



# Quantification of Uncertainty: Improving Efficiency and Technology



July 18–21, 2017

*SISSA, International School for Advanced Studies, Trieste, Italy*

## BOOK OF ABSTRACTS



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<http://indico.sissa.it/event/8>



## Welcome

Dear friends,

It is with great pleasure that we welcome you to the QUIET 2017 workshop, to SISSA, and to beautiful Trieste.

It is also a great pleasure to thank each and everyone of you for participating in the workshop. We look forward to all the lectures and posters and to the sessions at which exciting discussions we hope will take place. We have endeavored to structure the workshop so that ample time is provided not only for lectures and poster presentations, but for more informal interactions among participants.

We wish you all the best for a fruitful and enjoyable workshop. We also hope you will enjoy Trieste and, last but not least, SISSA!

Marta D'Elia  
Max Gunzburger  
Gianluigi Rozza

## Venue/Committees/Support

### Venue

SISSA, International School for Advanced Studies  
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Florida State University (Department of Scientific Computing), Tallahassee, USA.

## Scope/Goals/Themes/Structure

### Scope

QUIET 2017 - Quantification of Uncertainty: Improving Efficiency and Technology - is focused on the review of recent algorithmic and mathematical advances and the development of new research directions for uncertainty quantification in the setting of partial differential equations with random inputs. As such, the workshop impacts the scientific, engineering, financial, economic, environmental, social, and commercial milieus.

### Goals

The workshop focuses on some of the most promising approaches for near-future improvements in the way uncertainty quantification problems in the partial differential equation setting are solved. The goals of the workshop include:

- the construction of guidelines for the most promising directions of near-future research
- synergistic exchanges across topics facilitated by the commonality of algorithms used for more than one topic
- the exchange, among participants in each focus theme of the workshop, of recent and even unpublished progress and results
- exposure of a sizable group of junior researchers already active in uncertainty quantification research to new problem areas and new directions for their research.

### Themes

To maximize the probability of success in meeting the workshop goals and to therefore have maximum impact on the UQ community, the workshop focuses on problems with a high number of random parameters and on specific avenues of inquiry that have recently shown considerable promise. Specifically, the themes of the workshop are:

- reduced order modeling
- more efficient solvers
- high-dimensional approximation
- applications

### Structure

The workshop will be of 3.5 days; each day is dedicated to one of the four workshop themes during which invited talks are delivered by both senior and junior speakers. Two poster sessions will be held during which students and early postdocs present their research results. Each day will end with a discussion session at which the participants will review the talks of the day and discuss what are the most important research directions that should be pursued in the future.



# Invited Talks

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# Weighted reduced order methods for parametrized PDEs with random inputs

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In this talk we discuss a weighted approach for the reduction of parametrized PDEs with random input. Reduction methods based on weighted reduced basis (wRB) [1, 2] and a weighted proper orthogonal decomposition (wPOD) approach [3] will be presented.

Concerning wPOD, a first topic of discussion is related to the choice of samples and respective weights according to a quadrature formula. As a proof of concept (applicable only to lower dimensional parameter spaces), we use both Monte-Carlo and tensor product quadrature rules, and discuss the reliability of the resulting wPOD-reduced problem depending on the chosen quadrature formula. Moreover, to reduce the computational effort in the offline stage of wPOD for higher dimensional parameter space, we test Smolyak quadrature rules. The accuracy of the resulting method will be discussed [3].

Concerning wRB, we present a stabilized weighted reduced basis method for random input parameters on advection diffusion problems with dominant convection. Comparisons between offline-online stabilization and offline-only stabilization will be shown [2].

## References

- [1] P. Chen, A. Quarteroni, and G. Rozza. A weighted reduced basis method for elliptic partial differential equations with random input data. *SIAM Journal on Numerical Analysis*, 51(6):3163–3185, 2013.
- [2] D. Torlo, F. Ballarin, and G. Rozza. Stabilized reduced basis methods for advection dominated partial differential equations with random inputs. *In preparation*, 2017.
- [3] L. Venturi, F. Ballarin, and G. Rozza. Weighted POD–Galerkin methods for parametrized partial differential equations in uncertainty quantification problems. *In preparation*, 2017.

# Recent advances in compressed sensing techniques for the numerical approximation of PDEs

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*Compressed Sensing* (CS) is a signal processing technique that allows to acquire a signal using far fewer measurements than those prescribed by the so-called Nyquist-Shannon barrier. In particular, we can recover the best  $s$ -sparse approximation to an  $N$ -dimensional signal, where  $s \ll N$ , by performing  $m \sim s \cdot \text{polylog}(N)$  linear randomized measurements. This approximation is recovered by means of computationally efficient strategies such as  $\ell^1$ -minimization or greedy algorithms.

The aim of this talk is to present the main ideas that recently led to the application of CS to numerical methods for deterministic PDEs and to the uncertainty quantification of parametric PDEs with random inputs.

On the one hand, CS can be employed as a *dimension reduction* technique for the class of Petrov-Galerkin discretizations of PDEs in weak form. We will discuss the so-called **CORSING** technique, where the dimensionality of the stiffness matrix and of the load vector are reduced by exploiting the sparsity of the unknown solution with respect to a suitable basis of trial functions (e.g., wavelets or Fourier-like bases) [4, 5, 3].

On the other hand, in the case of the uncertainty quantification of high-dimensional parametric PDEs with random inputs, CS has been recently proved to be a useful tool for the construction of nonintrusive, highly parallelizable schemes that are able to alleviate the *curse of dimensionality*. These approaches are able to recover the best  $s$ -sparse approximation to a quantity of interest of the solution map with respect to a suitable universal sparsity basis (e.g., tensorized orthogonal polynomials) by means of a few random pointwise samples in the parametric space. In particular, we will present some recent results that show the robustness of this approach when the samples are subject to unknown error [2, 1].

In both cases, we will illustrate the benefits and the limits brought by CS from a numerical analyst's perspective and present some open challenges.

## References

- [1] B. Adcock and S. Brugiapaglia. Correcting for unknown errors in sparse high-dimensional function approximation. *In preparation*, 2017.
- [2] B. Adcock, S. Brugiapaglia, and C. G. Webster. Polynomial approximation of high-dimensional functions via compressed sensing. *arXiv preprint arXiv:1703.06987*, 2017.
- [3] S. Brugiapaglia. *COMpRessed SolvING: sparse approximation of PDEs based on compressed sensing*. PhD thesis, MOX - Politecnico di Milano, 2016.
- [4] S. Brugiapaglia, S. Micheletti, and S. Perotto. Compressed solving: A numerical approximation technique for elliptic PDEs based on Compressed Sensing. *Comput. Math. Appl.*, 70(6):1306–1335, 2015.
- [5] S. Brugiapaglia, F. Nobile, S. Micheletti, and S. Perotto. A theoretical study of COMpRessed SolvING for advection-diffusion-reaction problems. *Math. Comput.*, to appear, 2017.

# Hessian-based sampling for goal-oriented model reduction

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Model reduction techniques for parametric partial differential equations have been well developed to reduce the computational cost in many-query or real-time applications, such as optimal design/control, parameter calibration, and uncertainty quantification. However, it remains a great challenge to construct an efficient and accurate reduced order model (ROM) for high-dimensional parametric problems. One reason is that sampling in the high-dimensional parameter space for the construction of the ROM often faces curse of dimensionality, i.e., the computational complexity grows exponentially with respect to the number of parameter dimensions. The other is that the parametric solution manifold may be essentially high-dimensional such that a very large number of reduced basis functions have to be used in order to achieve certain required accuracy, which limits the efficacy of the computational reduction.

In this talk, we present a Hessian-based sampling method for goal-oriented model reduction to effectively construct a ROM that has good approximation property for some given quantity of interest (QoI) as a function of the parametric solution [1]. The rationale is that even the dimension of the solution manifold is high, the dimension of the quantity of interest, such as an average of the solution in a particular physical domain, is relatively low. To capture this low-dimensionality, we explore the curvature of the QoI in the parameter space informed by its Hessian [2, 3]. More specifically, take a (infinite-dimensional) parameter field  $m$  with Gaussian measure  $N(m_0, C)$  for example, where  $m_0$  is the mean and  $C$  is the covariance. A QoI  $Q$  that depends (implicitly through the solution) on the parameter  $m$  can be approximated by a truncated Taylor expansion up to the quadratic term as

$$Q_{\text{quad}}(m) = Q(m_0) + \langle Q_m, m - m_0 \rangle + \frac{1}{2} \langle Q_{mm}(m - m_0), m - m_0 \rangle.$$

Then the expectation of  $Q$  can be approximated by

$$\mathbb{E}[Q_{\text{quad}}] = Q(m_0) + \frac{1}{2} \text{tr}(H),$$

where  $\text{tr}(\cdot)$  is a trace operator, and  $H = C^{1/2} Q_{mm} C^{1/2}$  is the (covariance-preconditioned) Hessian. Thus, the variation of  $Q_{\text{quad}}$  is captured by the trace of the Hessian and the most sensitive directions of the parameter for the QoI are the eigen-directions of the Hessian corresponding to its leading eigenvalues. Therefore, we project the parameter  $m$  to the subspace spanned by the eigen-directions of the Hessian and sampling from this subspace for the construction of the ROM. We demonstrate by several numerical experiments that this Hessian-based sampling gives much smaller ROM approximation error for the QoI than that by a random sampling method.

## References

- [1] P. Chen and O. Ghattas. Hessian-based sampling for goal-oriented model reduction. *in preparation*, 2017.
- [2] P. Chen, U. Villa, and O. Ghattas. Hessian-based adaptive sparse quadrature for infinite-dimensional Bayesian inverse problems. *preprint*, 2016.
- [3] P. Chen, U. Villa, and O. Ghattas. Taylor approximation and variance reduction for PDE-constrained optimal control under uncertainty. *preprint*, 2016.

# Collocation Methods for Exploring Perturbations in Linear Stability Analysis

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We show that the methods of sparse-grid collocation used in uncertainty quantification can be used to develop new efficient algorithms to explore the stability of dynamical systems. In particular, eigenvalue analysis is a well-established tool for stability analysis, but there are situations where eigenvalues miss some important features of physical models. For example, in models of incompressible fluid dynamics, there are examples where linear stability analysis predicts stability but transient simulations exhibit significant growth of infinitesimal perturbations. This behavior can be predicted by pseudo-spectral analysis. In this study, we show that an approach similar to pseudo-spectral analysis can be performed inexpensively using stochastic collocation methods and the results can be used to provide quantitative information about instability. In addition, we demonstrate that the results of the perturbation analysis provide insight into the behavior of unsteady flow simulations.

# Operator based multi-scale analysis of simulation bundles

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We propose a new mathematical data analysis approach, which is based on the mathematical principle of symmetry, for the post-processing of bundles of finite element data from computer-aided engineering, which we consider as data points in a high-dimensional space, whose dimension is the number of grid points. Since all those numerical simulation data stem from the numerical solution of the same partial differential equation, there exists a set of transformations, albeit unknown, which map simulation to simulation. The transformations can be obtained indirectly by constructing a transformation invariant positive definite operator valid for all simulations.

The eigenbasis of such an operator turns out to be a convenient basis for the handled simulation set due to two reasons. First, the spectral coefficients decay very fast, depending on the smoothness of the function being represented, and therefore a reduced multi-scale representation of all simulations can be obtained, which depends on the employed operator. Second, at each level of the eigendecomposition the eigenvectors can be seen to recover different independent variation modes like rotation, translation or local deformation. Furthermore, this representation enables the definition of a new distance measure between simulations using the spectral coefficients. From a theoretical point of view the space of simulations modulo a transformation group can be expressed conveniently using the operator eigenbasis as orbits in the quotient space with respect to a specific transformation group.

Based on this mathematical framework we study several examples. We show that for time dependent datasets from engineering simulations only a few spectral coefficients are necessary to describe the data variability, while the coarse variations get separated from the finer ones. Low dimensional structures are obtained in this way, which are able to capture information about the underlying high dimensional simulation space. An effective mechanism to deal effectively with the analysis of many numerical simulations is obtained, due to the achieved dimensionality reduction. Furthermore, we investigate if the derived representation of the simulation space can also be used in the context of reduced basis methods.

# Modeling variability in cardiac electrophysiology

J.-F. Gerbeau<sup>1,2</sup>, D. Lombardi<sup>1,2</sup>, and E. Tixier<sup>1,2</sup>

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Many phenomena are modeled by deterministic differential equations, whereas the observation of these phenomena, in particular in life science, exhibit an important inter-subject variability. We will address the following question: how the model can be adapted to reflect the variability observed in a population?

We will present a non-parametric and non-intrusive procedure based on offline computations of the deterministic model [1]. The algorithm infers the probability density function of uncertain parameters from the matching of the observable statistical moments at different points in the physical domain. This inverse procedure is improved by incorporating a point selection algorithm that both reduces its computational cost and increases its robustness.

The method will be illustrated for different models, based on Ordinary or Partial Differential Equations. In particular, applications to experimental data sets in cardiac electrophysiology will be presented.

## References

- [1] J.-F. Gerbeau, D. Lombardi, and E. Tixier. A moment-matching method to study the variability of phenomena described by partial differential equations. *Preprint hal-01391254*, 2016. <https://hal.archives-ouvertes.fr/hal-01391254>.

# Sparse Grid Methods in Uncertainty Quantification

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In this presentation, we give an overview on generalized sparse grid methods for stochastic and parametric partial differential equations as they arise in various forms in uncertainty quantification. We focus on the efficient approximation and treatment of the stochastic/parametric variables and discuss both, the case of finite and infinite/parametric stochastic dimension. Moreover, we deal with optimal numerical schemes based on sparse grids where also the product between the spatial and temporal variables and the stochastic/parametric variables is collectively taken into account. Overall, we obtain approximation schemes which involve cost complexities that resemble just the cost of the numerical solution of a constant number of plain partial differential equations in space (and time), i.e. without any stochastic/parametric variable. Here, this constant number depends only on the covariance decay of the stochastic fields of the input data of the overall problem. We give examples from incompressible non-Newtonian fluid simulations.



# Structure Preserving Reduced Order Models

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The development of reduced order models for complex applications, offering the promise for rapid and accurate evaluation of the output of complex models under parameterized variation, remains a very active research area. Applications are found in problems which require many evaluations, sampled over a potentially large parameter space, such as in optimization, control, uncertainty quantification and applications where near real-time response is needed.

