsymbol{u}^*(t) = \boldsymbol{f}(t) \quad \text{a.s.} \tag{12}$$

and the flow rule

$$\forall \boldsymbol{z}^* \in \mathcal{K} : \ \langle\langle \dot{\boldsymbol{u}}(t), \boldsymbol{z}^* - \boldsymbol{u}^*(t) \rangle\rangle \leq 0 \quad \text{a.s.} \tag{13}$$

which states that the rate of change $\dot{\boldsymbol{u}}$ is in the normal cone of $\mathcal{K}$ at $\boldsymbol{u}^*$. Here, some of parameters such as the constitutive tensor (operator A), external loadings $\boldsymbol{f}$, the convex domain of admissible stresses $\mathcal{K}$ etc. are assumed to be uncertain. This results in an uncertain state variable $\boldsymbol{u} = (\boldsymbol{v}, \boldsymbol{\epsilon}_p, \boldsymbol{\nu})$ consisting of the displacement $\boldsymbol{v}$, the plastic strain $\boldsymbol{\epsilon}_p$ and the vector of internal variables $\boldsymbol{\nu}$.

After the time (backward Euler) and spatial (finite element) discretisations, the process of solving previously described problem consists of two phases: the global and local one, see Fig. 10. The global phase solves the equilibrium Eq. 12 for the unknown increment of displacement $\boldsymbol{v}(\omega)$. Taking the polynomial chaos expansion [7, 8] for the ansatz of $\boldsymbol{v}$, the solution is computed by a stochastic Galerkin projection of the nonlinear residual equation onto the finite stochastic subspace [3, 4, 1]. For this purpose are used the stochastic Newton-like algorithms which evaluate the correction of the displacement increment in each iteration by solving the corresponding system of stochastic linear equations with the help of the preconditioned Krylov subspace methods [6, 2]. Once

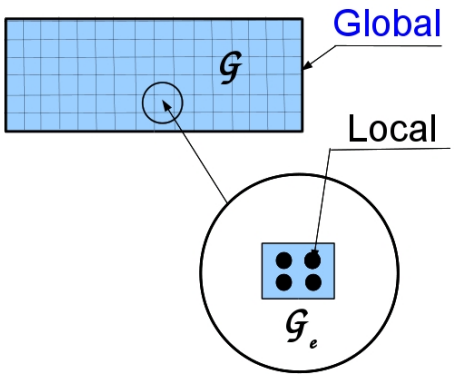


Figure 9: Schematic representation of the global and local phase of numerical algorithm used to integrate the evolution provlem

the solution is found, the displacement, the elastic strain and hence the global configuration are updated.

On the other side, the local phase of the algorithm solves the convex optimization problem coming from Eq. 13 in each integration point of the finite element mesh. The unique minimiser is found via the stochastic closest point projection algorithm, i.e. the new numerical scheme obtained by a generalisation of the very well known deterministic counterpart [5]. The procedure consists of non-dissipative (reversible) and dissipative (irreversible) steps, also called elastic predictor and plastic corrector. The non-dissipative step defines the trial state, while actual projection happens in the corrector step if certain conditions are fulfilled. More precisely, if the stress lies outside of the elastic domain the dissipative step searches for the closest distance in the energy norm of a trial state to a convex set of elastic domain and projects the stress back to the yield surface.

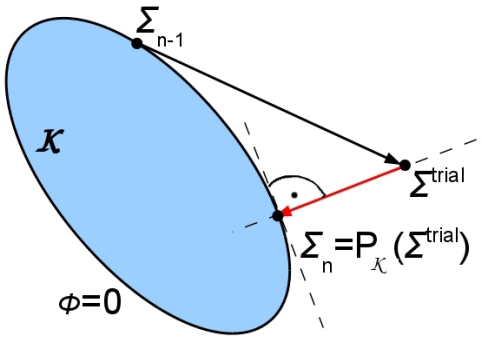
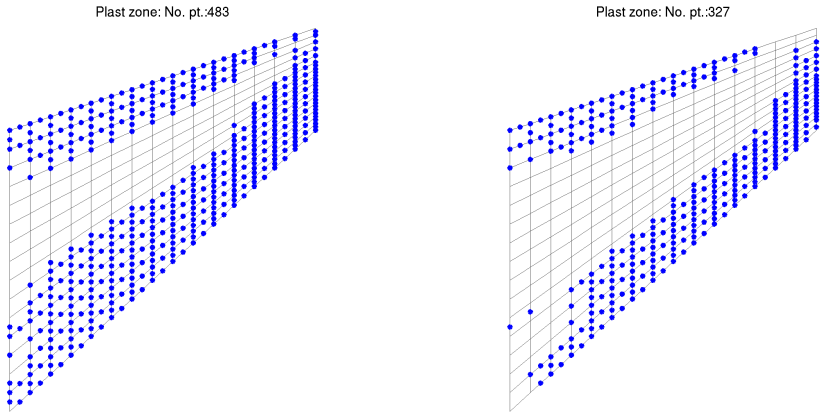


Figure 10: Schematic representation of the stochastic closest point projection algorithm

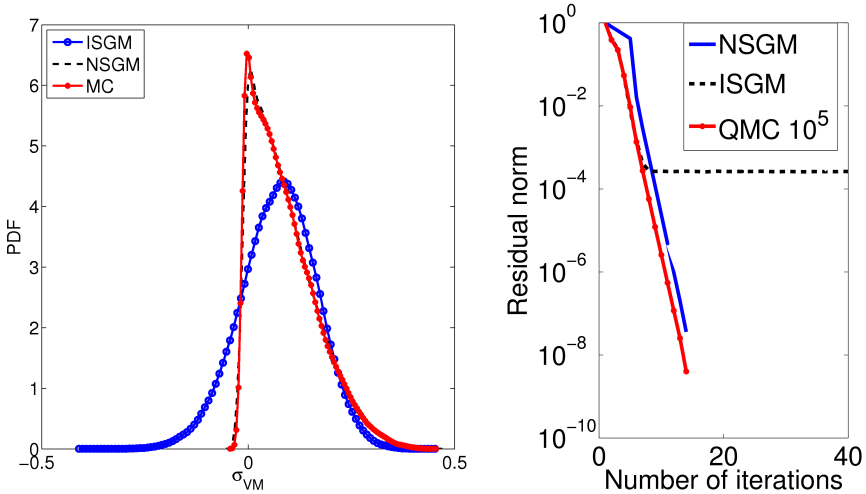
The numerical implementation of the closest point projection is realised in the non-intrusive and intrusive way. The first approach computes the projection with the help of the numerical integration, while the second is purely algebraic approach whose implementation requires significant changes of the deterministic software (i.e. simulator). Hence, the name “intrusive” method.



a) p_{75} b) p_{99}

Figure 11: The plastyfing zone with a) 75% and b) 99% probability

The intrusive stochastic closest point projection employs the property of the smoothness of the integrand and computes the projection with the help of the polynomial chaos algebra. The major issue of such an computation lies in the approximation of the convex set whose definition involves random inequalities. This further means that the decision regarding the elastic or plastic state has to be made with respect to some weaker criterion than the almost sure one. For example, in Fig. 11 one may see how the plasticity region changes with the increase of the probability level in decision criteria.



a) b)

Figure 12: The comparison of the non-intrusive (NSGM) and intrusive (ISGM) methods to the Monte Carlo solution with 10^6 samples: a) probability density function of plastic strain b) residual convergence

In comparison to the intrusive the non-intrusive approach gives more accurate approximation of the result. This conclusion is made with respect to the reference solution obtained by Monte Carlo simulation with 10^6 samples, see Fig. 12 a). For the same polynomial order the

intrusive approach delivers bigger error due to the accumulation of the local errors in polynomial chaos algebra operations. This causes the stagnation of the residual convergence in comparison to the non-intrusive approach as shown in Fig. 12 b).

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2.12 Uncertainty Updating in the Description of Heterogeneous Materials

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The investigation of the uncertainty updating methods is done in the framework of two projects QUANTIMAT (Deutsche Forschungsgemeinschaft project) and BEWUF (Deutscher Akademischer Austauschdienst travel project), both realised in cooperation with the Technical University in Prague. These projects are focusing on the uncertainty quantification and updating in the description of heat and moisture transport in heterogeneous materials. The goal is to develop a fast and reliable Bayesian updating procedure for the transport properties of building materials, such as masonry.

Durability of buildings is significantly influenced by damage processes driven by moisture. Structural degradation and extensive damage are just some of examples the high moisture levels, thermal expansion and contraction may cause. With this respect the proper modelling of heterogeneous building materials is of high practical importance. In order to describe material one may try to measure its characteristics. However, material properties very often cannot be directly measured, but determined from noisy experimental measurements of the system response. This process is known as identification or inverse problem. The identification of material properties can be approached in different ways, either in form of proper deterministic regularisation procedure [1] or via probabilistic Bayesian inference [8]. The first kind of approaches is providing the unique estimate, i.e. the identified value is one-point estimate which may differ from the reality depending on the number of the measurements being performed. On the other side, the Bayesian estimation provides the probabilistic description of the estimate (i.e. the probability density function) which is obtained from the priorly assumed probabilistic description of the unknown quantity and the existing measurement data. This method provides more information than one-point estimate, such as the posterior mean, mode, probability exceedance etc.