However, many challenges remain to secure the flexibility, robustness, and efficiency needed for general large scale applications, in particular for nonlinear and/or time-dependent problems.

In this talk, we discuss recent developments of reduced methods that conserve chosen invariants for nonlinear time-dependent problems. We pay particular attention to the development of reduced models for Hamiltonian problems and propose a greedy approach to build the basis [1]. As we shall demonstrate, attention to the construction of the basis must be paid not only to ensure accuracy but also to ensure stability of the reduced model. The performance of the approach is demonstrated for both ODEs and PDEs.

We discuss how to extend the approach to include more general dissipative problems through the notion of port-Hamiltonians, resulting in reduced models that remain stable even in the limit of vanishing viscosity [2]

To extend this to more general classes of problems, not endowed with a Hamiltonian structure, we consider methods that preserve specific quantities, e.g., mass conservation or Casimirs, and show that the combination of structure preserving Runge-Kutta methods with a carefully chosen basis results in stable reduced order methods for general classes of nonlinear time-dependent problems.

## References

- [1] B. Afkham and J. Hesthaven. Structure-preserving model-reduction of parametric hamiltonian systems. - *submitted*, 2016.
- [2] B. Afkham and J. Hesthaven. Structure-preserving model-reduction of dissipative hamiltonian systems. - *submitted*, 2017.

# Reduced-order models with space-adapted snapshots

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Space-adaptive numerical methods have recently found their way into reduced-order modeling of parametrized PDEs [1, 2, 3]. Standard techniques assume that all snapshots are computed with one and the same spatial mesh, which is often not appropriate for multi-scale problems. Instead, we consider unsteady adaptive finite elements, where the spatial discretization varies over time or stochastic sampling. Our focus is on reduced-order models obtained by a Galerkin projection onto a proper orthogonal decomposition (POD) of solution samples. In this context, adaptive snapshot computations allow a reduction of computational complexity in the offline-phase of the reduced-order model.

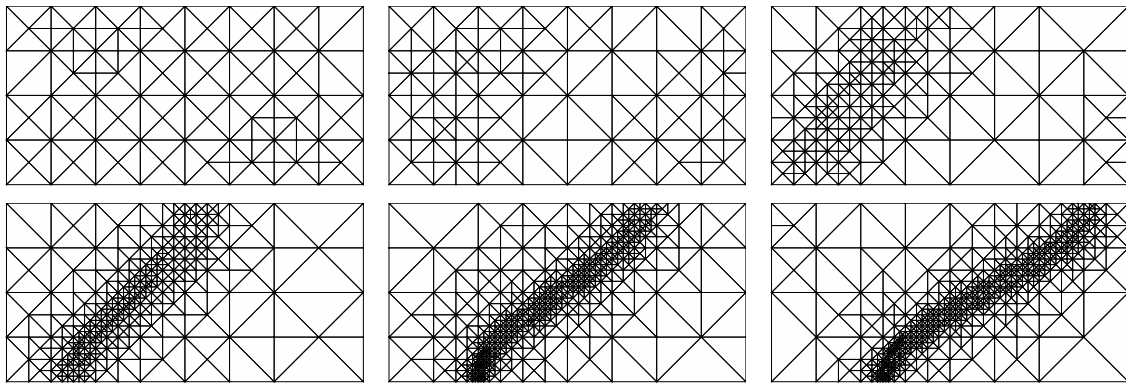


Figure 1: Adaptive finite element spatial discretizations.

The following points will be discussed in the talk:

- How can the effort for creating reduced-order models with space-adapted snapshots be minimized?
- How can the union of all snapshot meshes be avoided?
- What is the main difference between static and adaptive snapshots in the error analysis of Galerkin reduced-order models?

Numerical test cases illustrate the convergence properties with respect to the number of POD basis functions.

## References

- [1] M. Ali, K. Steih, and K. Urban. Reduced basis methods with adaptive snapshot computations. *Adv. Comput. Math.*, doi:10.1007/s10444-016-9485-9, 2016.
- [2] S. Ullmann, M. Rotkvic, and J. Lang. POD-Galerkin reduced-order modeling with adaptive finite element snapshots. *J. Comput. Phys.*, 325:244–258, 2016.
- [3] M. Yano. A minimum-residual mixed reduced basis method: exact residual certification and simultaneous finite-element reduced-basis refinement. *ESAIM: M2AN*, 50:163–185, 2016.

# Stabilization of EIM and PBDW Methods with Noisy Observations

Y. Maday<sup>1,2</sup>, J.-P. Aragaud<sup>3</sup>, B. Bouriquet<sup>3</sup>, G. Helin<sup>1,3</sup>, O. Mula<sup>4</sup>, A. T. Patera<sup>5</sup>, J. D. Penn<sup>5</sup>, T. Taddei<sup>1</sup>, and M. Yano<sup>6</sup>

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Empirical Interpolation Methods (EIM) and their Generalizations (GEIM) allow to provide, in the frame of model order reduction methods, rapid, stable and accurate reconstruction of function that we have been able to learn the behavior in an off line stage. It is complemented with the parametrized-background data-weak (PBDW) formulation to possibly correct a bias between the learning process, synthesized in a reduce basis and the true behavior.

In this talk we shall present an overview of the qualities of these approach when noisy data are available and how to best use the knowledge of the reduced space in order to diminish the negative effect of the noisy data.

This presentation will synthesize the collaborations through many contributions.

# Model order reduction for real time decisions from incomplete and uncertain measurements

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Next generation of autonomous vehicles will be able to make operational decisions in real-time to face and cope with unplanned circumstances without compromising the successful completion of their tasks. Accounting for unplanned circumstances requires the ability to monitor and capture both the evolution of the system health (self-awareness) and the dynamic change of the surrounding environment (situational awareness). This form of autonomous reasoning can be formalized as instance of the general paradigm of a Sense-Infer-Plan-Act flow able to process data into information, information into knowledge, and knowledge into intelligent decisions. In the Sense-Infer-Plan-Act framework, awareness encompasses the ability to (i) sense informative quantities, (ii) use measured data to infer the state of the system, and (iii) use this estimate to update system capabilities and re-plan operational strategies. Our studies [1, 2, 3, 4] address the specific problem of supporting self-awareness and propose to associate the Sense-Infer-Plan-Act flow with measurements (physical quantities that can be monitored with sensors) and capabilities (quantities that evolve with the state of the system and limit the operational space). In this framework, we tackle the time-constrained problem of obtaining efficient estimates of capabilities from sensor measurements; in particular, we consider measured data that may be incomplete and affected by uncertainties in both sensor location and sensor accuracy. To achieve this goal, we develop an offline-online methodology that combines model order reduction and localization techniques into a Multi-Step Reduced Order Modeling (MultiStep-ROM) procedure. In addition, we propose a novel approach for the identification of the most informative sensor locations: this strategy couples unsupervised learning techniques with MultiStep-ROM and allows for a drastic reduction in the number of sensors required to achieve reliable predictions of capabilities and well-informed decisions. We apply our methodologies to the practical case of autonomous aerospace vehicles that dynamically adapt their mission to the evolution of their structural state. In particular, our approaches are demonstrated for the real-time structural assessment of a composite wing panel undergoing a variety of damage conditions.

## References

- [1] D. Allaire, D. Kordonowy, M. Lecerf, L. Mainini, and K. Willcox. Multifidelity DDDAS methods with application to a self-aware aerospace vehicle. *Procedia Computer Science*, 29:1182–1192, 2014.
- [2] L. Mainini and K. Willcox. Sensitivity analysis of surrogate-based methodology for real-time structural assessment. *AIAA SciTech 2015*, AIAA Paper 2015-1362, 2015.
- [3] L. Mainini and K. Willcox. Surrogate modeling approach to support real-time structural assessment and decision making. *AIAA Journal*, 53:1612–1626, 2015.
- [4] L. Mainini and K. Willcox. Data to decisions: Real-time structural assessment from sparse measurements affected by uncertainty. *Computers & Structures*, 182:296–312, 2017.

# Conditional Expectation as the Basis of Bayesian Updating

H. G. Matthies<sup>1</sup>

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Introducing new information into a probabilistic description of knowledge is typically performed via some kind of application of Bayes's by now classical theorem. To avoid ambiguities (which did arise historically), the mathematically precise description of conditional probabilities in Bayes's theorem, especially when conditioning on events of vanishing probability, is formulated via conditional expectations, and is due to Kolmogorov. Nevertheless, most sampling approaches to Bayesian updating typically start from the classical formulation involving conditional measures and densities. These are usually the distributions of some random variables describing the prior knowledge. Here an alternative track is taken, in that the notion of conditional expectation is also taken computationally as the prime object. Being able to numerically approximate conditional expectations, one has a complete description of the posterior probability. A further task is to construct a new – transformed, or filtered – random variable which has a distribution as required by the (posterior) conditional expectations. In the talk, the abstract task and its solution will be presented first, and then different computational approximations will be sketched, as well as different ways of stochastic discretisations, adding another level of approximation. It is also possible – although not necessary – to formulate these concepts in a more algebraic/functional analytic setting. Here the fundamental notions are algebras of random variables and a distinguished linear functional called expectations. These connections will be shortly sketched, and show a possible joint theoretical and computational basis.

# Multivariate approximation in downward closed polynomial spaces

G. Migliorati<sup>1</sup>

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We present some results for multivariate approximation in polynomial spaces associated with downward closed index sets. By means of such results:

- we derive error estimates and convergence rates for the approximation on downward closed polynomial spaces of the solution to some relevant elliptic PDEs with parametric or stochastic diffusion coefficient,
- and we discuss adaptive and nonadaptive numerical algorithms based on interpolation or discrete least-squares approximation.

# Dictionary measurement selection for state estimation with reduced basis

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Parametric PDEs of the general form

$$\mathcal{P}(u, a) = 0$$

are commonly used to describe many physical processes, where  $\mathcal{P}$  is a differential operator,  $a$  is a high-dimensional vector of parameters and  $u$  is the unknown solution belonging to some Hilbert space  $V$ . A typical scenario in state estimation is the following: for an unknown parameter  $a$ , one observes  $m$  independent linear measurements of  $u(a)$  of the form  $\ell_i(u) = (w_i, u)$ ,  $i = 1, \dots, m$ , where  $\ell_i \in V'$  and  $w_i$  are the Riesz representers, and we write  $W_m = \text{span}\{w_1, \dots, w_m\}$ . The goal is to recover an approximation  $u^*$  of  $u$  from the measurements. Due to the dependence on  $a$  the solutions of the PDE lie in a manifold and the particular PDE structure often allows to derive good approximations of it by linear spaces  $V_n$  of moderate dimension  $n$ . In this setting, the observed measurements and  $V_n$  can be combined to produce an approximation  $u^*$  of  $u$  up to accuracy

$$\|u - u^*\| < \beta^{-1}(V_n, W_m) \text{dist}(u, V_n)$$

where

$$\beta(V_n, W_m) := \inf_{v \in V_n} \frac{\|P_{W_m} v\|}{\|v\|}$$

plays the role of a stability constant. For a given  $V_n$ , one relevant objective is to guarantee that  $\beta(V_n, W_m) > \gamma > 0$  with a number of measurements  $m > n$  as small as possible. We present results in this direction when the measurement functionals  $\ell_i$  belong to a complete dictionary.

# Multi-Index polynomial chaos methods for random PDEs

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In this talk we consider the problem of computing statistics of the solution of a partial differential equation with random data, where the random coefficient is parametrized by means of a finite or countable sequence of terms in a suitable expansion. We focus in particular on polynomial chaos type approximations with respect to the random parameters combined with hierarchical discretizations in the physical space.

When the polynomial chaos approximation is computed by Stochastic Collocation, this gives rise to a Multi-Level or more generally a Multi-Index Stochastic Collocation (MISC) method [2, 1, 4]. MISC is a combination technique based on mixed differences of spatial approximations and quadratures over the space of random data. Provided enough mixed regularity is available, MISC can achieve better complexity than a single level Stochastic Collocation method. Moreover, we show that in the optimal case the convergence rate of MISC is only dictated by the convergence of the deterministic solver applied to a one-dimensional spatial problem. We propose optimization procedures to select the most effective mixed differences to include in MISC. Such optimization is a crucial step that allows us to make MISC computationally effective.

Alternative to Stochastic Collocation methods, we present also Multi-level / Multi-index versions of discrete (weighted) least squares approximations on polynomial spaces, based on evaluations in random points and with different accuracy levels [3]. In particular, we show rigorous results on the minimum number of evaluations to acquire on each level to have a stable approximation and optimal complexity.

We show the effectiveness of multi-level / multi-index Stochastic Collocation and least squares methods on some computational tests, including tests with a infinite countable number of random parameters.

## References

- [1] A.-L. Haji-Ali, F. Nobile, L. Tamellini, and R. Tempone. Multi-index stochastic collocation convergence rates for random PDEs with parametric regularity. *Found. Comp. Math.*, 16(6):1555–1605, 2016.
- [2] A.-L. Haji-Ali, F. Nobile, L. Tamellini, and R. Tempone. Multi-Index Stochastic Collocation for random PDEs. *Comput. Methods Appl. Mech. Engrg.*, 306:95–122, 2016.
- [3] A.-L. Haji-Ali, F. Nobile, R. Tempone, and S. Wolfers. Multilevel weighted least squares polynomial approximation. in preparation.
- [4] F. Nobile, R. Tempone, and S. Wolfers. Sparse approximation of multilinear problems with applications to kernel-based methods in UQ. arXiv:1609.00246.



# Scalable Hierarchical Sampling of Gaussian Random Fields for Large-Scale Multilevel Monte Carlo Simulations

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We consider the numerical simulation of physical phenomena governed by partial differential equations (PDEs) with uncertain input data in a multilevel Monte Carlo (MLMC) framework. Generating samples of random fields with prescribed statistical properties efficiently is an important component of MLMC methods. We present a highly scalable multilevel, hierarchical sampling technique that involves solving a mixed formulation of a stochastic partial differential equation. This formulation allows us to leverage existing scalable methods for solving the resulting sparse linear systems arising from the mixed finite element discretization. The proposed sampling technique is then used to generate different realizations of random fields to be used as input coefficient realizations within the MLMC method.

Multilevel Monte Carlo techniques typically rely on the existence of hierarchies of computational meshes obtained by successive refinement. Instead, we use specialized element-based agglomeration techniques to construct hierarchies of coarse spaces that possess stability and approximation properties for wide classes of PDEs on unstructured meshes. An application to subsurface flow using the MLMC method with algebraically coarsened spaces with the proposed sampling technique will be presented to demonstrate the scalability of the method for large-scale simulations.