The main disadvantage of Bayesian updating lies in the significant computational effort that results from the sampling-based estimation of posterior densities. For each evaluation the method requires the approximate solution of a partial differential equation, i.e. the solution of the stochastic forward problem. Regarding this, the sampling-kind of methods are shown to be computationally exhaustive when used in practical applications. Typical example is the Markov chain Monte Carlo

(MCMC) method often used in numerical computation of full Bayesian update. In order to overcome this issue, we recently developed much faster but still reliable updating procedure by replacing the computationally expensive forward simulation with the surrogate solution in a form of a polynomial chaos expansion (PCE), please see [2, 6]. Such an approximation leads to a significant reduction of the computation time as the evaluation of the PCE is cheap. However, one may show that this reduction is not enough if the method is supposed to be used in real-time systems. This is caused by slow convergence of MCMC method, which often requires more than 10^6 samples to approach a stationary posterior distribution.

Due to previously mentioned reasons, we have built a new fast and reliable computational procedure [6, 4, 7], which works completely deterministically. The method updates the random variable by transforming its prior functional approximation (i.e. PCE) into the posterior one with the help of polynomial approximation of measurements. This is completely different procedure from the previously mentioned as the update of the probability measure is substituted with the random variable update. The estimator is of a minimum-variance type and represents the generalisation of Gauss-Markov theorem [3]. It minimises the quadratic loss function, i.e. the squared distance to the original random variable over the probability space generated by prior information and the measurement. The method does not rely on the assumption of Gaussianity or the linearity in the model. However, in order to simplify the computation we assumed linearity in the mapping between the parameter and the measurement space—linear Bayesian update. This further means that the solution of the minimisation problem is found in smaller subspace than available as not all given information has been used. The linear estimator has for a special case the very well-known Kalman filter when the Gaussianity is assumed.

The measurement error (and possibly model error) in the linear Bayesian update is taken as independent from the prior distribution and the measurement. However, such an error may significantly influence the update procedure as enlarges the stochastic subspace we project onto. Namely, with each new measurement one is more close to the desired estimate on the expense of the increase of the stochastic dimension, i.e. the number of random variables. In order to avoid this situation another procedure has been applied as described in [5]. The idea comes from the square root filtering, where the evaluation of the posterior is achieved by simple additive decomposition of the prior on the mean and the varying part, and their separate transformation to the corresponding posterior terms. In this manner the update consists of two stages: the update of the mean via Kalman filter and the update of the varying part via

the spectral square root filter. As the measurement error does not directly enter the formula, the additional random variables do not appear in computations, and thus the update procedure becomes more efficient. However, one has to keep in mind that the spectral square root filter is not equivalent to the linear Bayesian estimate as does not provide the updates of the higher order moments.

The comparison of proposed numerical methods is performed on a simple example of the steady state heat transfer described by a scalar homogeneous thermal conductivity parameter. The true value of the thermal conductivity (the so-called truth) is assumed to be one realisation of a lognormal random variable described independently from the a priori distribution, also taken to be lognormal. The prior distribution is chosen such that the truth lies in its high probability region, while the data set is obtained by measuring the temperature in a set of randomly chosen points in computational domain. For such an assumption, the MCMC and linear Bayesian update give similar results as shown in Fig. 13. Here one may notice that the posterior uncertainty decreases with the increase of the number of measurements as more information in the update process is involved.

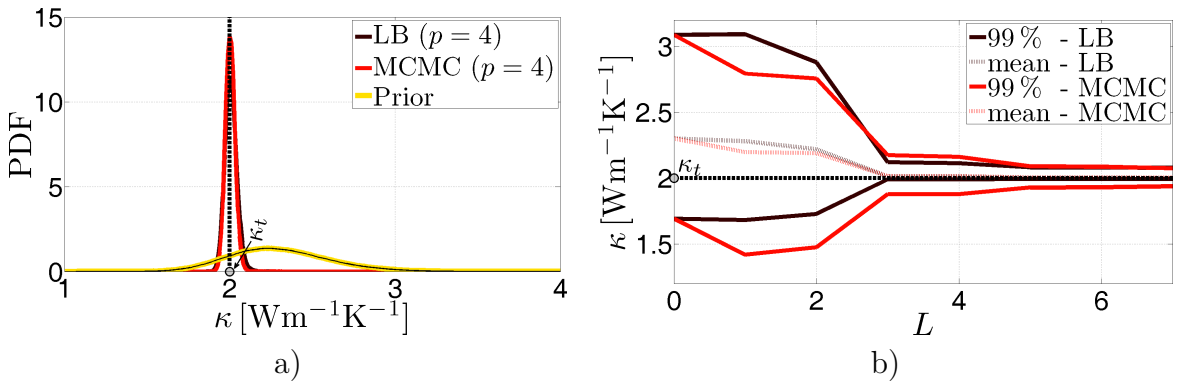

Figure 13: a) Comparison of the posterior PDFs obtained by MCMC and linear Bayesian update for the PCE of order 4 and 7 measurements b) Comparison of the 99% percentiles obtained by MCMC and linear Bayesian update for different number of the measurement points

With previous comparison one of the most important assumptions of the linear Bayesian update has not been satisfied. Namely, by measuring the temperature the linear mapping between the measurement and the parameter set is broken, and thus the update cannot be optimal. Regarding this, in Fig. 14 we compared the linear Bayesian update and the square root algorithm for both linear and nonlinear measurement. Additionally, we considered more complex situation than before as the truth is chosen to belong to lower probability region of the prior. As expected, the updates give similar results for the linear measurement, i.e. the uncertainty in the prior is reduced and the posterior mode is near to the truth, see Fig. 14 a). However, in case of nonlinear mea-

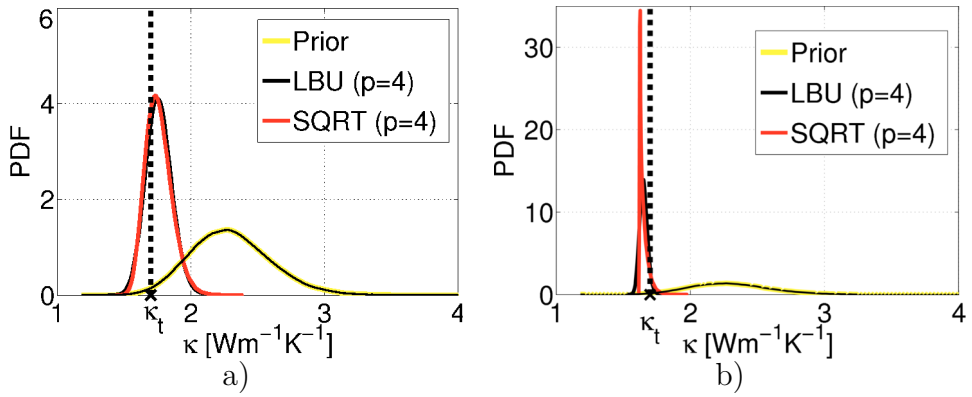

Figure 14: Comparison of the posterior PDFs obtained by linear Bayesian update and spectral square root algorithm for the PCE of order 4 and a) the linear measurement b) the nonlinear measurement

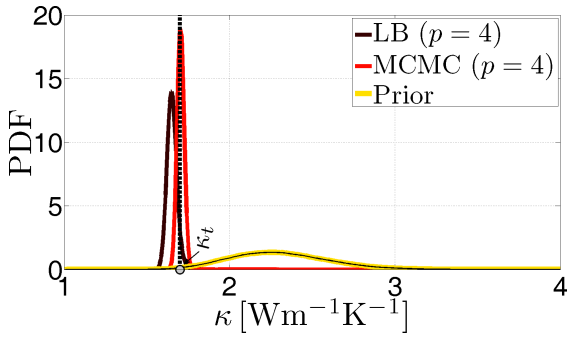

Figure 15: Comparison of the posterior PDFs obtained by MCMC and linear Bayesian update for the PCE of order 4 and the truth equal to 1.7

surement the spectral square root algorithm results in more skewed and narrowed probability density function than the linear Bayesian update. Also, both methods deliver the posterior mode which overshoots the truth, see Fig. 14. This is, however, not the case with the full MCMC update as shown in Fig. 16.

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2.13 Solving Multiphysics Problems with the software PAK

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The main objective of this DAAD travel project is the development of the software package PAK Multiphysics for solving complex problems which involve multiple physical models or multiple simultaneous physical phenomena. The goal is to merge the PAK modules, FEA software modules developed at the Faculty of Engineering, Kragujevac, Serbia, with the help of the CTL (Component Template Library) [4] developed at the Institute of Scientific Computing, Braunschweig, Germany. Each component of the PAK software solves a system of differential equations which describes constitutive model of one specific physical phenomenon. In order to describe more complex physical processes the modules have to be coupled in a determined way as further described.

Another project objective is improvement of the coupled material models with the help of the theory of stochastic modelling. Namely, the uncertainties will be introduced into the mutliphysics modelling in a form of random fields and processes after their identification from the measurement data in an updated Bayesian fashion has been done. Regarding this, an additional goal of this project is to develop a fast and reliable computational procedure using modern stochastic computational developments, and to implement these within a general software component framework.

2.13.1 Thermo-mechanical coupling

The heat transfer and structural engineering problems can be solved using finite element method (FEM) software, independently. However, in many scientific areas of research one has to deal with the thermo-mechanical problems in which the thermal changes induce the thermal strains and mechanical changes induce the appearance of the thermal energy. Regarding this, there is an increasing demand on the exchange of the data between the mentioned independent software components [1, 2, 3, 9]. Typical example represent the materials such as shape memory alloys, whose numerical computation requires the thermo-mechanical interaction for the accurate simulation of the material behavior.

During the last year the numerical algorithm for the coupling of two PAK software components with the help of CTL, namely the PAK-T component for heat transfer [11] and the PAK-S component for struc-

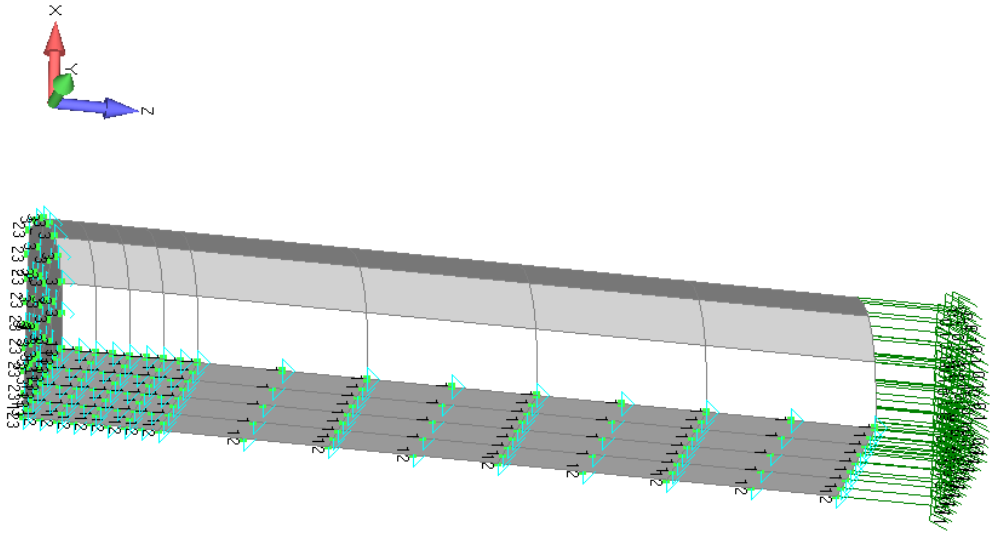


Figure 16: Model geometry and boundary conditions

tural analysis [10], has been developed. The PAK-S component contains many material models which describe the specific material behavior for various areas of interest. One of models of particular interest for this project is the thermo-plasic material model, which was extended to work for the case of large deformations as a more realistic scenario. To this end the code was provided with the subroutines which compute the induced dissipation energy during plastic deformation. The PAK-T component plays an important role in coupling as one has to evaluate the change in temperature due to the formation of dissipation energy. This change has a great impact on the alteration of material properties and the plastic deformations. Therefore, the data exchange between the PAK components is done for each iteration of the PAK-S solver. In this way the PAK-T component resolves the full time step for each new iteration and hands the temperature results back to the PAK-S component. This complex feedback-loop between the plastic strains and the temperature field is carefully tuned to converge accurately and efficiently.

The coupling algorithm is verified on the necking of cylindrical bar example. This example is concerned with the thermo-mechanical necking triggered by a non-homogeneity in the temperature field induced via self-heating of the specimen due to the plastic deformation. The boundary conditions of the bar are prescribed to allow free contraction of the specimen leading to an initially homogeneous state of stresses in the absence of geometric imperfections, see Fig. 16. Owing to the symmetry of the problem, only a eighth of the specimen is discretized with a finite element mesh which consists of 96 twenty-noded three-dimensional elements. Initially, the bar is at a homogeneous reference temperature 293K, which is identical to the temperature of the surrounding medium. As time evolves, the specimen is stretched with constant velocity applied

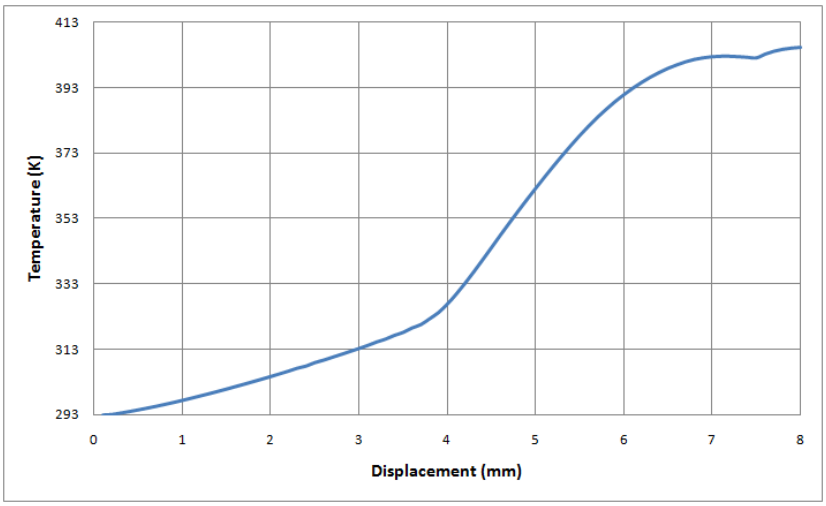
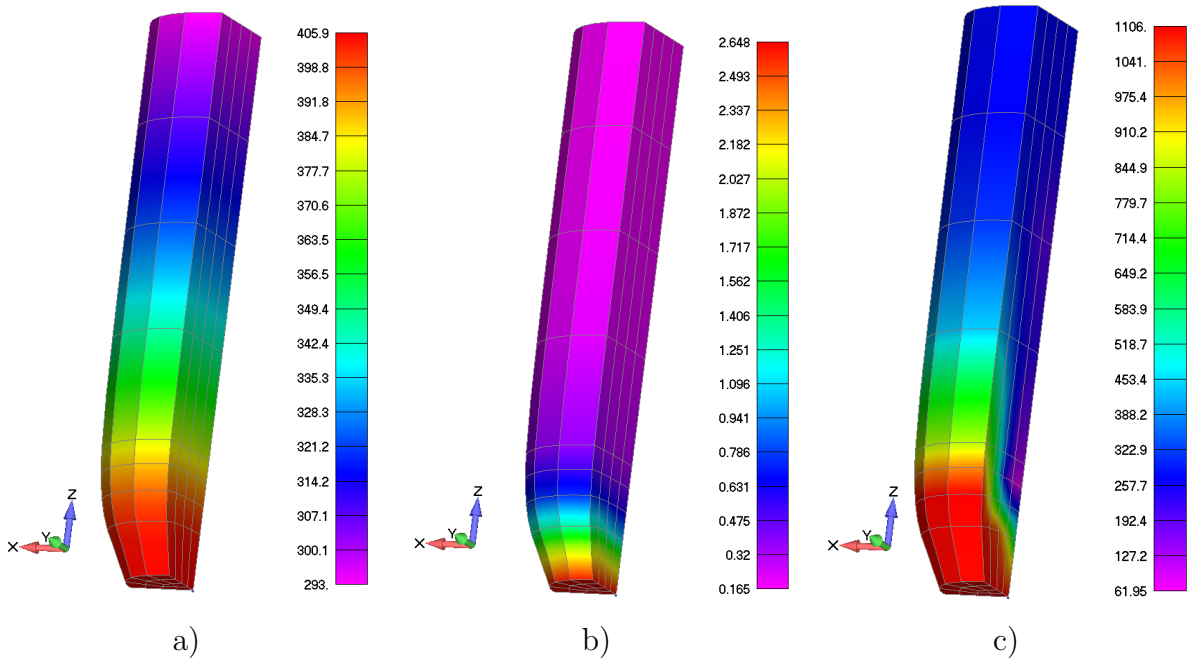


Figure 17: The evolution of the relative temperature with respect to the displacement



a) b) c)

Figure 18: a) The temperature field b) plastic strain c) effective stress

in 80 equal time steps until a final elongation 16 mm is attained.

The obtained results are compared with the results from [8]. Namely, we obtained the same evolution path of the relative temperature (the difference between the specimen and reference temperature) as in [8], see Fig. 17 and corresponding results in [8]. To this corresponds the temperature field in Fig. 18 a) induced by the self-heating of the specimen. Similarly, the field of effective stress is given in Fig. 18 c) with the maximal effective stress of 1106 MPa, and the minimal effective stress of 61.95 MPa.