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# Multifidelity methods for uncertainty propagation and rare event simulation

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In many situations across computational science and engineering, multiple computational models are available that describe a system of interest. These different models have varying evaluation costs and varying fidelities. Typically, a computationally expensive high-fidelity model describes the system with the accuracy required by the current application at hand, while lower-fidelity models are less accurate but computationally cheaper than the high-fidelity model. Uncertainty quantification typically requires multiple model solves at many different inputs, which often leads to computational demands that exceed available resources if only the high-fidelity model is used. We present multifidelity methods for uncertainty propagation and rare event simulation that leverage low-cost low-fidelity models for speedup and occasionally make recourse to the expensive high-fidelity model to establish unbiased estimators. Our methods combine low-fidelity models of any type, including projection-based reduced models, data-fit models and response surfaces, coarse-grid approximations, and simplified-physics models. Our numerical results demonstrate that our multifidelity methods achieve significant speedups while providing unbiased estimators, even in the absence of error control for the low-fidelity models.

# Improving Sampling-based Uncertainty Quantification Performance Through Embedded Ensemble Propagation

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A key component of computational uncertainty quantification is the forward propagation of uncertainties in simulation input data to output quantities of interest. Typical approaches involve repeated sampling of the simulation over the uncertain input data, and can require numerous samples when accurately propagating uncertainties from large numbers of sources. Often simulation processes from sample to sample are similar and much of the data generated from each sample evaluation could be reused.

In this talk, we explore a new method for implementing sampling methods that simultaneously propagates groups of samples together in an embedded fashion, which we call embedded ensemble propagation [3]. We show how this approach exploits properties of modern computer architectures to improve performance by enabling reuse between samples, reducing memory bandwidth requirements, improving memory access patterns, improving opportunities for fine-grained parallelization, and reducing communication costs. We describe a software technique for implementing embedded ensemble propagation based on the use of C++ templates, and demonstrate improved performance for the approach when applied to model diffusion problems on a variety of contemporary architectures.

A challenge with this method however is ensemble-divergence, whereby different samples within an ensemble choose different code paths. This can reduce the effectiveness of the method and increase computational cost. Therefore grouping samples together to minimize this divergence is paramount in making the method effective for challenging computational simulations. We also present several grouping approaches [1, 2] that attempt to minimize this divergence through surrogate models of ensemble computational cost. These approaches are developed within the context of locally adaptive stochastic collocation methods and Voronoi piecewise surrogate methods [4], and are applied to highly anisotropic diffusion problems where computational cost is driven by the number of (preconditioned) linear solver iterations, which vary widely from sample to sample.

## References

- [1] M. D’Elia, H. Edwards, J. Hu, E. Phipps, and S. Rajamanickam. Ensemble grouping strategies for embedded stochastic collocation methods applied to anisotropic diffusion problems. *Submitted to SIAM Journal on Uncertainty Quantification*, 2016.
- [2] M. D’Elia, E. Phipps, A. Rushdi, and M. Ebeida. Surrogate-based ensemble grouping strategies for embedded sampling-based uncertainty quantification. *Submitted to SIAM Journal on Uncertainty Quantification*, 2017. <https://arxiv.org/abs/1705.02003>.
- [3] E. Phipps, M. D’Elia, H. C. Edwards, M. Hoemmen, J. Hu, and S. Rajamanickam. Embedded ensemble propagation for improving performance, portability, and scalability of uncertainty quantification on emerging computational architectures. *SIAM Journal on Scientific Computing*, 39(2):C162–C193, 2017.
- [4] A. Rushdi, L. Swiler, E. Phipps, M. D’Elia, and M. Ebeida. VPS: Voronoi piecewise surrogate models for high-dimensional data fitting. *International Journal for Uncertainty Quantification*, 7(1):1–21, 2017.

# An Efficient Reduced Basis Solver for Stochastic Galerkin Matrix Equations

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Stochastic Galerkin finite element approximation of PDEs with random inputs leads to linear systems of equations with coefficient matrices that have a characteristic Kronecker product structure. By reformulating the systems as multiterm linear matrix equations, we develop (see [1]) a memory-efficient solution algorithm which generalizes ideas from rational Krylov subspace approximation. Our working assumptions are that the number of random variables characterizing the random inputs is modest (in the order of a few tens) and that the dependence on these variables is linear, so that it is sufficient to seek only a reduction in the complexity associated with the spatial component of the approximation space. The new approach determines a low-rank approximation to the solution matrix by performing a projection onto a low-dimensional space and provides an efficient solution strategy whose convergence rate is independent of the spatial approximation. Moreover, it requires far less memory than standard preconditioned Krylov methods applied to the Kronecker formulation of the linear systems.

## References

- [1] C. E. Powell, D. Silvester, and V. Simoncini. An efficient reduced basis solver for stochastic galerkin matrix equations. *SIAM Journal on Scientific Computing*, 39(1):A141–A163, 2017.

# Goal-oriented error estimation for fast approximations of nonlinear problems

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Numerical simulation is a key component of numerous domains: industry, environment, engineering, physics for instance. In some cases time is the limiting factor, and the numerical simulation should be very fast and accurate. The computing time must be very short, either because the computation is repeated many times in a relatively short interval (*many-query context*) or because the result cannot wait (*real-time context*).

To tackle this issue, several procedures of accelerating existing numerical models have been proposed. The general idea of such procedures consists in replacing the existing model, called the *full* model, by a fast and accurate approximation, called *metamodel*, or *surrogate model*. It is possible in some cases to design metamodels which include a certified error bound. In this latter case, the user does not know exactly the approximation error, but the error is guaranteed to be lower than the provided bound. Moreover, the error bound computation is included in the metamodel, so that its computational burden stays small compared to the full model. For example, we can cite [3] where the authors provide such bounds in the framework of the reduced basis method (dimension reduction).

Providing such error bound for nonlinear problems is the aim of this work. More precisely, let  $\mathcal{P} \subset \mathbb{R}^d$  denote a parameter space, and let  $P$  be a probability distribution on  $\mathcal{P}$ . Let  $X$  (*resp.*  $Y$ ) be a finite dimensional vector space endowed with a scalar product  $\langle \cdot, \cdot \rangle_X$  (*resp.*  $\langle \cdot, \cdot \rangle_Y$ ). We consider a nonlinear function  $\mathcal{M} : \mathcal{P} \times X \rightarrow Y$ . Given a parameter  $\mu \in \mathcal{P}$ , we denote by  $u(\mu) \in X$  a solution to the equation:

$$\mathcal{M}(\mu, u(\mu)) = 0, \quad (1)$$

and we define the *output* by  $s(\mu) = \langle \ell, u(\mu) \rangle_X$ , for a given  $\ell \in X$ .

We assume that for every  $\mu \in \mathcal{P}$ , Equation (1) admits a unique solution in  $X$ , so that the application  $s : \mathcal{P} \rightarrow \mathbb{R}$  is well-defined. Denote  $\mathcal{N}$  the dimension of  $X$ .

As already mentioned, it is common in a *many-query context*, or in a *real-time context*, to call for model reduction (*metamodelling*). More precisely, let  $\tilde{X}$  be a subspace of  $X$ , of dimension  $N$  such that  $N \ll \mathcal{N}$ . We consider  $\tilde{u} : \mathcal{P} \rightarrow \tilde{X}$  a surrogate model (in a very wide sense of the term) of  $u : \mathcal{P} \rightarrow X$ . Let us define the approximate output  $\tilde{s}(\mu)$  by  $\tilde{s}(\mu) = \langle \ell, \tilde{u}(\mu) \rangle_X$ .

The objective is then to provide some probabilistic error bound between  $s(\mu)$  and  $\tilde{s}(\mu)$ . In other words, one accepts the risk of this bound  $\epsilon(\mu; \alpha)$  being violated for a set of parameters having "small" probability measure  $\alpha \in (0, 1)$ :  $(|s(\mu) - \tilde{s}(\mu)| \geq \epsilon(\mu; \alpha)) \leq \alpha$ . This quantity  $\epsilon(\mu; \alpha)$  is a so-called *goal-oriented probabilistic error bound*.

The methodology we propose here in the nonlinear framework [2] is an extension of the one in [1].

## References

- [1] A. Janon, M. Nodet, and C. Prieur. Goal-oriented error estimation for the reduced basis method, with application to sensitivity analysis. *Journal of Scientific Computing*, 68(1):21–41, 2016.
- [2] A. Janon, M. Nodet, C. Prieur, and C. Prieur. Goal-oriented error estimation for fast approximations of nonlinear problems. Research report, 2016.
- [3] N. Nguyen, K. Veroy, and A. Patera. Certified real-time solution of parametrized partial differential equations. In *Handbook of Materials Modeling*, pages 1523–1558. Springer, 2005.

# Tackling UQ in DARMA, a Programming Model for Task-Based Execution at Extreme-Scale

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This talk focuses on the advantages of task-based implementations and execution models for UQ problems. Task-based models show the potential to mitigate critical challenges posed by extreme-scale architectures such as exposing maximal parallelism, managing data locality and deep memory hierarchies, and hiding communication latency. Specifically, we demonstrate how to tackle UQ using DARMA (Distributed Asynchronous Resilient Models and Applications) (<http://www.sandia.gov/darma/>), an abstraction layer for asynchronous many-task (AMT) runtimes [2] that uses C++ template metaprogramming to facilitate the capture of data-task dependencies [1]. In this talk we (a) summarize how concurrency and parallelism are expressed using DARMA among independent UQ tasks, and (b) present an analysis of the benefits of reusing, within a pool of samples, tasks results to accelerate the execution time of other independent tasks. We demonstrate a set of basic UQ examples written in the DARMA, and then focus on a Multi-Level Monte Carlo test case.

## References

- [1] D. S. Hollman, J. C. Bennett, H. Kolla, J. Lifflander, N. Slattengren, and J. Wilke. Metaprogramming-enabled parallel execution of apparently sequential c++ code. In *Proceedings of the Second International Workshop on Extreme Scale Programming Models and Middleware*, pages 24–31, 2016.
- [2] J. J. Wilke, J. C. Bennett, D. S. Hollman, N. L. Slattengren, H. Kolla, F. Rizzi, R. L. Clay, and K. Teranishi. The darma approach to asynchronous many-task programming. Technical report, Presented at ECP Review 2016, Sandia National Laboratories, 2016.

# Stochastic sensitivity analysis to grid resolution and closure modeling in large-eddy simulation

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Nowadays, large-eddy simulation (LES) is increasingly applied to complex flow configurations of interest in technological or environmental applications. In this context, the assessment of the quality and reliability of LES results has become a topic of increasing interest. A systematic exploration of the sensitivity to the different parameters involved in the computational set up or in physical modeling is difficult for LES, due to the large costs of each single simulation, and it may become unaffordable for complex cases or when a large number of parameters is involved. A possible approach, which is being increasingly used in recent years in computational fluid dynamics, is Uncertainty Quantification (UQ), in which the uncertain or unknown parameters are modeled as input random variables with a given probability distribution. These uncertainties can be propagated through the computational model to statistically quantify their effect on the results. Since this propagation process implies large computational costs, especially for LES, a computationally inexpensive surrogate model is usually adopted to build continuous response surfaces in the parameter space.

As an example of stochastic sensitivity analysis to discretization and modeling parameters, we consider herein the flow around a 5:1 rectangular cylinder, which is the object of an international benchmark (BARC) collecting experimental and numerical flow realizations [1]. The BARC configuration is of practical interest, e.g. in civil engineering, and, in spite of the simple geometry, the related flow dynamics and topology is complex. Significant dispersion of the BARC predictions was observed for some quantities, also in LES, and deterministic sensitivity analyses were not conclusive. LES are carried out here by using a spectral-element numerical method. An explicit quadratic low-pass filter in the modal space is used, characterized by a cut-off value and by a weight function, which provides dissipation of the modes higher than the cut off and acts as a SGS dissipation. The uncertain parameters are the size of the spectral elements in the spanwise direction and the weight of the explicit filter. The latter has been chosen because it directly controls the amount of SGS dissipation, while the sensitivity to the grid resolution in the spanwise direction is investigated because of the high impact of this parameter shown in some of the LES simulations (see the discussion in [1]). The impact of the uncertainty in these parameters is evaluated through generalized polynomial chaos. The most-probable values and the stochastic variance of the results are compared with the ensemble average and with the overall dispersion of the BARC predictions respectively.

## References

- [1] L. Bruno, M. V. Salvetti, and F. Ricciardelli. Benchmark on the Aerodynamics of a Rectangular 5:1 Cylinder: an overview after the first four years of activity. *J. Wind Eng. Ind. Aerod.*, 126:87–106, 2014.

# Uncertainty Quantification in Materials Modeling

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Uncertainty is ubiquitous in nature. In materials modeling, uncertainty can arise from many sources, including constitutive relations, material microstructure, and source terms, as well as boundary and/or initial conditions. In this presentation, we will provide an overview of uncertainty quantification (UQ) for materials modeling, with application examples from fracture mechanics. We will review the peridynamics theory of solid mechanics, a nonlocal reformulation of classical continuum mechanics suitable for material failure and damage simulation, and we will demonstrate the application of UQ methodologies to various peridynamic problems of interest, including crack propagation in glass, fiber-reinforced composites, and ceramics.



# Sensitivity Analysis and Active Subspace Construction for Surrogate Models Employed for Bayesian Inference

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For many complex models, the computational cost of high-fidelity codes precludes their direct use for Bayesian inference and uncertainty propagation. For example, the considered neutronics and nuclear thermal hydraulics codes can take hours for a single run. Furthermore, models often have tens to thousands of inputs – comprised of parameters, initial conditions, or boundary conditions – many of which are nonidentifiable or noninfluential in the sense that they are not uniquely determined by measured responses. In this presentation, we will discuss techniques to isolate influential inputs and construct surrogate models for Bayesian inference and uncertainty propagation.

As detailed in [1, 5], global sensitivity analysis is commonly employed to isolate subsets of influential parameters. Since parameter distributions are not typically known *a priori*, one often assumes that parameters are independent and uniformly distributed. However, we will demonstrate for a problem arising in quantum-informed continuum modeling for ferroelectric materials that this can yield incorrect conclusions for correlated parameter sets.