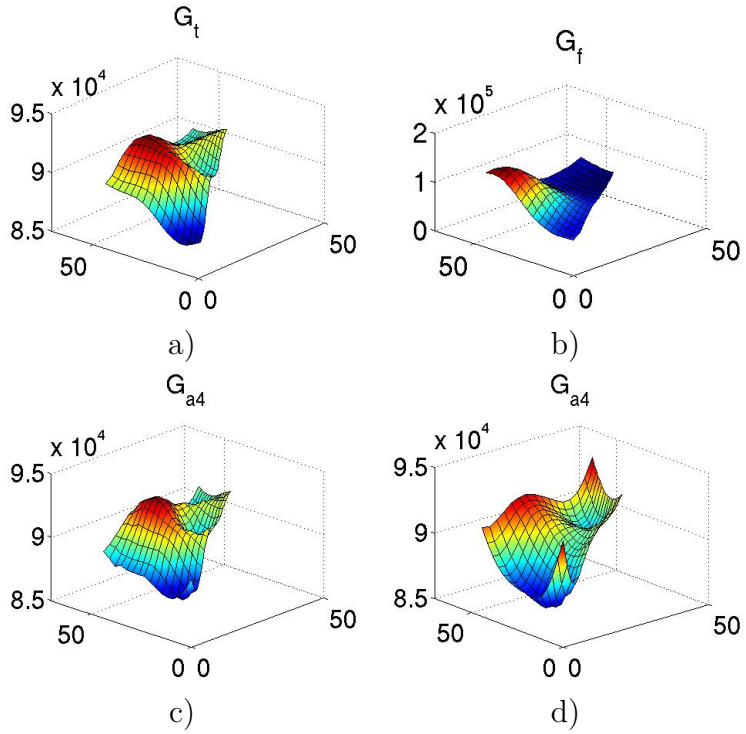


Figure 19: Shear modulus G: a) truth b) prior c) update (linear model) d) update (nonlinear model). For PCE is used $p = 3$ and $M = 10$.

2.13.2 Bayesian identification of material parameters describing elasto-plastic material

The numerical methods presented in Section 2.12 are also applied for the identification of material properties of elastoplastic material. The elasto-plastic behaviour is mathematically speaking the variational inequality of the second kind characterised by a state variable consisting of the displacement, plastic deformation and internal variable. The model is more complex than the one presented in Section 2.12 due to the non-smooth evolution of the internal variables, for more information please see [6]. In addition, the unknown parameters are modelled as random fields, not random variables as before.

The methods are numerically tested on a simple example of Cook's membrane clamped on one end and loaded by force in the vertical direction at the other end. The shear modulus G is taken to be identified from the measurements of the shear stress in several randomly distributed points of domain, for more details please see [5, 7]. Both the true value of parameter (in virtual experiment) and the prior distribution are modelled as independent modified lognormal random fields. The truth is taking the value of only one realisation of the corresponding field.

The linear Bayesian update is computed with the help of polynomial approximations of the third order and the Karhunen-Loève expansions with 10 random variables. The update is performed in sequential way, i.e. each new update takes for the prior the last obtained posterior and

Table 3: The relative mean error $\epsilon_m[\%]$ and relative variance $\epsilon_v[\%]$ as a function of the PCE order and the number of the measurement points. The measurement is the first stress component.

		Yield stress					
	p	2	3	4	5	6	7
ϵ_m	2	30.62	30.76	20.54	16.32	0.50	0.27
	3	30.73	30.79	20.60	16.42	0.78	0.11
	4	30.73	30.54	20.62	16.36	0.76	0.10
ϵ_v	2	99.42	97.66	87.65	82.37	48.32	44.06
	3	99.37	97.37	87.16	82.12	48.24	44.10
	4	99.37	99.37	87.12	82.08	48.12	44.03

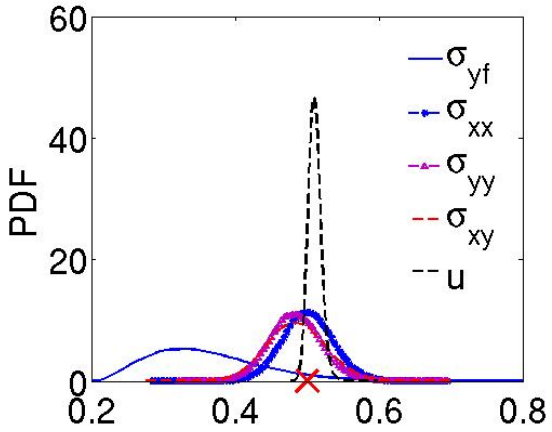


Figure 20: The posterior density function of yield stress in different experiments. The truth is denoted with red X.

provides new measurements of shear stress by setting up different loading conditions than before. In this manner the six stage sequential update process is carried out for both linear and nonlinear model (i.e. purely elastic and elastoplastic model). As expected, the update in case of pure elastic response gives much better result than the update for the elastoplastic response, see Fig. 19. This phenomenon is already explained in Section 2.12. Namely, the measurement of elastoplastic response is nonlinear in parameter set and thus the update is not optimal.

Besides the shear stress, another material property has been investigated, namely the yield stress which characterises the strength of material before the plastic deformation occurs. For this, the first stress component is measured and the prior is also taken to be lognormal distribution (see [7]). The comparison to the true value is done with the help of two error indicators, the error in the mean and variance. As plotted in Table 3, the mean value converges very fast with the number of the measurement points, while the variance has much slower convergence. However, this can be improved by measuring another quantity or moving the sensors to the strong plastyfing zone, see Fig. 20.

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2.14 Data validation and reconciliation

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The validation of measured data in energy conversion and power plants is governed in Germany by the VDI guideline 2048 [1, 2]. The basic problem solved in this guideline is that of measured values x and free variables y, having to fulfil certain balance and material equations $f(x, y) = 0$. Usually, the measured values do not fulfil the balance equation so that a reconciliation procedure needs to be applied. Given that the errors in the measurements can be described by a covariance matrix S_X the mathematically equivalent statement is

$$\min_v v^\top S_X^{-1} v \quad \text{s.t. } f(x+v, y+w) = 0 \tag{14}$$

which minimises over the admissible v and simultaneously finds an admissible w, such that the balance equations are fulfilled. Furthermore, a covariance matrix for the corrected values needs to be computed.

In the original VDI guideline, the system is linearised, and the free variables y are eliminated, because otherwise the system to be solved would become singular. After computation of the correction v, the system is solved for w and then the covariance matrix of the corrected values is computed. A drawback of the method is that the free variables need to be eliminated beforehand, which can become complicated, and that the corrections need be applied afterwards in a postprocessing step to get the values of the free variables.

An approach to get around this difficulty had been proposed by Witkowski to endow the free variables with artificial very high variances [3]. The advantage of this method is, that the free variables can then be included in the minimisation (14). However, if the artificial variance is not high enough the results of the reconciliation process can change. In contrast, if the variance is too high the process may become numerically instable.

An approach that circumvents these difficulties is to solve the linearised problem as one large system of equations

$$\underbrace{\begin{bmatrix} S_X^{-1} & 0 & F^\top \\ 0 & 0 & G^\top \\ F & G & 0 \end{bmatrix}}_{Z} \begin{bmatrix} v \\ w \\ \lambda \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ -f(x,y) \end{bmatrix}. \tag{15}$$

An advantage of this approach is, that everything is in one equation and no pre- and postprocessing is necessary. Further, compared to [3], there

are no trade-offs in accuracy. The size of the linear system to be solved is larger than in the VDI guideline, however, Z is a sparse matrix and the size of the system is still small enough to be solved efficiently on modern hardware with linear algebra subroutines.

The computation of the covariance matrix of the corrected values $\tilde{x} = x + v$ is a bit more involved than in the VDI guideline. However, using the restrictions P_x, P_y, and P_λ defined by

$$P_x = \begin{bmatrix} I_x & 0_y & 0_\lambda \end{bmatrix}, \quad P_y = \begin{bmatrix} 0_x & I_y & 0_\lambda \end{bmatrix}, \quad P_\lambda = \begin{bmatrix} 0_x & 0_y & I_\lambda \end{bmatrix} \tag{16}$$

this can be written succinctly as

$$S_{\tilde{x}} = S_x - S_v = S_x - \left(\frac{\partial v}{\partial x}\right) S_x \left(\frac{\partial v}{\partial x}\right)^\top \tag{17}$$

$$= S_x - (P_x Z^{-1} P_\lambda^\top)(F_x S_x F_x^\top)(P_x Z^{-1} P_\lambda^\top)^\top. \tag{18}$$

It could further be proved that the covariance matrix of the corrected values $S_{\tilde{x}}$ can be taken as one block of the inverse matrix Z^{-1} by

$$S_{\tilde{x}} = P_x Z^{-1} P_x^\top. \tag{19}$$

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2.15 Centre for Scientific Computing

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Das Centre for Scientific Computing (CSC) ist ein Zusammenschluss der Institute für Wissenschaftliches Rechnen (Prof. Matthies) und Computational Mathematics (Prof. Sonar) zu einem Technologietranszferzentrum (TTZ) innerhalb der Innovationsgesellschaft der TU Braunschweig (iTUBS). Zielsetzung ist die Beratung und Bearbeitung von Fragestellungen aus dem Kontext des wissenschaftlichen Rechnens und der angewandten Mathematik.

2.15.1 Durchgeführte Arbeiten

In 2012 wurden ein Projekt zur Datenassimilation mit dem Institut für Geophysik und Extraterrestrische Physik aus dem Jahre 2011 weitergeführt. Dabei werden vorhandene experimentelle Daten benutzt, um parametrisch beschriebene, numerische Vorhersagemodelle zu kalibrieren. Eine solche Inversionsaufgabe wird derzeit für die plasmaphysikalischen Vorgänge der Wechselwirkung zwischen dem Sonnenwind und der Erdmagnetosphäre bearbeitet. Satellitenmessungen dienen hier als Referenzwerte für ein magnetohydrodynamisches Simulationsmodell des Sonnenwindes.
Darüber hinaus wurde mehre Schulung zur CFD-Toolbox OpenFOAM und zum PostprocessingTool ParaView sowohl in Braunschweig wie auch bei Kunden vor Ort durchgeführt. Auf dem 7. OpenFOAM Workshop in Darmstadt wurde ein öffentliches User-Training bzgl. Außenaerodynamiksimulation mit OpenFOAM vom CSC abgehalten.
Im Folgenden werden die Projekte genannt. Die Arbeiten und Berichte unterliegen den jeweiligen Geheimhaltungsvereinbarungen.

- **Machbarkeitsstudie zur Rekonstruktion des inneren und äußeren Anteils des Merkur-Magnetfeldes aus In-situ-Messungen in der Merkur-Magnetosphäre**
  Projektabschnitt Ia – Rekonstruktion für ein Ersatzmodell, Vorwärtsaufgabe
  Projektpartner: Inst. f. Geophysik und Extraterrestrische Physik
  In 2012 geleistete Arbeiten:
  - Analytische und numerische Umsetzung
  - Berechnung diverser Szenarien
- **OpenFOAM – Introduction**
  Einführender Schulungskurs für Teilnehmer aus Industrie und Wis-

senschaft in die Simulations-Toolbox OpenFOAM®
Durchgeführt am

  - 11./12.06.2012
  - 11./12.12. 2012

- **OpenFOAM – Advanced**
  Weiterführender Schulungskurs für Teilnehmer aus Industrie und Wissenschaft in die Simulations-Toolbox OpenFOAM®
  Durchgeführt am

  - 25./26.07.2012

- **ParaView**
  Einführung in die Visualisierung mit ParaView®
  Durchgeführt am

  - 13.06.2012
  - 13.12.2012

- **Generic external aerodynamic simulation training**
  7th OpenFOAM®Workshop, Darmstadt, Germany. 25 – 28 June 2012

2.16 Seismic Risk Analysis for Hospital Structures

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2.16.1 Introduction

Italy is a nation with a relevant seismic activity: in the last decades, lots of serious earthquakes have occurred in the Italian territory, causing several collapses of structures and many human casualties. The attention of the scientific community on this problem is growing day by day: the seismic risk evaluation for the built environment is a very current topic, in particular for those types of buildings which have a primary importance for the community [3]. Hospital buildings belong to this category of structures and they are object of seismic risk analyses. In order to perform a seismic risk analysis, three aspects must be considered:

- structural vulnerability, that describes the features of the structure, without considering the characteristics of the site of construction
- seismic hazard, that expresses the probability that, in a given period and in a given place, a certain earthquake event occurs
- exposure, that measures the quality and quantity of the contents of the buildings that is exposed to risk (in terms of persons and objects)

The combination of these three aspects leads to the identification of the seismic risk, which can be expressed by means of an index of risk. In the present work, the attention will be mainly focused on the evaluation of the structural vulnerability.

2.16.2 Vulnerability of the Hospitals in Tuscany Region (Italy): an Empirical Approach

The evaluation of the structural vulnerability can be performed by means of different levels of accuracy: the first methods, developed since the 70', are called empirical methods: they are based on qualitative evaluations and they are necessary in case of the examination of a large number of buildings, for which detailed analyses are too time-consuming. On the other hand, analytical methods are characterized by a direct physical meaning: they allow the study of the vulnerability by means of analyses of the mechanical behavior of the structure, using numerical models. The results of this type of analysis are expressed in terms of PGA of

capacity, which is the peak ground acceleration of the soil that causes the collapse of the analyzed structure.

Some recent developments have led to hybrid methods, which represent a combination of the two methods described above. Talking about the Tuscany Region (Italy), the Hospital Buildings Heritage is composed of 533 Structural Units (S.U., which means a structurally independent building): in order to analyze the structural vulnerability of all of them, an empirical method has been used [5]: in particular, the Vulnerability Index Method [1] has been considered. The method consists in the filling in of the II Level Vulnerability Form [4], composed of 11 parameters that describe the structure (type and organization of the resistant system, quality of the materials, typology of roofs...); for each parameter the surveyor must give a judgment, which corresponds to a specific score. By means of a weighted sum, it is possible to obtain a normalized index within the range 0-100%, where a high index corresponds to a high vulnerable structure. The application of this procedure to the entire sample of analysis has led to a classification of vulnerability.

2.16.3 Structural Vulnerability: an Analytical Approach

The method of evaluation of the vulnerability described above considers, in a simplified way, all the problems of a structure under seismic action and it is generally used for all the typologies of structures. Since Hospital Buildings have specific requirements due to their social function, a study of detail on the vulnerability of these systems has been performed.

The idea of the work is to analyze in a detailed way some buildings of the sample, by means of static non linear analyses: so far, this analysis process has been performed on some masonry structures. This typology of analysis requires the creation of a numerical model that represents the "equivalent frame structure" of the masonry building [2]; each element of the model has a non linear behavior, taking into account the mechanical properties of the materials and the geometries of the structural elements.

Until now, 14 masonry structural units have been analyzed: for each building, 8 pushover analyses have been done, considering 2 main directions of the seismic action, 2 different lateral load profiles (one proportional to the masses and one proportional to the first modal form) and 2 different configurations of eccentricity of the lateral load (centered profile on the barycenter of the masses of the structure and eccentric profile, with 5% of the building dimension eccentricity).

Each analysis gives its pushover curve as result. These curves show the relation among the displacement of a control point (usually chosen on the upper floor of the structure in a baricentric position) and the

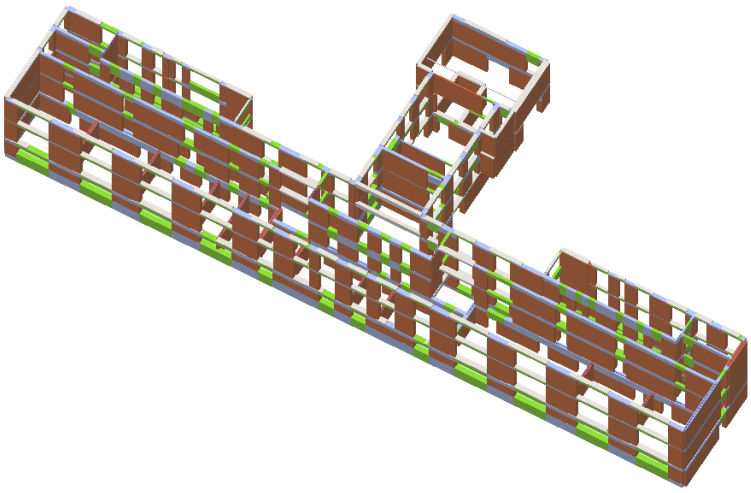

Figure 21: analytical model of a structural unit

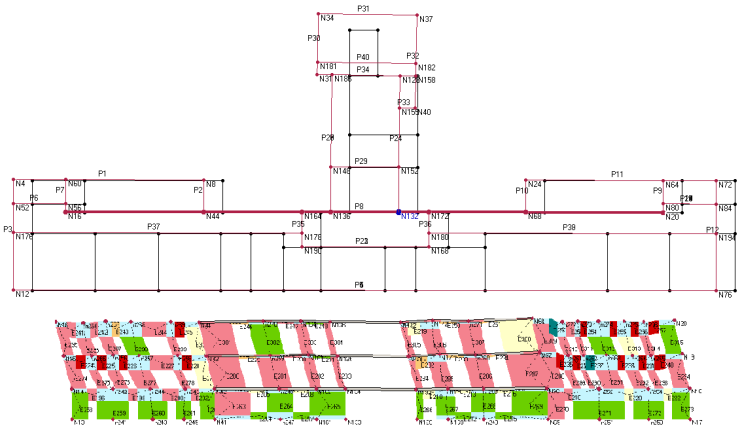

Figure 22: planimetric and a front view of the model during one analysis in the longitudinal direction

total base shear. The lowest value of PGA obtained from the 8 analyses has been considered as the capacity of the structure.