Alternatively, one can employ QR or SVD analysis to construct active subspaces comprised of linear combinations of parameters [2, 6]. We will motivate this analysis by considering gradient-based techniques but focus primarily on gradient-free active subspace techniques for codes that do not have adjoint capabilities [3]. We illustrate these techniques for a neutronics code having approximately 5000 inputs.

Finally, by employing activity scores to rank parameter sensitivity, we will demonstrate the manner in which Bayesian inference using surrogate models constructed on active subspaces can be used to construct posterior densities for nonidentifiable physical parameter sets [4]. We illustrate these techniques for an elliptic PDE having 91 input parameters and a closure relation employed in a two-phase nuclear thermal hydraulic code.

## References

- [1] F. Campolongo, J. Cariboni, and A. Saltelli. An effective screening design for sensitivity analysis of large models. *Environmental Modelling and Software*, 22:1509–1518, 2007.
- [2] P. G. Constantine. *Active Subspaces: Emerging Ideas for Dimension Reduction in Parameter Studies*. SIAM, Philadelphia, PA, 2015.
- [3] A. Lewis, R. C. Smith, and B. Williams. Gradient-free active subspace construction using Morris screening elementary effects. *Computers and Mathematics with Applications*, 72:1603–1615, 2016.
- [4] A. Lewis, R. C. Smith, and B. Williams. Bayesian model calibration on active subspaces. *Proceedings of the 2017 American Control Conference*, Paper 978-1-5090-5994-2, 2017.
- [5] R. C. Smith. *Uncertainty Quantification: Theory, Implementation, and Applications*. SIAM, Philadelphia, PA, 2014.
- [6] M. Stoyanov and C. G. Webster. A gradient-based sampling approach for dimension reduction of partial differential equations with stochastic coefficients. *International Journal for Uncertainty Quantification*, 5(1):49–72, 2015.

# Spectral stochastic finite elements for two nonlinear problems

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We study applications of spectral stochastic finite element methods (SSFEM) in two nonlinear problems: inverse subspace iteration for eigenvalue computations and Navier-Stokes equations.

In the first part we focus on random eigenvalue problems in the context of spectral stochastic finite elements [1]. In particular, given a parameter-dependent, symmetric positive-definite matrix operator, we explore the performance of algorithms for computing its eigenvalues and eigenvectors represented using polynomial chaos expansions. We formulate a version of stochastic inverse subspace iteration, which is based on the stochastic Galerkin finite element method, and we compare its accuracy with that of Monte Carlo and stochastic collocation methods. The coefficients of the eigenvalue expansions are computed from a stochastic Rayleigh quotient. Our approach allows the computation of interior eigenvalues by deflation methods, and we can also compute the coefficients of multiple eigenvectors using a stochastic variant of the modified Gram-Schmidt process. The effectiveness of the methods is illustrated by numerical experiments on benchmark problems arising from vibration analysis.

In the second part we study the steady-state Navier-Stokes equations in the context of stochastic finite element discretizations [2]. Specifically, we assume that the viscosity is a random field given in the form of a generalized polynomial chaos expansion. For the resulting stochastic problem, we formulate the model and linearization schemes using Picard and Newton iterations in the framework of the stochastic Galerkin method, and we explore properties of the resulting stochastic solutions. We also propose a preconditioner for solving the linear systems of equations arising at each step of the stochastic (Galerkin) nonlinear iteration and demonstrate its effectiveness for solving a set of benchmark problems.

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## References

- [1] B. Sousedík and H. C. Elman. Inverse subspace iteration for spectral stochastic finite element methods. *SIAM/ASA Journal on Uncertainty Quantification*, 4(1):163–189, 2016.
- [2] B. Sousedík and H. C. Elman. Stochastic Galerkin methods for the steady-state Navier-Stokes equations. *Journal of Computational Physics*, 316:435–452, 2016.

# Sparse grid approximation of elliptic PDEs with lognormal diffusion coefficient

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This talk is concerned with sparse grid methodologies to efficiently approximate the solution,  $u$ , of an elliptic PDE whose diffusion coefficient is modeled as a lognormal random field. The presentation is divided in two parts.

In the first part, we build upon previous works available in the literature to establish a convergence result (in  $L^2$  norm in probability) for the approximation of  $u$  by sparse collocation with Gauss–Hermite points, see [1]. More specifically, we first link the error to the size of the multi-index set defining the sparse collocation and then derive a bound on the number of points in the associated sparse grid. The result of the analysis is an algebraic convergence rate of the approximation error with respect to both the size of the multi-index set and the number of points in the sparse grid; interestingly, the analysis gives also an explicit “a-priori” estimate of the optimal multi-index set. We validate the results against numerical tests: in particular, we consider a family of random fields parameterized by a coefficient that sets the spatial smoothness of the field, in the spirit of the Matérn family.

As expected, the convergence rate for very rough fields turns out to be quite slow, even for optimized grids (be it the above-mentioned “a-priori” grids or the classical “a-posteriori”-adaptive grids). Thus, in the second part of the talk, we propose a remedy based on using the solution of the PDE on a smoothed versions of the random field as control variate for a Monte Carlo sampling of  $u$ , see [2].

## References

- [1] O. G. Ernst, B. Sprungk, and L. Tamellini. Convergence of sparse collocation for functions of countably many gaussian random variables (with application to lognormal elliptic diffusion problems). *ArXiv e-prints 1611.07239*, 2016.
- [2] F. Nobile, L. Tamellini, F. Tesei, and R. Tempone. *An Adaptive Sparse Grid Algorithm for Elliptic PDEs with Lognormal Diffusion Coefficient*, volume 109 of *Lecture Notes in Computational Science and Engineering*, pages 191–220. Springer International Publishing Switzerland, 2016.

# Improving sparse recovery guarantee for Legendre expansions using envelope bound

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The sample complexity of polynomial approximation using  $\ell_1$  minimization has usually been derived via the uniform bound of the underlying basis. In this work, we prove a sufficient condition for sparse Legendre expansion without using this uniform boundedness condition. Our sample complexity, independent of maximum polynomial degree, is established using the restricted eigenvalue property and the unbounded envelope of all Legendre polynomials. Our analysis also reveals some easy-to-test criteria for random sample sets under which the reconstruction error can be slightly improved.

# Multilevel Sequential<sup>2</sup> Monte Carlo for Bayesian Inverse Problems

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The identification of parameters in mathematical models using noisy observations is a common task in uncertainty quantification. We employ the framework of Bayesian inversion: we combine monitoring and observational data with prior information to estimate the posterior distribution of a parameter. Specifically, we are interested in the distribution of a diffusion coefficient of an elliptic PDE. In this setting, the sample space is high-dimensional, and each sample of the PDE solution is expensive.

To address these issues we propose and analyse a novel Sequential Monte Carlo (SMC) sampler for the approximation of the posterior distribution. Classical, single-level SMC constructs a sequence of measures, starting with the prior distribution, and finishing with the posterior distribution. The intermediate measures arise from a tempering of the likelihood, or, equivalently, a rescaling of the noise. The resolution of the PDE discretisation is fixed. In contrast, our estimator employs a hierarchy of PDE discretisations to decrease the computational cost. Importantly, we construct a sequence of intermediate measures by decreasing the temperature and increasing the discretisation level at the same time. We present numerical experiments in 2D space, comparing our estimator to single-level SMC and other alternatives.

# Sparse approximation of high-dimensional functions via convex and nonconvex regularizations

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In this talk, we present and analyze a novel compressed sensing approach for optimal polynomial recovery of both high-dimensional complex-valued and Hilbert-valued signals. The latter typically comes from the solution of parameter PDEs, where the target function is smooth, characterized by a rapidly decaying orthonormal expansion, whose most important terms are captured by a lower (or downward closed) set. By exploiting this fact, we develop a novel weighted minimization procedure with a precise choice of weights, and a modification of the iterative hard thresholding method, for imposing the downward closed preference. We will also present theoretical results that reveal our new computational approaches possess a provably reduced sample complexity compared to existing compressed sensing, least squares, and interpolation techniques. In addition, the recovery of the corresponding best approximation using our methods is established through an improved bound for the restricted isometry property. Finally, we will present an entirely new theory for compressed sensing that reveals that nonconvex minimizations are at least as good as  $\ell_1$  minimization in exact recovery of sparse signals. Our theoretical recovery guarantees are developed through a unified null space property based-condition that encompasses all currently proposed nonconvex functionals in literature. Several nonconvex functionals will be explored and the specific conditions in order to guarantee improved recovery will be given. Numerical examples, related to polynomial approximation of several functions in high dimensions, will be provided to support the new theory and demonstrate the computational efficiency of both weighted  $\ell_1$  and nonconvex regularizations.

# It's Really Dark Down There: UQ in Groundwater Hydrology

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In this talk I will briefly survey the history of UQ in groundwater hydrology, review some current methods for carrying it out, and identify research opportunities for applied mathematicians. Uncertainty about the states of groundwater systems arises primarily from lack of knowledge of system parameters, which in turn is usually due to the combined effects of sparse sampling and the high degrees of heterogeneity found on multiple scales. Since the most common UQ models used to resolve uncertainty in groundwater hydrology are based on stochastic partial differential equations (SPDEs) in some way, I will focus my review on SPDE methods ranging from naive Monte Carlo simulations of large parameter systems to direct estimates of the forms of probability density function of system states. I will also survey models of reduced complexity like continuous time random walks and other Markov-type models based on SPDEs. Topics will include stochastic representations of uncertain distributions of system parameters in space and time, methods to reduce uncertainty about the specific forms of models, and the so-called "scaling problem" that arises mostly from the mismatch in scales of measurements (the laboratory and field) and scales of application (aquifers and regions). The need for UQ will be motivated by the effects of anomalous transport of groundwater contaminants and their potential impacts on human health.

# Scalable solvers for meshless methods on many-core clusters

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Our goal is to solve large-scale stochastic collocation problems in a high-order convergent and scaling fashion. To this end, we recently discussed the radial basis function (RBF) kernel-based stochastic collocation method [1]. In this meshless method, the higher-dimensional stochastic space is sampled by (quasi-)Monte Carlo sequences, which are used as centers of radial basis functions in a collocation scheme. This non-intrusive approach combines high-order algebraic or even exponential convergence rates of spectral (sparse) tensor-product methods with good pre-asymptotic convergence of kriging, the profound stochastic framework of Gaussian process regression and parts of the simplicity of Monte Carlo methods.

Preliminary applications for this uncertainty quantification framework were (elliptic) model problems and incompressible two-phase flows with applications in chemical bubble reactors and river engineering. All solvers were parallelized to run on clusters of many-core hardware (Graphics Processing Units, GPUs) with profound scalability results.

One specific challenge of the discussed approach is the solution of a well-structured large to huge dense linear system of the type

$$\begin{pmatrix} k(\vec{y}_1, \vec{y}_1) & \dots & k(\vec{y}_1, \vec{y}_N) \\ \vdots & \ddots & \vdots \\ k(\vec{y}_N, \vec{y}_1) & \dots & k(\vec{y}_N, \vec{y}_N) \end{pmatrix} \vec{\alpha} = \begin{pmatrix} \int_{\Gamma} k(\vec{y}_1, \vec{y}) \rho(\vec{y}) d\vec{y} \\ \vdots \\ \int_{\Gamma} k(\vec{y}_N, \vec{y}) \rho(\vec{y}) d\vec{y} \end{pmatrix}$$

to compute the quadrature weights. Here, the  $\vec{y}_i$  are the (quasi-)Monte Carlo samples in stochastic space and  $N$  is the sample count. Linear systems of similar type arise in Gaussian process regression and several machine learning approaches. In those cases  $N$  is the number of instances to learn from.

Classical direct factorization techniques to solve the above linear system for a large to huge kernel sample count are barely tractable, even on large parallel computers. Therefore, we discuss iterative approaches to solve such linear systems on large parallel clusters with a special emphasis on many-core hardware. To keep the iteration count small, a large-scale preconditioner with excellent strong scalability properties has been developed for GPU clusters. Moreover, we work on an optimal-complexity matrix approximation by hierarchical matrices on many-core hardware.

The presentation will cover the latest results with respect to numerical methods and applications. Performance and scalability results will be given based on studies on the Titan GPU cluster at Oak Ridge National Lab.

This work is partly based on joint work with Michael Griebel, Helmut Harbrecht and Christian Rieger.

## References

- [1] P. Zaspel. *Parallel RBF Kernel-Based Stochastic Collocation for Large-Scale Random PDEs*. Dissertation, Institute for Numerical Simulation, University of Bonn, Germany, 2015.





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# Identification of a Visco-plastic Model with Uncertain Parameters using Bayesian Methods

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The evaluation of the performance of engineering structures includes models of behavior of materials, structural elements, loadings, external excitations etc. In assessment studies, there are several classes of uncertainty related to the lack of information on loading conditions/excitations, behavior of material properties over time, geometry and boundary conditions which may be identified and reduced by the means of quality control or system monitoring and identification. The reader of more interest is referred to [3].

In this work the focus is on the propagation of the uncertainty into a visco-plastic model and quantification of the uncertainty in the response of the model described by model parameter uncertainty. To do so, Stochastic Finite Element Method (SFEM) is applied for different tests e.g. relaxation test and creep test. [2]

Once the forward model, which is a much more realistic model than the discrete model, is provided, in order to identify the model parameters, solving the inverse problem is studied. Employing some Bayesian approaches like Polynomial Chaos Expansion based update, leads us to update and identify the model parameters which are set as uncertain values in the first step. The results confirm the efficiency of the used methods. [1]

## References

- [1] B. R. A. L. Hermann G. Matthies, E. Zander. Parameter estimation via conditional expectation: a bayesian inversion. *Advanced Modeling and Simulation in Engineering Sciences*, 3:24, 2016.
- [2] H. G. Matthies. Uncertainty quantification with stochastic finite elements. *Encyclopedia of Computational Mechanics*, 27, 2007.
- [3] R. E. Melchers. Structural reliability analysis and prediction. *John Wiley and Sons*, 2, 1999.