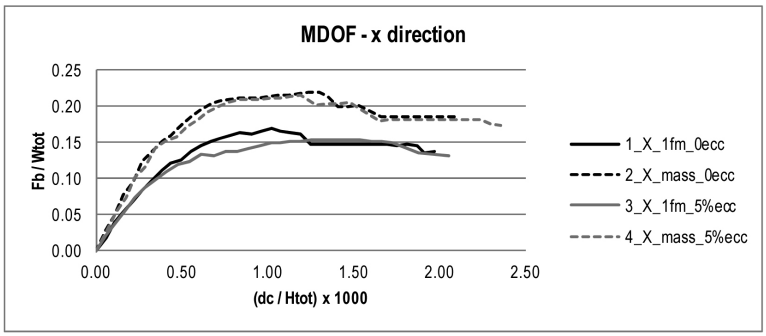

Figure 23: pushover curves for the analyzed S.U. in the longitudinal direction

2.16.4 Structural Vulnerability: the Correlation Study

On this reduced subset of buildings, analyzed both in an empirical and analytical way, it has been possible to perform a correlation study, in order to understand if the empirical approach can give a direct information about the acceleration of collapse of the considered structure.

The empirical method, for its nature, can be employed only in a comparative way, obtaining an Index of Vulnerability for each of the analyzed structures and allowing the comparison of them, in order to assess which building is more vulnerable in the considered group, without giving information about the absolute level of security of the structure.

The results of this present work show that there is a quite evident correlation among the Index of Vulnerability I_v and the PGA of capacity: this relation, starting from the calculated I_v, allows the estimation of a plausible value of the PGA_c for the analyzed structure (referred to a ground category A and a topographic category T1) and consequently, to get a qualitatively indication on the objective safety index of the building, calculating the ratio between the PGA of capacity and of demand, related to the site of construction seismic hazard.

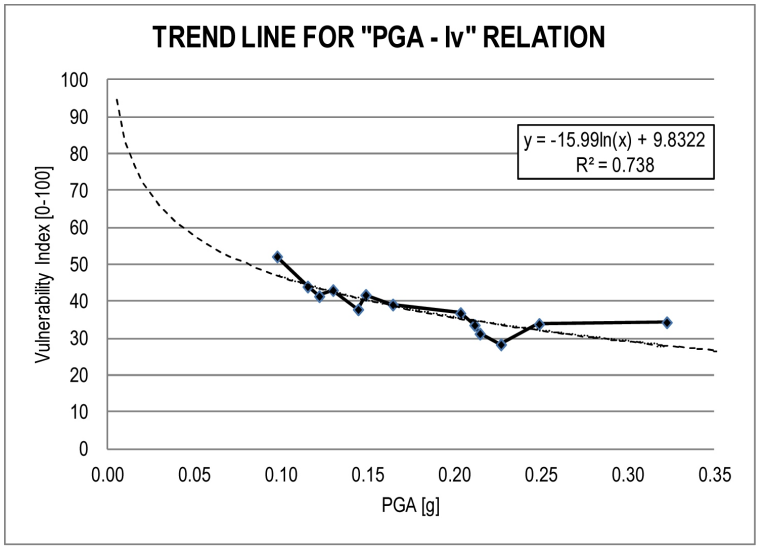

Figure 24: correlation among the Index of Vulnerability and the PGA of capacity

The equation of the correlation will be improved in the future with the enlargement of the sample of analysis.

2.16.5 Future Developments on the Vulnerability Assessment

The targets of this research consist, at first, in the enlargement of the sample of analysis for the masonry structures, in order to guarantee a more reliable result for this type of buildings.

A similar procedure will be applied for a group of reinforced concrete buildings belonging to the investigated sample, in order to obtain, even in this case, a correlation law among I_v and PGA_c.

In this way, it will be possible to find an unique vulnerability classification in terms of PGA_c, based from one side on the consolidated efficacy of the empirical evaluation with 11 parameters and, on the other side, on results carried out with detailed elaborations, performed with non

linear analyses that are able to take into account the real behavior of the structure, considering the effective structural configuration.

2.16.6 Hospital Buildings: the Definition of the Exposure

The evaluation of the seismic risk of a building must consider not only the vulnerability of the structure, but even the exposure of the analyzed object, which measure the quality and quantity of the elements exposed to risk: for example, a certain building will have different level of the Index of risk if it is used as a warehouse or as a first aid within the Hospital system.

The structural vulnerability represents therefore only one part of the seismic risk; one Hospital system should continue to be operative even after a low-medium event: this feature is more related to the typology and quality of the non-structural systems that are contained in the buildings. In this type of structures (hospitals), particular attention should be given to the health systems such as medical gas distributions, all the equipments for medical interventions and so on. It is also necessary to consider the importance of the electrical and plumbing systems, that assume a crucial importance for the medical equipments mentioned above, as well as all the architectural components (such as light ceilings, non structural walls) that can cause several damage with their local collapses.

Some studies on this argument have been performed by the Federal Emergency Management Agency (F.E.M.A.), which has produced some guidelines, such as the "N.E.H.R.P. (National Earthquake Hazards Reduction Program) Guidelines and Commentary for Seismic Rehabilitation of Buildings" - F.E.M.A. 273 (1997), document that at first introduces the concept of *building seismic performance levels*; a further development in this direction has been done by the A.S.C.E. (American Society of Civil Engineers) with the "Prestandard and commentary for the seismic rehabilitation of buildings" - F.E.M.A. 356 (2000). These documents define the building's expected performances, investigating the typology and extension of the damage of each component of the building system. In particular, for the non-structural components, there are three tables that separately describe the behavior of:

- architectural components
- mechanical, electrical and plumbing systems/components
- contents

Starting from this, some detailed studies will be performed in the last part of the PhD Course, in order to take into account these aspects within the seismic risk analysis of hospital structures.

2.16.7 Conclusions

The research will lead to a procedure of analysis of the seismic risk specifically for Hospital structures, considering all the three aspects mentioned in the beginning: seismic hazard of the site of construction, structural vulnerability and value of the exposure. This procedure is characterized by a fast assessment method that is based on detailed analyses and on a reliable empirical method, used in the Italian territory since the 80's.

A reliable seismic risk analysis of the Hospital buildings allows the creation of a seismic risk classification, which is a useful tool for the Public Administrations in order to plan the interventions for the seismic improvement/retrofitting of the structures.

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3 Lehre im WS 2011/2012 and SS 2012

3.1 Wintersemester 2011/2012

Advanced Object Oriented C++ Techniques	2+2	Rainer Niekamp
Seminar zum wissenschaftlichen Rechnen	0+2	Hermann G. Matthies, Alexander Litvinenko
Weiterführendes Programmieren/ Intermediate Programming	0+4	Hermann G. Matthies, Rainer Niekamp, Elmar Zander
Einführung in das Programmieren (für Nicht-Informatiker)	0+4	Hermann G. Matthies, Rainer Niekamp, Elmar Zander
Einführung in das Wissenschaftliche Rechnen (ODE I)	2+1	Hermann G. Matthies, Joachim Rang
Visualisierung wissenschaftlicher Daten	2+1	Joachim Rang, Elmar Zander
Bionische Methoden der Optimierung I	2+1	Joachim K. Axmann, Oliver Pajonk
Discontinuous Galerkin Methods I	2+1	Ralf Hartmann
Einführung in PDE und Numerische Methoden für PDEs	2+1	Hermann G. Matthies, Alexander Litvinenko
Praktikum zum Wissenschaftlichen Rechnen	0+4	Alexander Litvinenko

3.2 Sommersemester 2012

Fortgeschrittene Methoden für ODEs und DAEs	2+1	Hermann G. Matthies, Joachim Rang
Partitioned Methods for Multifield Problems	2+1	Joachim Rang, Martin Krosche
Advanced Object Oriented C++ Techniques	2+1	Rainer Niekamp
Seminar zum wissenschaftlichen Rechnen	0+2	Hermann G. Matthies, Dominik Jürgens
Industrielles Software-Entwicklungsmanagement	2+0	Joachim K. Axmann, Oliver Pajonk
Weiterführendes Programmieren/ Intermediate Programming	0+4	Hermann G. Matthies, Rainer Niekamp, Dominik Jürgens
Einführung in das Programmieren (für Nicht-Informatiker)	0+4	Hermann G. Matthies, Rainer Niekamp, Dominik Jürgens
Praktikum zum Wissenschaftlichen Rechnen	0+4	Hermann G. Matthies, Alexander Litvinenko
Software Entwicklungspraktikum	0+4	Hermann G. Matthies, Oliver Pajonk
Parallel Computing I	3+1	Thorsten Grahs
Introduction to High Performance Computing	3+1	Josef Schüle

4 Veröffentlichungen und Vorträge

4.1 Schriften und Proceedings

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[1] M. Espig, W. Hackbusch, A. Litvinenko, H. G. Matthies, and P. Wähnert, *Efficient low-rank approximation of the stochastic Galerkin matrix in tensor formats*, Tech. report, DFG-Schwerpunktprogramm 1324 *Extraktion quantifizierbarer Information aus komplexen Systemen*, 121, URL: http://www.dfg-spp1324.de/download/preprints/preprint121.pdf.

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4.3 Vorträge

Alexander Litvinenko, Mike Espig, Wolfgang Hackbusch, Hermann G. Matthies and Elmar Zander, *Efficient Analysis of High Dimensional Data in Tensor Formats*, GAMM Seminar “Analysis and Numerical Methods in Higher Dimensions”, Leipzig, January 2012

Alexander Litvinenko, Mike Espig, Wolfgang Hackbusch, Hermann G. Matthies and Elmar Zander, *Efficient Analysis of High Dimensional Data in Tensor Formats*, Forschungsseminar, Universität Trier, February 2012

Alexander Litvinenko, Mike Espig, Wolfgang Hackbusch, Hermann G. Matthies and Elmar Zander, *Efficient Analysis of High Dimensional Data in Tensor Formats*, Workshop "High-Order Numerical Approximation for Partial Differential Equations", Hausdorff Center for Mathematics, University of Bonn, Februar 2012

Alexander Litvinenko, Hermann G. Matthies, *Uncertainty Quantification in numerical Aerodynamic via low-rank Response Surface*, GAMM Conference, Darmstadt, March 2012

Alexander Litvinenko, *Multilinear algebra and different tensor formats with applications*, Forschungsseminar Technische Universität Braunschweig, May 2012

Alexander Litvinenko, Mike Espig, Wolfgang Hackbusch, Hermann G. Matthies and E. Zander. *Efficient Analysis of High Dimensional Data in Tensor Formats*, SIAM UQ Conference, Raleigh, NC, USA, April 2012

Alexander Litvinenko, H. G. Matthies, B. Rosić, O. Pajonk and E. Zander. *Tensor Approximation Methods for Parameter Identification*, SIAM Conference on Applied Linear Algebra, Valencia, Spain, Juni 2012

Alexander Litvinenko, Bojana. V. Rosić, Elmar Zander, Oliver Pajonk, Hermann G. Matthies. *Sampling-free linear Bayesian update of polynomial chaos representations*, Forschungsseminar Technische Universität Braunschweig, December 2012

Hermann G. Matthies, *Stochastic PDEs and Inverse Problems.* Conference of Australia and New Zealand Industrial and Applied Mathematics (ANZIAM), Warrnambool, Australia, February 2012

Hermann G. Matthies, *Parameter Identification in Continuum Mechanics* Priority Research Centre for Geotechnical and Materials Modelling, University of Newcastle, NSW, Australia, February 2012

Hermann G. Matthies, A. Litvinenko and T. El-Moselhy, *Sampling and low-rank tensor approximations.* MCQMC, 10th International Conference on Monte Carlo and quasi-Monte Carlo methods in Scientific Computing, Sydney, Australia, February 2012

Hermann G. Matthies, Keynote Lecture *System Identification in a Probabilistic Setting*, IASS-IACM 7th International Conference on Computational Mechanics for Spatial Structures, GF Sarajevo, Bosnia and Herzegovina, 3. April 2012

Hermann G. Matthies, *A stochastic setting for parameter identification*, Jacobs University Bremen, Fraunhofer MEVIS, 3. May 2012

Hermann G. Matthies, Laudatio for Roger Ohayon, FEM Class of 42 Anniversary, Barcelona, Spain, May 2012

Hermann G. Matthies, A. Litvinenko, B. Rosić and O. Pajonk. *Tensor approximation methods for parameter identification.* SIAM Conference on Applied Linear Algebra, Valencia, Spain, June 2012

Hermann G. Matthies, B. Rosić, O. Pajonk, A. Kučerová and J. Sýkora. *Bayesian Identification of Parameters Describing Nonlinear Models of Heterogeneous media.* IUTAM Symposium on Multiscale Problems in Stochastic Mechanics, Karlsruhe, June 2012

Hermann G. Matthies, *A Stochastic Setting for Inverse and Parameter Identification Problems*, Humboldt Universität Berlin, 4 July 2012

Hermann G. Matthies. *Uncertainty Quantification and High Dimensional Parametric Problems*, 10th World Congress On Computational Mechanics (WCCM 2012), São Paulo, Brazil, 11 July 2012

Hermann G. Matthies and B. Rosić. *Tensor Approximation for Parameter Identification.* European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS), Vienna, Austria, September, 2012

Rainer Niekamp: *Non-Intrusive Coupling of Simulations based on Software-Component-Technique*, invited lecture, Prague, 5 December 2012

Joachim Rang: *An analysis of the Prothero-Robinson example for constructing new DIRK and ROW methods*, Numdiff-13, Martin-Luther Universität Halle, Halle/Saale, 13.09.2012

Hermann G. Matthies, *Uncertainty Quantification and Parameter Identification*, Siemens AG Corporate Technology, München, 30.10.12

Hermann G. Matthies, *Notes on Model Reduction*, and *Probabilistic Methods for Parameter Identification*, Tyché Workshop on stochastic methods in high dimension, Paris, France, 6-7 December 2012

Joachim Rang, *Time discretisation methods for the incompressible Navier-Stokes equations*, Workshop Recent Developments in the

Numerics of Nonlinear Hyperbolic Conservation Law, Oberwolfach, January 2012

Joachim Rang: *Adaptive time step control for the incompressible Navier–Stokes equations*, Workshop Adaptive Methods with Applications in Fluid Dynamics, Berlin, April 2012

B. Rosić, O. Pajonk, A. Kučerová, J. Sýkora and H. G. Matthies. *Bayesian Parameter Identification for Nonlinear Systems.* ESCO 2012: 3rd European Seminar on Computing, Pilsen, Czech Republic, June 2012

B. Rosić, O. Pajonk, A. Litvinenko and H. G. Matthies. *Inverse Problems for Nonlinear Elastoplastic Models via Bayesian Parameter Identification.* European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS), Vienna, Austria, September 2012

O. Pajonk, B. Rosić, A. Litvinenko, and H. G. Matthies. *Comparison of Square Root Updating Schemes — Sampling vs. Spectral Implementation.* EnKF Workshop, Bergen, Norway, June 2012

O. Pajonk, B. Rosić, A. Litvinenko, and H. G. Matthies. *A Spectral Approach to Linear Bayesian Updating.* SIAM Conference on Uncertainty Quantification, Raleigh, USA, April 2012

O. Pajonk, B. Rosić, and H. G. Matthies. *Deterministic Linear Bayesian Updating of State and Model Parameters.* ECMOR XIII, Biarritz, France, September 2012

4.4 Projekttreffen

Alexander Litvinenko, *Non-linear Bayesian Update*, Codecs Project meeting, RWTH Aachen, Aachen, May 2012

Alexander Litvinenko, *Efficient Uncertainty Quantification for the Complete Field Solution*, MUNA Final Project meeting, DLR Braunschweig, October 2012

4.5 Organisation von Minisymposia/Konferenzen

A. Litvinenko, C. Schillings: Young Researchers Ḿinisymposium "Stochastic partial differential equations (SPDEs) and applications", GAMM Conference, Darmstadt, March 2012

H.G. Matthies, A. Ibrahimbegović: Minisymposium on heterogeneties and uncertainties in inelastic materials, 10th WCCM Sao Paolo, Brazil, July 2012

F. Chinesta, P. Ladevèze, A. Huerta, H. G. Matthies: Minisymposium on Matthies Reduced basis, POD and PGD model reduction techniques, European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS), Vienna, Austria, September, 2012

A. Ibrahimbegović, H. G. Matthies: Minisymposium on Heterogeneties and uncertainties in inelastic materials, European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS), Vienna, Austria, September, 2012

4.6 Teilnahme und Lehre an Workshops und Weiterbildung

A. Litvinenko, Workshop on High-Order Numerical Approximation for Partial Differential Equations, Hausdorff Center for Mathematics, University of Bonn, February 6-10, 2012.

A. Litvinenko, Workshop on Stochastic Analysis and Stochastic PDEs, University of Warwick, Coventry, England, April 2012

Hermann G. Matthies, GAMM Arbeitsgruppe UQ Workshop on Uncertainty Quantification for Computational Science and Engineering, KIT Karlsruhe, 17.-19. July 2012

Hermann G. Matthies, Adnan Ibrahimbegović, Short Course on *NONLINEAR COMPUTATIONAL MECHANICS OF STRUCTURES: Models, Computations, Probability, Interaction, FE Code Coupling*, at 7th International Conference on Computational Mechanics for Spatial Structure, GF Sarajevo, Bosnia and Herzegovina, 1.-4. April 2012

Hermann G. Matthies, Tyché Workshop on stochastic methods in high dimension, Paris, France, 6-7 December 2012

O. Pajonk, EnKF Workshop, Bergen, Norway, June 2012

Joachim Rang, Workshop on Recent Developments in the Numerics of Nonlinear Hyperbolic Conservation Law. Oberwolfach, 16-21.01.2012

Joachim Rang, Workshop on Adaptive Methods with Applications in Fluid Dynamics. WIAS Berlin, 19.-21.04.2012

4.7 Habilitation und Dissertationen

Josef Schüle, Antrittsvorlesung: Hochleistungsrechnen - heute und morgen, 03.02.2012. Habilitationsschrift: *Paralleles Rechnen: Performancebetrachtungen zu Gleichungslösern*, Oldenbourg Verlag, München, 2010.