# Stochastic sensitivity analysis applied to URANS simulations of high-pressure injectors

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This work focuses on numerical simulation of high-pressure injectors for automotive applications. Several investigations have shown that the flow behavior inside the injector has a significant impact on emission level of vehicles. The flow in injectors is complex, since turbulence interacts with cavitation in channels of very small size, making measurements and simulations very challenging. Physical models taking the previously listed phenomena into account are needed in numerical simulations and it is reasonable to infer that these models may significantly affect the reliability of the numerical predictions. As for turbulence modeling, from an industrial point of view, the unavoidable compromise between computational costs and accuracy makes interesting to investigate the capabilities of the "cheap" Unsteady Reynolds-averaged Navier-Stokes (URANS) approach. Another key issue is the modeling of cavitation phenomena. Several models are proposed in the literature of different levels of complexity and it is not clear yet which kind of model is better suited for this type of problems. Moreover, cavitation models typically contain a number of parameters to be a-priori specified. We adopt an approach widely used for the simulation of this kind of flows, also available in commercial CFD codes, in which a transport equation for the void fraction is considered containing a source term modeled through the classical Rayleigh-Plesset equation. This model contains four free parameters, which strongly affect the source term and therefore the cavitating flow behavior. The considered flow configuration is a rectangular cross-section channel for which LES and experimental results are available in the literature ([1] and [2]). For this 3D geometry, a classical deterministic sensitivity analysis would imply huge computational costs also for URANS. Therefore, a stochastic approach is used in order to obtain continuous response surfaces of the quantities of interest in the parameter space, starting from a few deterministic simulations. First of all, a preliminary screening using generalized Polynomial Chaos (gPC) or Stochastic Collocation (SC) and 2D URANS simulations is carried out to identify the cavitation model parameters having the largest impact on the numerical predictions. Based on this analysis, we select the two most important parameters and we carry out a sensitivity analysis for the real 3D geometry using gPC. To investigate the impact of turbulence closure, the analysis is repeated for two turbulence models:  $k-\omega$  SST and Reynolds stress model. The quantities of interest are the mass-flow-rate (MFR) at the channel outlet, the pressure along the channel-axis and the cavitation length inside the channel. The stochastic range of variability of URANS results always contains the reference LES and experimental data. The cavitation length and the pressure distribution are sensitive to the turbulence closure, while the MFR predictions are practically the same for both models. A parameter optimization procedure is finally carried out minimizing the differences on pressure and MFR.

## References

- [1] M. Altimira and L. Fuchs. Numerical investigation of throttle flow under cavitating conditions. *International Journal of Multiphase Flow*, 75:124–136, 2015.
- [2] E. Winklhofer, E. Kull, E. Kelz, and A. Morozov. Comprehensive hydraulic and flow field documentation in model throttle experiments under cavitation conditions. In *Proceedings of the ILASS-Europe Conference, Zürich*, pages 574–579, 2001.

## Adaptive Multi-Level Monte-Carlo method

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In this work we focus on a variation of MLMC method for elliptic PDEs and variational inequalities with stochastic input data. Adaptive Multi-Level Monte-Carlo Finite Element method combines the ideas of Multi-Level Monte-Carlo Finite Element (MLMC-FE) method and a posteriori error estimation for adaptive solution of deterministic spatial problems. Whereas the classical MLMC-FE method is based on a hierarchy of uniform meshes, in the adaptive version of the method we use meshes generated by adaptive mesh refinement and levels are characterized by a hierarchy of FE-error tolerances. Under suitable assumptions on the problem, convergence of adaptive MLMC-FE method is shown and upper bounds for its computational cost are obtained. We illustrate advantages of the adaptive method in comparison to the classical MLMC by applying the method to model stochastic elliptic problems.

# Numerical Sensitivity Analysis and Reduced-order Modeling for Cardiac Conductivity Estimation by a Variational Data Assimilation Approach

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An accurate estimation of cardiac conductivity tensors is crucial for extending computational electrocardiology from medical research to clinical practice. However, experimental results in the literature significantly disagree on the values and the ratios between longitudinal and tangential coefficients.

With this motivation, we investigate a novel variational data assimilation approach for the estimation of the cardiac conductivity parameters [1]. The procedure relies on the least-square minimization of the misfit between simulations and experiments, constrained by the underlying mathematical model, which in our case is represented by the classical Bidomain system, or its common simplification given by the Monodomain problem. Regarding the conductivity tensors as control variables of the minimization, a parameter estimation procedure is derived.

As the theory of this approach currently provides only an existence proof and it is not informative for practical experiments, we perform a numerical sensitivity analysis of the estimation with respect to the size and the location of the measurement sites for *in silico* test cases reproducing experimental and realistic settings. This will be finalized with a real validation of the variational data assimilation procedure. Results indicate the presence of lower and upper bounds for the number of sites which guarantee an accurate and minimally redundant parameter estimation. Moreover, the location of sites are in general non critical for properly designed experiments.

Since the solver demands high computational costs, we investigate possible model reduction techniques for the inverse conductivity problem. The Proper Orthogonal Decomposition (POD) approach is taken for forward model reduction, along with the Discrete Empirical Interpolation Method (DEIM) for tackling nonlinearity. In the application of this POD-DEIM combination, we obtain a rather small set of samples by sampling the parameter space based on polar coordinates and densifying the “boundary layer” of the sample space utilizing Gauss-Lobatto nodes. Replacing the full order model in the optimization process with a low-dimensional model, the computational effort is finally reduced by at least 90% in conductivity estimation.

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## References

- [1] H. Yang and A. Veneziani. Estimation of cardiac conductivities in ventricular tissue by a variational approach. *Inverse Problems*, 31(11):115001, 2015.

# Measure transport approaches to uncertainty quantification

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Inference problems arise naturally in many engineering applications, where unobservable quantities of interest need to be inferred from indirect observations and approximate mathematical models. The results of the inference process can be used, e.g, for the calibration of numerical schemes, for taking decisions under uncertainty, for tracking the states of dynamical systems, etc. Among other methods, Bayesian inference is a versatile framework capable of addressing very ill-posed inference problems.

All Bayesian inference problems can be condensed into the problem of finding a **computable transport** between a tractable reference distribution and the intractable target distribution resulting from the Bayesian inference process. We identify this transport as the solution of a **variational**

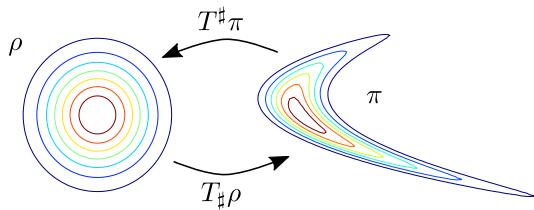


Figure 1: The transport  $T$  maps mass from the reference density  $\rho$  to the target density  $\pi$ .

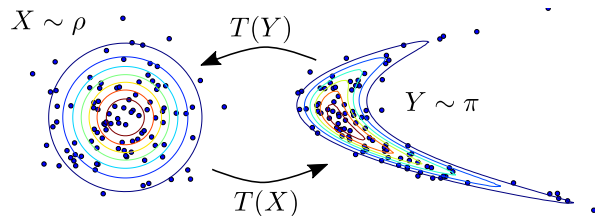


Figure 2: The transport  $T$  transforms quadratures for  $\rho$  to quadratures for  $\pi$ .

**problem** minimizing the Kullback-Leibler divergence between the approximate push-forward density  $T_{\#}\rho$  and the target density  $\pi$ , over the set of Knothe-Rosenblatt rearrangements [2, 3]. This leads to an unconstrained optimization problem, whose convergence can be reliably monitored<sup>1</sup>.

Even though practical problems often involve inference over high-dimensional parameter spaces (such as the fields governing some PDE or the long run states of a dynamical system), many of them have a rich **low-dimensional structure** which can be exploited. With the help of a number of engineering applications we will outline several types of structure (independence [4], smoothness [1] and separability) and ways to take advantage of them during the construction of transports.

## References

- [1] D. Bigoni, A. Spantini, and Y. Marzouk. On the computation of monotone transports. *In preparation*, 2017.
- [2] T. El Moselhy and Y. Marzouk. Bayesian inference with optimal maps. *Journal of Computational Physics*, 231(23):7815–7850, oct 2012.
- [3] Y. Marzouk, T. Moselhy, M. Parno, and A. Spantini. Sampling via Measure Transport: An Introduction. In R. G. Ghanem, D. Higdon, and H. Owhadi, editors, *Handbook of Uncertainty Quantification*, pages 1–41. Springer International Publishing, Cham, 2016.
- [4] A. Spantini, D. Bigoni, and Y. Marzouk. Inference via low-dimensional couplings. 2017.

<sup>1</sup>We recently released **TransportMaps v1.0** which is capable of representing and identifying the transport  $T$ . The software is freely available at <https://transportmaps.mit.edu>.



# Effective Conductivity in Heterogeneous Composite Porous Media

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The effective hydraulic conductivity of a porous medium is a single parameter that represents the aggregate effect of the conductivity field for the variable coefficient poisson equation,  $\nabla \cdot K(x)\nabla H = f$ . The logistical difficulties of sampling the medium on scales fine enough to resolve the spatial heterogeneity lead to incomplete information of the associated conductivity field and uncertainty in the effective hydraulic conductivity. Since the conductivity field is never exactly known, direct simulation of fluid flow through the *actual* aquifer is impossible, so hydrologists must rely on statistical characterizations (either known or assumed) of the conductivity field to generate multiple realizations of (hopefully) representative random fields for analysis or numerical simulation.

We develop a phenomenological model for the effective conductivity of highly heterogeneous composite media. We use thresholded random fields to model porous media that consist of the compositions of different materials that have been deposited by geologic processes into disjoint, irregular configurations (e.g clay lenses in a sandy aquifer). The effective conductivity of the medium depends on the relative proportion of the two materials, on degree of heterogeneity between the two materials and on the spatial distribution of the materials. As the degree of heterogeneity increases, the irregular geometry and topology of the configuration has increasing influence on the flow. This is particularly pronounced for volume fractions near the percolation threshold of the more conductive material, and the event of percolation marks a transition between two different regimes. The focus of our model is to quantify this transition.

# Scalable Domain Decomposition Solvers for Uncertainty Quantification in High Performance Computing.

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Spectral stochastic finite element models of realistic engineering systems may involve solutions of linear systems or linearized systems for non-linear problems with billions of unknowns. For stochastic modeling, it is therefore essential to design robust, parallel and scalable algorithms that can efficiently utilize the high-performance computing to tackle such large-scale systems. Domain decomposition method for stochastic PDEs formulated by Sarkar et. al. [4] are shown to exhibit excellent scalabilities when implemented using Krylov iterative solvers for the high-resolution finite element (FE) meshes in the cases of a few random variables [5]. However, for the systems with high dimensional stochastic fields which requires a large number of random variables to characterize the underlying stochastic process, these algorithms exhibit significant algorithmic and implementational challenges.

Intrusive polynomial chaos expansion based domain decomposition algorithms for uncertainty quantification developed by Subber and Sarkar [5] are extended here to concurrently handle high resolution in both spatial and stochastic domains using an in-house implementation. Sparse iterative solvers with efficient preconditioners are employed to solve the resulting global and subdomain level local problems through multi-level iterative solvers. To enhance the capability to undertake the problems with a high-dimensional stochastic field, the proposed solver uses an in-house stochastic assembly code written based on FEniCS assembly procedure [2]. The pre-processing procedures required for employing polynomial chaos expansion (PCE), Karhunen-Loeve expansion (KLE) and multidimensional inner products are adapted from UQ Toolkit (UQTK) [3]. PETSc based sparse matrix-vector objects and routines are utilized to cut the floating-point operations and memory requirements [1]. The sparse iterative KSPCG solvers with mean-based preconditioners from PETSc are employed to accelerate the solution of the subdomain level local problems [1]. Numerical and parallel scalabilities of these algorithms are presented for the stochastic diffusion equation with random diffusion coefficient modeled by a non-Gaussian stochastic process.

## References

- [1] S. Balay et al. PETSc users manual revision 3.6. Technical report, Argonne National Laboratory (ANL), 2016.
- [2] A. Logg, K. A. Mardal, and G. Wells. *Automated solution of differential equations by the finite element method: The FEniCS book*, volume 84. Springer Science & Business Media, 2012.
- [3] K. Sargsyan, C. Safta, K. Chowdhary, S. Castorena, S. de Bord, and B. Debusschere. UQTK version 3.0.1 User Manual. Technical report, Sandia National Laboratory (SNL), 2016.
- [4] A. Sarkar, N. Benabbou, and R. Ghanem. Domain decomposition of stochastic PDEs: theoretical formulations. *International Journal for Numerical Methods in Engineering*, 77(5):689–701, 2009.
- [5] W. Subber and A. Sarkar. A domain decomposition method of stochastic PDEs: An iterative solution techniques using a two-level scalable preconditioner. *Journal of Computational Physics*, 257:298–317, 2014.

# Global Reconstruction of Solutions to Parametric PDEs Via Compressed Sensing

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We present a novel theoretical framework for solving parametric PDEs via compressed sensing over tensor-products of Hilbert spaces. This work builds on the existing theory for the recovery of compressible solutions via  $\ell_1$ -minimization, and guarantees convergence in terms of the errors of the best  $s$ -term approximation and the residual in a given polynomial subspace. Compared to other approaches that only recover a functional of the solution [1, 3, 4], e.g. evaluation at a single point, our approach recovers the solution globally over the physical domain. We also provide extensions to the fixed point continuation and Bregman iterative algorithms [2, 5] for solving the basis pursuit problem in this context. We conclude with numerical results demonstrating the efficacy of our approach in high-dimensions and comparisons with sparse grids and stochastic Galerkin approximations.

## References

- [1] A. Doostan and H. Owhadi. A non-adapted sparse approximation of pdes with stochastic inputs. *Journal of Computational Physics*, 230:3015–3034, 2011.
- [2] E. Hale, W. Yin, and Y. Zhang. Fixed-point continuation for  $\ell_1$ -minimization: methodology and convergence. *SIAM J. Optim.*, 19(3):1107–1130, 2008.
- [3] L. Mathelin and K. Gallivan. A compressed sensing approach for partial differential equations with random input data. *Commun. Comput. Phys.*, 12:919–954, 2012.
- [4] X. Yang and G. E. Karniadakis. Reweighted  $\ell_1$ -minimization method for stochastic elliptic differential equations. *Journal of Computational Physics*, 248:87–108, 2013.
- [5] W. Yin, S. Osher, D. Goldfarb, and J. Darbon. Bregman iterative algorithms for  $\ell_1$ -minimization with applications to compressed sensing. *SIAM J. Imaging Sci.*, 1(1):143–168, 2008.