Elmar Zander *Tensor Approximation Methods for Stochastic Problems.* 22.05.12

Oliver Pajonk *Stochastic Spectral Methods for Linear Bayesian Inference.* 20.07.12

Martin Krosche *A generic component-based software architecture for the simulation of probabilistic models.* 13.11.12

Bojana Rosić *Variational formulations and functional approximation algorithms in stochastic plasticity of materials.* 16.11.12

4.8 Abschluss- und Studienarbeiten

Torben Rodermund *Leistungsanalyse von parallelen Beschleunigungsframeworks am Beispiel von physikalischen Berechnungen aus der Raumfahrt*, Masterarbeit. Betreuer: Josef Schüle

5 Sonstiges

Alexander Litvinenko, Elmar Zander, TU-Night 30. June 12

5.1 Gäste am Institut

Fritz-Adrian Lülf, Ph.D.-student at ONERA, France. Lectures: *Reduzierte Modelle nicht-linearer Strukturen*, 12. Januar 12, und *Numerische Lösung des dynamischen Verhaltens einer geometrisch nicht-linearen und im Raum diskretisierten Struktur*, 10. Dezember 12
Another research visit at the institute Juni-September 12.

Habib N. Najm, PhD, Distinguished Member Tech. Staff at Sandia National Laboratories, Livermore, CA, USA. Research visits 16.-20. Januar 12, lecture on *Uncertainty Quantification in Computational Models*, and 12.-16.11.12, lecture on *Challenges in Uncertainty Quantification*

Antonio Falco Montesino, Associate Professor at Departamento de Ciencieas fisicas, Matematicas y de la Computation, Universidad CEU Cardenal Herrera, Valencia, Lecture on *Tensor approximation*, 20. January 12

Youssef Marzouk, PhD, Boeing Assistant Professor of Aeronautics and Astronautics, Massachusetts Institute of Technology, Boston, USA. Research visit 26.-29. March 2012, Lecture on *Bayesian inference with spectral approximations and optimal maps*

Anthony Nouy, PhD, Professor at the Department of Mathematics and Informatics, École Centrale de Nantes, France. Research visit 21.-23. May 12

Emmanuel Roubin, Ph.D.-student at LMT-Cachan (ENS Cachan/CNRS/UPMC/PRES UniverSud Paris) Secteur Génie Civil, France. Research visit 4.-22. June 12

Dr. Noémi Friedman, Budapest Univ. of Techn. and Economics, and Szent István Univ., Budapest, Hungary. Guest lecture on *Analysis, experiments and application of an antiprismatic deployable space truss system characterized by snap-back behaviour*, 02 July 12

Paul Hauseux,Ph.D.-student at Laboratoire de Mécanique de Lille, research visit 10.-20. December 12

5.2 Einladungen an Mitglieder des Instituts

Hermann G. Matthies, invitation as visiting Professor to the Université des Sciences et Technologies de Lille UFR de Mathématiques, Département de Mécanique Laboratoire de Mécanique de Lille, 18.04.–20.4. and 28.11–5.12.12.

5.3 Beteiligung am SFB 880 Grundlagen des Hochauftriebs künftiger Verkehrsflugzeuge

Wissenschaftliches Ziel dieses SFB ist es, die technologischen Grundlagen von neuartigen Hochauftriebskonzepten für lärmarme Verkehrsflugzeuge mit Kurzstart- und Kurzlandeeigenschaften zu schaffen. Dabei wirken zahlreiche Forschungsstellen (z.B. Aerodynamik, Akustik, Turbomaschinen u.v.m.) zusammen. Dies wird durch die Beteiligung der Forschungsinstitute der TU Braunschweig, das LU Hannover-Institut für Turbomaschinen und Fluid- Dynamik und durch eine wesentliche Beteiligung des Deutschen Zentrums für Luft- und Raumfahrt (DLR) in Braunschweig erreicht. Eine eingehende Analyse heutiger Verkehrsflugzeuge ergibt einen zukünftigen Bedarf für Hochauftriebssysteme, der

nicht durch die derzeitig vorherrschende, evolutionäre Technologienentwicklung abgedeckt werden kann. Dieses gilt vor allem in den Bereichen der Lärmminderung und der verbesserten Skalierbarkeit der Leistungsparameter von Hochauftriebssystemen bei Start und Landung.

Das Teilprojekt „Quantifizierung der Unsicherheiten in Modellen der Hochauftriebsflugdynamik des Instituts für Wissenschaftl. Rechnens“ untersucht und charakterisiert die Robustheit des Fliegens in Hochauftriebskonfiguration und etwaiger Regelsysteme mit neuartigen, stochastischen Approximations-Verfahren. Bei der Modellierung derartiger Systeme treten meist Unsicherheiten auf, die durch nur ungenau bekannte Parameter, Messungen oder unbekannte Modelleinflüsse bedingt sind. Gegenwärtig wird die Quantifizierung von Unsicherheiten bei der Simulation des Flugverhaltens sowie die Berücksichtigung stochastischer dynamischer Vorgänge in der Atmosphäre in der Form von Monte-Carlo-Simulationen durchgeführt. Hier dagegen werden die Eingangsunsicherheiten und auch alle späteren Ergebnisse als Funktionen unabhängiger Zufallsvariablen modelliert. Um die Unsicherheiten bzgl. Rechenzeit und Speicherbedarf möglichst effizient quantifizieren zu können, wird eine Niedrig-Rang-Approximation mit dünnen Tensorprodukten verwendet.

Ein Graduiertenkolleg ist in den SFB integriert.

Weitere Informationen zum SFB 880 finden Sie unter https://www.tu-braunschweig.de/sfb880

5.4 Eurographics: European Association for Computer Graphics

Aided by Ina Müller the Institute of Scientific Computing is offering editorial and organisational support to the *Eurographics* (EG), which is the only truly Europe-wide professional Computer Graphics association. The association supports its members in advancing the state of the art in Computer Graphics and related fields such as Multimedia, Scientific Visualization and Human Computer Interfaces. Through a world-wide membership, EG maintains close links with developments in the US, Japan and other countries, promoting the exchange of scientific and technical information and skills on a global scale. Eurographics organises many different activities and services for its members, who include researchers, developers, educators and those who work in the computer graphics industry, both as users and providers of computer graphics hardware, software, and applications. The events and services of the Association are available to everyone. The Eurographics Annual Conference is the major annual computer graphics conference in Europe. It brings together graphics experts from around the world to describe

the latest developments. It offers an ideal opportunity to find out what is happening and to meet the people behind the developments. There are also courses at both introductory and advanced levels for managers and technical staff, offering a cost-effective training mechanism for specialised subjects.

Eurographics organises workshops to bring together those working in specific areas. Eurographics has a number of working groups, which promotes cooperation among researchers in the same field. Eurographics has a varied publication activity. See http://diglib.eg.org/ It publishes, among others:

- Computer Graphics Forum: A quarterly journal that has become a respected and authoritative source of information, stocked by many libraries, and is received automatically by EG members.
- Book series: Members of Eurographics can purchase a selection of the proceedings of the Workshop Programme.
- Eurographics Publication Series: Eurographics members are also entitled to discounts on purchases through the Eurographics website.

5.5 Beteiligung am Studiengang CSE

Professor Matthies ist stellvertretender Sprecher des internationalen Master-Studiengangs Computational Sciences in Engineering (CSE).

Der an der Technischen Universität Braunschweig zuerst angebotene und in Deutschland inzwischen kopierte Studiengang CSE wurde gegründet, um dem ständig wachsenden Bedarf der Industrie an qualifiertem Nachwuchs im Bereich Computersimulation gerecht zu werden. Er gibt Studierenden die Möglichkeit, eine spezifische Ingenieur- bzw. Naturwissenschaft zusammen mit dem Wissenschaftlichen Rechnen und der Informationsverarbeitung in einer internationalen und interdisziplinären Umgebung zu studieren.

Die internationale und interdisziplinäre Ausrichtung, die durch die englische Sprache, einen einsemestrigen Auslandsaufenthalt an einer Partneruniversität für deutsche Studierende sowie die Kooperation unterschiedlicher Studiengänge gegeben ist, erweitert die beruflichen Möglichkeiten der Absolventen entscheidend. Die Studienschwerpunkte liegen in den Bereichen Mechanik, Angewandte Mathematik und Angewandte Informatik.

Weitere Informationen zum Studiengang CSE findet man unter:
http://www.tu-braunschweig.de/cse

5.6 Board Memberships

Professor Matthies is Associate Editor for the *ASA- and SIAM Journal on Uncertainty Quantification* as well as a member of the Editorial Advisory Board for the recently launched journal *Advanced Modelling and Simulation in Engineering Sciences* (AMSES).
He is also a member of the Advisory Boards of the SRI - Center for Uncertainty Quantification in Computational Science Engineering at King Abdulla Unviersity of Science and Technology (KAUST), Saudi Arabia.