# Parabolic PDEs with random coefficients on moving hypersurfaces

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Sometimes the partial differential equations with random coefficients can be better formulated on moving curved domains, especially in biological applications. We will introduce and analyse the advection-diffusion equations with random coefficients on moving hypersurfaces. We will consider two cases, uniform and log-normal distributions of coefficients. In the uniform case, under suitable regularity assumptions, using Banach-Nečas-Babuška theorem, we will prove existence and uniqueness of the weak solution and also we will give some regularity results about the solution. For log-normal case, we will prove the measurability and p-integrability of the path-wise solution. For discretization in space, we will apply the evolving surface finite element method. In order to deal with uncertainty, we will use Monte Carlo method.

# Multilevel Stochastic Collocation in Linear Gyrokinetics

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The simulation of micro-turbulence in plasma fusion is essential for understanding the properties of the confinement of fusion plasmas with magnetic fields. In this contribution, we employ the established plasma micro-turbulence simulation code GENE (<http://genecode.org/>) and we focus on linear gyrokinetic eigenvalue problems defined on a five dimensional phase space. The major outcomes of linear simulations are the growth rates and modes of micro-instabilities, representing the real and imaginary parts of the dominant eigenvalue.

Since input parameters such as temperature gradients of ions and electrons are intrinsically uncertain, these plasma simulations need be performed within the framework of uncertainty quantification. In this contribution, we model seven input parameters, such as the temperature gradients of ions and electrons, the plasma  $\beta$  parameter, and the safety factor, as uniform random variables. Although seven is not typically regarded as a high dimensionality, given the complexity of the underlying application, standard full grid-based approaches are computationally prohibitive. Thus, the underlying stochastic problem suffers from the curse of dimensionality.

To overcome the curse of dimensionality, we employ multilevel stochastic collocation [2] and generalized polynomial chaos expansion. In this approach, we perform a hierarchical decomposition in both phase space and parameter domains. In the phase space, we consider a hierarchy of discretization grids with a resolution increasing by a constant factor, whereas in the parameter domain, we employ sparse grids, using the library SG++ [1]. In particular, we use the adaptive sparse grid combination technique, constructed using non-uniform, nested Leja points, to create a surrogate for the calculation of polynomial chaos expansion's coefficients. Furthermore, we exploit the non-intrusiveness of our stochastic approach and we simulate the underlying problem using two layers of parallelism.

Using a multilevel stochastic collocation approach, we reduce the computational cost of the overall simulation, while keeping the errors small. Moreover, using adaptivity and multiple layers of parallelism, we efficiently use the available resources, while controlling the required number of runs.

## References

- [1] D. Pflueger. *Spatially Adaptive Sparse Grids for High-Dimensional Problems*. Verlag Dr. Hut, Muenchen, Aug. 2010.
- [2] A. L. Teckentrup, P. Jantsch, C. G. Webster, and M. Gunzburger. A Multilevel Stochastic Collocation Method for Partial Differential Equations with Random Input Data. *eprint arXiv:1404.2647*, 37916, 2014.

# Multilevel-Multifidelity estimators for the analysis of cardiovascular flows under uncertainty

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Hemodynamics numerical modeling is rapidly becoming a reliable tool for the diagnosis and treatment of cardiovascular disease and surgical planning. Examples are non-invasive detection of stenosis in the coronary and peripheral arteries or testing of surgical designs. Hemodynamic modeling consists in the solution of the incompressible Navier-Stokes equations particularized to blood flow in elastically deformable vessels, therefore expensive high-fidelity fully coupled fluid-structure solutions are generally required. Despite the complexity of such models, 1D or 0D simplified formulations can be obtained assuming a Newtonian fluid flowing in the axial direction of deformable cylindrical vessels or linearizing the incompressible Navier-Stokes equations around rest conditions, respectively.

Computations of biological and biomedical systems are intrinsically affected by multiple sources of uncertainty, therefore a single deterministic simulation can only provide a limited amount of information. A more comprehensive analysis of such systems should instead rely on a stochastic framework where all parameters affecting boundary conditions, material constitutive behavior and model geometry are defined in probability with distributions either assumed or assimilated from available patient-specific data.

In the presence of a fairly large number of parameters a natural and common choice to perform non-intrusive UQ analysis is to use the Monte Carlo (MC) method. MC is a robust and reliable approach which retains its order of convergence independently from the regularity of the solution and the number of parameters. However, the order of convergence is only  $\mathcal{O}(N^{-1/2})$  where  $N$  is the number of simulations, therefore a large number of realizations might be still necessary to obtain reliable statistics. More recently a multilevel-multifidelity [2] extension of MC has been proposed to improve the quality of the statistical predictions for a fixed computational budget. The pivotal idea is that low resolution/low fidelity models can be used as control variates to reduce the variability of the estimator. In particular, an optimal sample allocation across resolutions/fidelities is obtained by minimizing the overall computational cost.

In this work we explore the possibility to leverage the automated pipeline [1] implemented in SimVascular [3], which is able to generate a cascade of model fidelities for cardiovascular models, into the multilevel-multifidelity [2] framework for UQ analysis in presence of large number of uncertainty parameters.

## References

- [1] C. M. Fleeter, D. Schiavazzi, and A. Marsden. Towards a multi-fidelity hemodynamic model pipeline for the analysis of cardiovascular flow under uncertainty. *5th International Conference on Computational and Mathematical Biomedical Engineering, CMBE2017*, 2017.
- [2] G. Geraci, M. Eldred, and G. Iaccarino. A multifidelity control variate approach for the multilevel Monte Carlo technique. *Center for Turbulence Research, Annual Research Briefs 2015*, pages 169–181, 2015.
- [3] A. Updegrave, N. Wilson, J. Merkow, and *et al.* SimVascular: An open source pipeline for cardiovascular simulation. *Ann. Biomed. Eng.*, 44:1–17, 2016.

# Non-intrusive polynomial chaos method applied to problems in computational fluid dynamics in both high fidelity and reduced order settings

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Studying uncertainty quantification is very important in computational fluid dynamics (CFD) applications. Several sources of uncertainty (e.g. uncertainties in the model, lack of knowledge of the modeler, uncertainties in the input model parameters, discretization error) might in fact affect the results of the simulations.

Many methods have been developed to assess how input parameters uncertainties propagate, through the simulation model of the CFD problem, into the outputs of interest. The aim of this work is to carry out a study on the application of non-intrusive polynomial chaos expansion (PCE) on CFD problems. The polynomial chaos method is based on the spectral representation of the output with respect to the input parameters. One important feature of spectral representation of the uncertainty is the possibility of decomposing the random variable into separable deterministic and stochastic component [4, 2]. By a computational stand point, the main problem in PCE consists in finding the deterministic coefficients of the expansion. In non-intrusive polynomial chaos method, no changes are made in the simulations code, and the coefficients are computed in a post processing phase following the simulations. Thus, the deterministic terms in the expansion are obtained via a sampling based approach is used [3, 5] in which samples of the input parameters are prescribed and then CFD simulations are carried out for each sample. The properties of multivariate orthogonal Hermite polynomials are then used to obtain the expansion coefficients from the CFD simulation output.

In this work non intrusive polynomial chaos method is applied to one problem in CFD in both high fidelity and reduced order settings, for detailed theory on reduced order methods see [1]. The objective of this work is to assess whether non intrusive PCE is influenced by the use of a POD-Galerkin based model reduction approach. To this end, we will apply POD model reduction to CFD simulations based on incompressible Navier–Stokes equations, and compare the PCE coefficients and sensitivities obtained for the reduced order solution to the ones resulting from the full order simulations.

## References

- [1] J. S. Hesthaven, G. Rozza, and B. Stamm. Certified reduced basis methods for parametrized partial differential equations. *SpringerBriefs in Mathematics*, 2015.
- [2] S. Hosder, R. Walters, and R. Perez. A non-intrusive polynomial chaos method for uncertainty propagation in CFD simulations. In *44th AIAA aerospace sciences meeting and exhibit*, page 891, 2006.
- [3] S. S. Isukapalli. Uncertainty analysis of transport-transformation models. *Unpublished PhD diss. New Brunswick, NJ: Rutgers, The State University of New Jersey, Department of Chemical and Biochemical Engineering*, 1999.
- [4] M. Loeve. Probability theory, vol. ii. *Graduate texts in mathematics*, 46:0–387, 1978.
- [5] M. T. Reagana, H. N. Najm, R. G. Ghanem, and O. M. Knio. Uncertainty quantification in reacting-flow simulations through non-intrusive spectral projection. *Combustion and Flame*, 132(3):545–555, 2003.

# Techniques for reducing computational complexity of sparse grid stochastic collocation methods

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Sparse grid stochastic collocation (SC) methods are a valuable tool for solving problems in uncertainty quantification, yet they suffer from a dramatic increase in costs in high-dimensions. This poster demonstrates how to use SC methods to solve partial differential equations (PDEs) with random coefficients, exploiting multilevel and hierarchical structure in the spatial and stochastic approximation schemes to drastically improve the computation efficiency of the method. We demonstrate the savings of our methods for both linear and non-linear random PDEs.



# A Preconditioned Low-rank Projection Method with a Rank-reduction Scheme for Stochastic Partial Differential Equations

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In this study, we consider the numerical solution of large coupled systems of linear equations obtained from the stochastic Galerkin formulation [3] of stochastic partial differential equations. Consider the stochastic elliptic boundary value problem: Find  $u(\mathbf{x}, \xi) : \bar{D} \times \Gamma \rightarrow \mathbb{R}$  that satisfies

$$\mathcal{L}(a(\mathbf{x}, \xi))(u(\mathbf{x}, \xi)) = f(\mathbf{x}) \quad \text{in } D \times \Gamma, \quad (1)$$

where  $\mathcal{L}$  is a linear elliptic operator and  $a(\mathbf{x}, \xi)$  is a positive random field parameterized by a set of random variables  $\xi = \{\xi_1, \dots, \xi_M\}$ . The stochastic Galerkin discretization of (1) leads to a large coupled deterministic system  $Au = f$ , for which computations will be expensive for large-scale applications. When the coefficient  $a(\mathbf{x}, \xi)$  has an affine structure depending on a finite number of random variables, the system matrix  $A$  can be represented by a sum of Kronecker products of smaller matrices,

$$Au = \left( \sum_{k=0}^M G_k \otimes K_k \right) \left( \sum_{l=1}^{\kappa_u} v_l \otimes w_l \right) = f, \quad (\text{or, equivalently, } \text{mat}(Au) = \sum_{k=0}^M K_k U G_k^T = F), \quad (2)$$

where  $\otimes$  is the Kronecker product,  $\kappa_u$  is the rank of the solution  $u$  (i.e.,  $\kappa_u = \text{rank}(U)$ ),  $\text{mat}(\cdot)$  is a “matricization” operator,  $\{K_i\}$  are weighted stiffness matrices, and  $\{G_i\}$  are “stochastic” matrices. Matrix operations such as matrix-vector products that take advantage of the tensor format can be performed efficiently (i.e.,  $Au = \sum_{k=0}^M \sum_{l=1}^{\kappa_u} (G_k v_l \otimes K_k w_l)$  whose complexity is  $O(\text{nnz}(G_k) + \text{nnz}(K_k))$ ), which makes the use of iterative solvers attractive. In this study, we develop a new efficient iterative solution method for (2) that exploits the Kronecker product structure of the linear systems.

In particular, it has been shown that the solution of (2) can be approximated by a tensor of low rank (i.e.,  $U \approx \sum_{l=1}^{\tilde{\kappa}_u} v_l w_l^T$  with  $\tilde{\kappa}_u \ll \kappa_u$ ), which further reduces computational effort [2]. To compute a low-rank approximation of the solution efficiently, we propose a multilevel rank-reduction scheme, which identifies an important subspace in the stochastic domain inexpensively in a coarse spatial grid setting and compresses tensors of high rank on the fly during the iterations of a fine-grid computation. For fine-grid computations, we explore a variant of the generalized minimum residual (GMRES) method [1] combined with the new rank-reduction strategy. As opposed to expensive conventional singular-value-decomposition-based truncation, the proposed rank-reduction scheme achieves significant computational savings by employing the multilevel truncation approach. The efficiency of the proposed method is illustrated by numerical experiments on benchmark problems.

## References

- [1] J. Ballani and L. Grasedyck. A projection method to solve linear systems in tensor format. *Numerical Linear Algebra with Applications*, 20(1):27–43, 2013.
- [2] P. Benner, A. Onwunta, and M. Stoll. Low-rank solution of unsteady diffusion equations with stochastic coefficients. *SIAM/ASA Journal on Uncertainty Quantification*, 3(1):622–649, 2015.
- [3] R. G. Ghanem and P. D. Spanos. *Stochastic Finite Elements: a Spectral Approach*. Dover Publications, 2003.

# Uncertainty quantification embedded in software-component libraries: case study of thermomechanical modeling of an ITER spectroscopy

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In scientific computing, a new approach to coding is emerging, which involves a more modular and component-based software architecture. Computer science research centers are developing libraries of software components that package thoroughly verified, high-performance implementations of computational tasks that often occur in multiphysics simulation. The aim is to ease the development of new simulation software, or the improvement of existing codes, using these components. One of the leading software-component libraries is the Trilinos library developed at Sandia National Laboratories, USA.

The component-based software architecture provides new opportunities for UQ (uncertainty quantification): The developers of the software-component libraries may embed highly optimized implementations of intrusive UQ methods directly into the software components. Such an embedded approach eases for the end users the coding effort of introducing capabilities for efficiently and accurately propagating uncertainties in an existing software-component-based code. Such an embedded approach is currently being implemented in Trilinos based on the use of C++ templating and the dedicated software component Stokhos [2].

The present work addresses the embedded approach through its application to a thermomechanical analysis of the front mirror of the Charge eXchange Recombination Spectroscopy system of the ITER tokamak [1]. This thermomechanical analysis involves the prediction of the heat-induced optical distortion of the bolted mirror/holder assembly by means of a transient non-linear thermomechanical contact model. It involves several uncertain parameters, including the properties of the particles emitted by the plasma, material properties in the harsh ITER environment, and manufacturing tolerances.

The poster will present a Trilinos-software-component-based implementation of the transient non-linear thermomechanical contact model, based on the mortar finite element method, iterative solution methods, automatic differentiation, multigrid preconditioning, and hybrid parallelism. In addition, the poster will report on numerical experiments that assess the performance of Trilinos's existing embedded UQ capabilities for propagating uncertainties through the transient non-linear thermomechanical contact model, and it will discuss how the multiphysics coupling, nonlinearities, and contact inequalities pose challenges that motivate our ongoing further research on model reduction and embedded ensemble propagation to adequately extend the embedded UQ approach.

## References

- [1] Y. Krasikov, A. Panin, W. Biel, A. Krimmer, A. Litnovsky, Ph. Mertens, O. Neubauer, and M. Schrader. Major aspects of the design of a first mirror for the ITER core CXRS diagnostics. *Fusion engineering and design*, 96:812–816, 2015.
- [2] E. T. Phipps, M. D'Elia, H. C. Edwards, M. Hoemmen, J. Hu, and S. Rajamanickam. Embedded Ensemble Propagation for Improving Performance, Portability and Scalability of Uncertainty Quantification on Emerging Computational Architectures. *arXiv:1511.03703 [cs]*, Nov. 2015. arXiv: 1511.03703.

# Risk average optimal control problem for elliptic PDEs with uncertain coefficients

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We consider a risk averse optimal control problem for an elliptic PDE with uncertain coefficients. The control is a deterministic distributed forcing term and is determined by minimizing the expected  $L^2$ -distance between the state (solution of the PDE) and a target deterministic function. An  $L^2$ -regularization term is added to the cost functional. [5, 6]

We consider a finite element discretization [7] of the underlying PDE and derive an error estimate on the optimal control.

Concerning the approximation of the expectation in the cost functional and the practical computation of the optimal control, we analyze and compare two strategies.

In the first one, the expectation is approximated by either a Monte Carlo estimator or a deterministic quadrature on Gauss points [1], assuming that the randomness is effectively parametrized by a small number of random variables. Then, a steepest descent algorithm is used to find the discrete optimal control.

The second strategy, named Monte Carlo Stochastic Approximation [8, 9, 3, 4, 2] is again based on a steepest-descent type algorithm. However the expectation in the computation of the steepest descent is approximated with independent Monte Carlo estimators at each iteration using possibly a very small sample size. The sample size and possibly the mesh size in the finite element approximation could vary during the iterations. We present error estimates and complexity analysis for both strategies and compare them on few numerical test cases.

## References

- [1] I. Babuska, F. Nobile, and R. Tempone. A stochastic collocation method for elliptic partial differential equations with random input data. *SIAM Journal on Numerical Analysis*, 45(3):1005–1034, 2007.
- [2] A. Defossez and F. Bach. Averaged least-mean-squares: Bias-variance trade-offs and optimal sampling distributions. 2015.
- [3] A. Dieuleveut and F. Bach. Non-parametric stochastic approximation with large step-sizes. 2015.
- [4] N. Flammarion and F. Bach. From averaging to acceleration, there is only a step-size. 2015.
- [5] D. Kouri. *Optimization Governed by Stochastic Partial Differential Equations*. 2011.
- [6] D. Kouri. *An Approach for the Adaptive Solution of Optimization Problems Governed by Partial Differential Equations with Uncertain Coefficients*. PhD thesis, 2012.
- [7] A. Quarteroni. Numerical models of differential problems. 8, 2014.
- [8] M. Schmidt and F. Le Roux, N. Bachs. Minimizing finite sums with the stochastic average gradient. 2016.
- [9] A. Shapiro, D. Dentcheva, and A. Ruszczyński. Lectures on stochastic programming: Modeling and theory. 2009.

# Conjugate gradient methods for stochastic Galerkin finite element matrices with saddle point structure

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We consider linear systems of equations with saddle point structure resulting from the stochastic Galerkin finite element (SGFE) discretization of Stokes flow with random input data. The associated matrices are  $Q$  times as large as the finite element matrices of the underlying spatial problem, where  $Q$  is a factor depending on the modeling and discretization of the uncertain quantities. Furthermore, the stochastic Galerkin approach leads to a coupled problem in the general case, meaning the associated system of equations cannot be trivially decomposed into  $Q$  independent finite element problems. Due to this high dimensionality, iterative solvers and corresponding preconditioners are of particular interest in the context of the SGFE method. The efficient iterative solution of the SGFE discretized diffusion problem was for example investigated in [2] and [4], just to name two.

We focus on the concept of non-standard inner product conjugate gradient (CG) methods. The basic idea is to precondition the system matrix in a way, such that the resulting product is symmetric and positive definite in an inner product which is not necessarily the Euclidean one. This implies the existence of a well-defined CG method in that particular inner product, see [3]. While investigating a specific block triangular preconditioner for the Stokes problem with deterministic data, Bramble and Pasciak [1] discovered an inner product that fulfills the mentioned criteria and thus implies the existence of a non-standard inner product CG method. A preconditioned system which is in principle non-symmetric can thereby be solved using a short-recurrence Krylov subspace method.

We restate sufficient conditions for the existence of such a Bramble-Pasciak-type CG method and show how they can be fulfilled in the SGFE framework. In order to end up with an efficient iterative procedure, the block triangular preconditioner is constructed based on well-established techniques for the discrete Stokes problem with deterministic data. The theoretic findings are verified by means of numerical results. In particular, we investigate Stokes flow problems where the viscosity is a random field which can be described by a finite number of random variables using the Karhunen-Loève expansion. The performance and accuracy of the considered CG method is furthermore compared to that of other Krylov subspace methods.

## References

- [1] J. H. Bramble and J. E. Pasciak. A preconditioning technique for indefinite systems resulting from mixed approximations of elliptic problems. *Mathematics of Computation*, 50:1–17, 1988.
- [2] O. G. Ernst, C. E. Powell, D. J. Silvester, and E. Ullmann. Efficient solvers for a linear stochastic Galerkin mixed formulation of diffusion problems with random data. *SIAM Journal on Scientific Computing*, 31:1424–1447, 2009.
- [3] V. Faber and T. Manteuffel. Necessary and sufficient conditions for the existence of a conjugate gradient method. *SIAM Journal on Numerical Analysis*, 21:352–362, 1984.
- [4] E. Ullmann and C. E. Powell. Solving log-transformed random diffusion problems by stochastic Galerkin mixed finite element methods. *SIAM/ASA Journal on Uncertainty Quantification*, 3:509–534, 2015.

## Reduced basis methods for groundwater flow

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In this work we apply reduced basis methods to the Darcy flow problem with random coefficients which can be written as a parameter dependent PDE that depends on a vector  $\mathbf{y}$  of  $M$  random variables. Approximations to quantities of interest can be obtained using, for example, the stochastic collocation method which requires approximations of solutions to the PDE for many realisations of the parameter  $\mathbf{y}$ . For a given  $\mathbf{y}$  an approximation to each of these PDEs can be obtained by solving a deterministic saddle point problem whose solution can be approximated using mixed finite element methods. With a fine spatial discretisation the combined cost of solving all of the required deterministic systems can be prohibitively expensive. We shall present an efficient reduced basis algorithm and demonstrate through numerical experiments the significant computational savings that can be made by using this reduced model instead of standard finite element methods. We focus on uncertainty quantification for a groundwater flow problem.

## Towards Uncertainty Analysis for Multi-scale Models

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In the poster we will discuss intrusive and non-intrusive methods for uncertainty quantification (UQ) and sensitivity analysis (SA) for multi-scale simulations together with their advantages and disadvantages. Our goal is to formulate a generic mathematical description of uncertainty propagation in a multi-scale model in order to build computationally efficient techniques for uncertainty analysis. In this study, we present first results. Finally, we show two examples of uncertainty estimation and sensitivity analysis.

# Statistically optimal weights for distributed Tikhonov-regularization

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We consider the problem of recovering an unknown, spatially distributed parameter  $u$  occurring in a PDE from a limited (possibly finite) number of observations of the associated PDE solutions. To reconstruct the parameter, we consider the minimizer  $\hat{u}_w$  of a Tikhonov-regularized least-squares functional, where the regularization term contains a weighted  $L^2$ -norm with a fixed spatially varying weight  $w$ . Due to the under-determined nature of the inverse problem, an accurate recovery can only succeed in certain cases, depending also on the weight  $w$ . We follow the assumption that the parameter to be recovered follows a certain stochastic distribution, modeled by a random field. For the choice of the deterministic weight we propose to minimize the variance of  $u - \hat{u}_w$ , the difference between the reference parameter and the reconstruction. We analyze the associated stochastic control problem (for the case of linear observations) together with discretization and solution strategies. The numerical results demonstrate that significant reductions in variance are possible over the canonical choice  $w = 1$ , even if the reference parameters are sampled from a random field with a spatially uniform correlation.

# Optimal solvers for nonsymmetric linear systems with stochastic PDE origins ‘Balanced black-box stopping test’

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This poster discusses the design and implementation of efficient solution algorithms for nonsymmetric linear systems arising from FEM approximation of stochastic convection-diffusion equations. The novel feature of our preconditioned GMRES and BICGSTAB( $\ell$ ) solvers is the incorporation of error control in the ‘natural’ norm in combination with a reliable and efficient a posteriori estimator for the PDE approximation error. This leads to a robust and optimally efficient black-box stopping criterion: the iteration is terminated as soon as the algebraic error is insignificant compared to the approximation error. Our algorithms are optimal in the sense that they result in the savings of unnecessary computations. Also, using the black-box stopping test and a ‘good’ preconditioner, the suboptimal Krylov solvers like BICGSTAB( $\ell$ ) etc. can be stopped optimally. Currently scarce convergence theory exists for such iterative solvers. This work is an extension of our work on devising optimal black-box stopping test in iterative solvers for solving symmetric positive-definite linear systems arising from FEM approximation of stochastic diffusion equations [1]

## References

- [1] D. Silvester and Pranjal. An optimal solver for linear systems arising from stochastic fem approximation of diffusion equations with random coefficients. *SIAM/ASA Journal on Uncertainty Quantification*, 4(1):298–311, 2016.



# Uncertainty quantification in cardiac electrophysiology: fast multifidelity methods for clinical practitioners

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In cardiac electrophysiology, there are numerous sources of uncertainty, both in the parameters and in the modeling aspects. For instance, the *de facto* standard bidomain model is strongly nonlinear and has several parameters with large uncertainties: conductivities, location and timing of source currents, microstructure organization (fibers and sheets), anatomy, and electrodes location.

Computing the ECG from the bidomain equation is a computational demanding task. A single patient-tailored simulation can take several CPU hours on a large cluster. This makes uncertainty quantification (UQ) unfeasible, unless modeling reduction and/or approximation strategies are employed. One such strategy is to compute the activation time via the eikonal equation, which under common circumstances provides a physiologically-motivated solution [1].

While the eikonal approximation enables to perform UQ studies with an acceptable computational cost, the required time frame still exceeds that available to a clinical practitioner. Even by taking advantage of massively parallel GPU hardware, a plain Monte Carlo study would require at least several hours. Therefore, it would be desirable to reduce the cost by at least two orders of magnitude. This would allow to provide the sought information in less than a few minutes, opening up the possibility to employ mathematical tools in the everyday clinical practice.

Multi-fidelity methods have become very popular over the last years and their applications span the fields of UQ, inverse problems, and optimization [4]. The central idea of this approach is to build a hierarchy of extremely fast low-fidelity models, which might be inaccurate but exhibit some degree of correlation with the high-fidelity one. It is the control of the correlation, rather than of the error estimates, that is crucial to ensure that propagating uncertainties via the low-fidelity models provides useful information on the statistics of the high-fidelity quantity-of-interest [3].

There are several options to propagate information across models. In our work, we adopt a Bayesian viewpoint [2]. This choice allows to provide automatically confidence intervals on the estimated quantity-of-interest and to exploit non-linear dependencies between the models, rather than just correlation. This is achieved by fitting a Bayesian regression between the high-fidelity output and the low-fidelity ones. In practice, only  $\sim 100$  runs of the high-fidelity model are necessary, enabling the use of UQ in the everyday clinical practice.

## References

- [1] P. C. Franzone and L. Guerri. Spreading of excitation in 3-d models of the anisotropic cardiac tissue. i. validation of the eikonal model. *Mathematical biosciences*, 113(2):145–209, 1993.
- [2] P.-S. Koutsourelakis. Accurate uncertainty quantification using inaccurate computational models. *SIAM Journal on Scientific Computing*, 31(5):3274–3300, 2009.
- [3] B. Peherstorfer, K. Willcox, and M. Gunzburger. Optimal model management for multifidelity monte carlo estimation. Technical report, Technical report 15–2, Aerospace Computational Design Laboratory, MIT, 2015.
- [4] B. Peherstorfer, K. Willcox, and M. Gunzburger. Survey of multifidelity methods in uncertainty propagation, inference, and optimization. 2016.

# Multilevel Monte Carlo for transmission problems with geometric uncertainties

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When a quantity of interest depends non-smoothly on the high-dimensional parameter representing the uncertainty in the physical system, the multilevel Monte Carlo algorithm (MLMC) is a valid option to compute moments, as it allows to bypass the precise location of discontinuities in the parameter space.

Such lack of smoothness occurs when considering the point evaluation of the solution to a transmission problem with uncertain interface, if the point can be crossed by the interface for some realizations. Considering a Helmholtz transmission problem, we provide a space regularity analysis for the solution, in order to state converge results in the  $L^\infty$ -norm for the finite element discretization. The latter are then used to determine the optimal distribution of samples among the Monte Carlo levels. Particular emphasis is given on the robustness of our estimates with respect to the dimension of the parameter space. We present numerical experiments confirming the theoretical statements. The methodology used clearly conveys that MLMC is a viable approach also for other problems lacking smoothness with respect to the stochastic parameter.

## Reduced Basis Methods and Their Application to Ensemble Methods for the Navier-Stokes Equations

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The definition of partial differential equation (PDE) models usually involves a set of parameters whose values may vary over a wide range. The solution of even a single set of parameter values may be quite expensive. In many cases, e.g., optimization, control, uncertainty quantification, and other settings, solutions are needed for many sets of parameter values. We consider the case of the time-dependent Navier-Stokes equations for which a recently developed ensemble-based method allows for the efficient determination of the multiple solutions corresponding to many parameter sets. The method uses the average of the multiple solutions at any time step to define a linear set of equations that determines the solutions at the next time step. To significantly further reduce the costs of determining multiple solutions of the Navier-Stokes equations, we incorporate a proper orthogonal decomposition (POD) reduced-order model into the ensemble-based method.

# Reduced basis method for parabolic problems with random data

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We consider the reduced basis method applied to a parameter and time dependent PDE problem, given  $\xi \in \Gamma \subset \mathbb{R}^p$ , for  $t \in [0, T]$ , find  $u(t; \xi) \in X$  such that

$$\begin{aligned} (\partial_t u, v)_{L^2} + a(u, v; \xi) &= b(v; \xi), \quad \forall v \in X \\ u(0; \xi) &= 0. \end{aligned}$$

The uncertain input  $\xi$  is treated by the Monte Carlo (MC) method where the PDE needs to be solved for  $N_{MC}$  randomly chosen parameter samples. MC is attractive since it is easy to implement and its convergence rate is independent of the stochastic parameter dimension. However, a large number of samples  $N_{MC}$  is required in order to achieve reasonable accuracy, because of the low convergence rate of  $\mathcal{O}(N_{MC}^{-1/2})$ . Using standard numerical discretization methods to solve the PDE problem for each sample is computationally expensive.

The reduced basis method approximates the solution manifold on a low-dimensional subspace which is constructed by the *POD-greedy* procedure [2]. The method yields a rigorous a posteriori error estimator for the error between the finite element and the reduced solution.

We are interested in computing linear functionals of the solution evaluated at the final time  $T$ , i.e. in an output

$$s(\xi) = l(u(T; \xi)).$$

We consider a primal-dual approach, which uses the solution of an adjoint problem in order to obtain a better output estimation. The focus of this talk is to improve the error of statistical quantities using the idea of the weighted reduced basis method [1]. We illustrate the method based on an instationary heat conduction problem and show corresponding numerical results.

## References

- [1] P. Chen, A. Quarteroni, and G. Rozza. A weighted reduced basis method for elliptic partial differential equations with random input data. *SIAM Journal on Numerical Analysis*, 51:3163–3185, 2013.
- [2] B. Haasdonk and M. Oehlberger. Reduced basis method for finite volume approximations of parametrized linear evolution equations. *ESAIM Math. Model. Numer. Anal.*, 42:277–302, 2008.

# Bayesian identification in ROM for computational fluid dynamics

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When predicting the behavior of physical systems one has to deal with aleatoric and epistemic uncertainties describing the inherent nature of the phenomena or the lack of the modeller's knowledge. In this work the focus is put on the estimation of epistemic uncertainties present in the computational fluid dynamics models. The uncertainties describing solutions of Navier Stokes equations include discretization errors, modelling errors (e.g. turbulence modelling) and in the case of reduced order models also approximation errors. In the present work a Bayesian update procedure [1] is used to assimilate experimental or "true" data directly at reduced order level. The methodology is tested for the case of incompressible Navier-Stokes flows analysed with POD-Galerkin reduced order models [2].

## References

- [1] H. G. Matthies, E. Zander, B. Rosic, and A. Litvinenko. Parameter estimation via conditional expectation — A Bayesian inversion. *Advanced Modeling and Simulation in Engineering Sciences*, 3(1):24, 2016.
- [2] G. Stabile, S. Hijazi, A. Mola, S. Lorenzi, and G. Rozza. POD-Galerkin reduced order model for finite volume approximation of the Navier–Stokes equations: vortex shedding around a circular cylinder. *Submitted to Communications in Applied and Industrial Mathematics*, 2017.

# Deterministic Risk Prediction with Reduced Basis Methods

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A central problem in Uncertainty Quantification is predicting risk of failure of a system given uncertainties in its parameters. Catastrophic failure is usually modeled as certain system outputs exceeding a critical value, while outputs themselves are modeled as values taken by linear functionals acting on the solution of the parameter dependent system PDE. Ideally risk prediction is a deterministic problem – the goal is to identify all regions within the parameter set resulting in failure in the above sense. We call this set the domain of failure. Unfortunately deterministic approaches to find the domain of failure are rarely feasible; take, for instance, the EIT problem: here the goal is to recover a voxel-grid of the brain structure from measurements of the electric field on the skull. Each voxel is a single model parameter. Depending on the finesse of the model the amount of parameters may become massive.

This naturally lends itself to a stochastic problem formulation: the risk of failure is formulated as a probability and its corresponding expectation value. Monte Carlo methods seem to be a natural fit for this description as their convergence is independent of the parameter dimension. Unfortunately they converge slowly in the number of samples taken ( $O(N^{-\frac{1}{2}})$ ) and require many (costly) forward PDE evaluations. To alleviate the high evaluation cost several model reduction techniques have already been applied (see e.g. [1], [3]).

In this work we are looking at deterministic approaches to the problem. Such approaches naturally hinge on sampling the parameter domain and thus suffer greatly from high parameter dimensions. Under which circumstances can the curse of dimensionality be broken? Guided by the Karhunen-Loeve decomposition we explore the sampling complexity for elliptic systems with an infinite number of parameters in an anisotropic setting, i.e. the influence of parameters exhibits a well-known decay. The parametric behaviour of solutions of this problem class is well-understood [2] and well-suited for low-dimensional approximation. We exploit solution regularity to bound the domain of failure by sampling the parameter domain. We adaptively increase the parameter dimension depending on desired error bounds. Solving the PDE is sped up with the help of reduced basis methods to adaptively construct a low-dimensional basis. As reduced basis methods offer certified error bounds, we can control the dimension of the approximation. This makes it computationally possible to obtain deterministic bounds for the domain of failure, which can be used as a better starting point for stochastic methods.

## References

- [1] P. Chen, A. Quarteroni, and G. Rozza. Reduced order methods for uncertainty quantification problems. *ETH Report 03*, 2015.
- [2] A. Cohen and R. DeVore. Approximation of high-dimensional parametric pdes. *Acta Numerica*, pages 1–159, 2015.
- [3] A. Manzoni, S. Pagani, and T. Lassila. Accurate solution of bayesian inverse uncertainty quantification problems combining reduced basis methods and reduction error models. *SIAM/ASA J. Uncertainty Quantification*, 4(1):380–412, 2016.

# Model reduction for environmental marine optimal flow control problems

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Reduced order methods are a suitable approach to face parametrized optimal flow control problems governed by partial differential equations. Surely, this holds for optimal flow control applications in environmental and marine sciences and engineering. Environmental parametrized optimal control problems are usually studied for different configurations described by several physical and/or geometrical parameters representing different phenomena and structures. Optimal flow control theory can be adapted to several scientific interests and needs in this field, from monitoring and preservation of ecological populations, as well as protected natural areas, to data assimilation approach in forecasting models. These issues require a demanding computational effort. Reduced basis techniques are a reliable and rapid tool to solve them, in order to save and contain computational time. Two examples are briefly presented: a pollutant control in the Gulf of Trieste, Italy and a solution tracking governed by quasi-geostrophic equations describing North Atlantic Ocean dynamic. The two experiments show the capability of reduced order methods in this field of research: they underline how reduced order methods may be a reliable and convenient tool to manage several environmental optimal flow control problems, for different mathematical models, geographical scale as well as physical meaning.

## References

- [1] J. S. Hesthaven, G. Rozza, and B. Stamm. *Certified reduced basis methods for parametrized partial differential equations*. SpringerBriefs in Mathematics. Springer, 2015.
- [2] R. Mosetti, C. Fanara, M. Spoto, and E. Vinzi. Innovative strategies for marine protected areas monitoring: the experience of the Istituto Nazionale di Oceanografia e di Geofisica Sperimentale in the Natural Marine Reserve of Miramare, Trieste-Italy. In *OCEANS, 2005. Proceedings of MTS/IEEE*, pages 92–97. IEEE, 2005.
- [3] F. Negri, A. Manzoni, and G. Rozza. Reduced basis approximation of parametrized optimal flow control problems for the Stokes equations. *Computers & Mathematics with Applications*, 69(4):319–336, 2015.
- [4] F. Negri, G. Rozza, A. Manzoni, and A. Quarteroni. Reduced basis method for parametrized elliptic optimal control problems. *SIAM Journal on Scientific Computing*, 35(5):A2316–A2340, 2013.
- [5] M. Strazzullo, F. Ballarin, R. Mosetti, and G. Rozza. Reduced basis POD-Galerkin method for parametrized optimal control problems in environmental marine sciences and engineering. *Submitted*, 2017.
- [6] E. Tziperman and W. C. Thacker. An optimal-control/adjoint-equations approach to studying the Oceanic general circulation. *Journal of Physical Oceanography*, 19(10):1471–1485, 1989.

# Data-assimilation, parameter space reduction and reduced order methods in applied sciences and engineering

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We present the results of the first application in the naval architecture field of a new methodology for parameters space reduction [5]. The physical problem considered is that of the simulation of the hydrodynamic flow past the hull of a ship advancing in calm water. Such problem is extremely relevant at the preliminary stages of the ship design, when several flow simulations are typically carried out by the engineers to assess the dependence of the hull total resistance on the geometrical parameters of the hull. Given the high number of geometric and physical parameters which might affect the total ship drag, the main idea of this work is to employ the active subspaces method to identify possible lower dimensional structures in the parameters space. Thus, a fully automated procedure has been implemented to produce several perturbations of an original hull CAD geometry, use the resulting shapes to run high fidelity flow simulations with different structural and physical parameters as well, and collect data for the active subspaces analysis. The free form deformation procedure used to morph the hull shapes [1], the high fidelity solver based on potential flow theory with fully nonlinear free surface treatment [3, 4], and the active subspaces analysis tool employed in this work [2] have all been developed at mathLab, the applied mathematics lab of SISSA, at the International School for Advanced Studies in Trieste. The contribution will discuss several details of the implementation of such tools, as well as the results of their application to the target engineering problem. To show all the possibilities of the proposed pipeline we also present a biomedical engineering case where we deform a carotid using the radial basis function interpolation technique and perform a further reduction by POD-Galerkin ROM.

## References

- [1] PyGeM: Python Geometrical Morphing. <https://github.com/mathlab/pygem>.
- [2] P. G. Constantine. *Active subspaces: Emerging ideas for dimension reduction in parameter studies*, volume 2. SIAM, 2015.
- [3] A. Mola, L. Heltai, and A. DeSimone. A stable and adaptive semi-lagrangian potential model for unsteady and nonlinear ship-wave interactions. *Engineering Analysis with Boundary Elements*, 37:128–143, 2013.
- [4] A. Mola, L. Heltai, and A. DeSimone. A fully nonlinear semi-lagrangian potential model for ship hydrodynamics simulations directly interfaced with cad data structures. In *Proceedings of the Twenty-fourth International Ocean and Polar Engineering Conference*, volume 4, pages 815–822, 2014.
- [5] M. Tezzele, F. Salmoiraghi, A. Mola, and G. Rozza. Dimension reduction in heterogeneous parametric spaces: a naval engineering case. *submitted*, 2017.



## Features selection in models described by ODEs and PDEs.

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Computational models based on ODEs or PDEs provide a large number of outputs (or features). However, for several tasks such as classification, regression or parameter estimation, a large number of features generally leads to an ill-posed and computationally challenging problem. Therefore, a strategy needs to be developed in order to extract a few relevant features needed to perform such a task. We consider a generic model  $\mathcal{F}(\mathbf{u}; \boldsymbol{\vartheta}) = 0$ , where  $\mathbf{u}$  is the vector of state variables and  $\boldsymbol{\vartheta} = (\vartheta_1, \dots, \vartheta_p)$  is the vector of parameters of interest. Let  $\mathbf{v}(\mathbf{u}; \boldsymbol{\vartheta})$  denote the vector of model outputs. First, a dictionary of features  $\{f_1, \dots, f_{N_f}\}$  is built. These features are linear or non-linear transformations of the model outputs  $\mathbf{v}$ . Some are available in the literature and are known and commonly used by the community. For example, in cardiac electrophysiology, the common features associated to the action potential are its duration, amplitude, maximum time derivative, etc. Additional features are “agnostically” computed from the model outputs. Examples are integrals over time or space of the output fields, Fourier coefficients, values at certain points in time or space, etc. The parameters of interest are sampled and for each sample the model is evaluated and the outputs stored. This step is done *offline* and the set of the parameter samples and the corresponding model outputs is later referred to as the *training set*.

The goal of the present method is to compute an optimal feature, referred to as a numerical biomarker, for each parameter of interest. Such a feature is chosen to make the identification of the associated parameter as simple as possible. For a given parameter  $\vartheta_h$ , the numerical biomarker  $b_h$  is sought as a linear combination of the dictionary entries:  $b_h = \sum_{i=1}^{n_f} \beta_{hi} f_i$ . It must be maximally correlated with its associated parameter  $\vartheta_h$  and minimally correlated with all the other parameters. Furthermore, this numerical biomarker should have a sparse decomposition onto the dictionary entries. This sparsity condition is motivated by interpretational reasons and generalization performance. The requirements formulated above may be translated into a non-linear minimization problem with a  $\ell_1$ -norm penalty. The minimization is carried out using an accelerated gradient descent method. The hyperparameters corresponding to the  $\ell_1$ -norm regularization are calibrated using a hard threshold, the L-curve criterion or cross-validation techniques depending on the required properties of the numerical biomarkers.

We then present parameter estimation framework which takes advantage of the numerical biomarkers. The inverse problems we are interested in consist in minimizing the following generic cost function:

$$J(\boldsymbol{\vartheta}) = \frac{1}{2} \sum_{k=1}^M [y_k(\boldsymbol{\vartheta}) - y_k(\boldsymbol{\vartheta}^*)]^2,$$

where  $\boldsymbol{\vartheta}^*$  is the true parameters values and the  $y_k$  are transformations of the model outputs  $\mathbf{v}$ . The method is illustrated with ODE and PDE models and the influence of the hyperparameters is investigated. Finally, the method is applied to practical cases such as an electrophysiology heart cell model and a full-body cardiovascular model.

# Analysis of Model Inadequacy for Transport through Porous Media

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In this work, we consider contaminant transport due to incompressible flow through a porous media, characterized by an exponentially correlated permeability field. The transport is governed by a convection-diffusion equation and flow velocity as prescribed by Darcy's law [1]. We focus on uncertainty in model predictions for mean concentration of the contaminant due to inadequacy introduced by upscaling or depth-wise averaging a two-dimensional system. Specifically, the upscaling results in an unclosed second-order correlation term for which a suitable mathematical representation is sought. Our initial efforts are focused on assessing model predictability and quantifying uncertainty for the case when the unclosed term is approximated using the gradient diffusion model as commonly implemented in RANS modeling for turbulent flow applications [2]. Furthermore, we explore the suitability of multiple stochastic formulations for the unclosed term to be able to calibrate bounds on uncertainty in predictions of the upscaled model in each case. Synthetic data as generated using the original two-dimensional formulation, regarded as the *truth* model is used in our analysis.

## References

- [1] H. Darcy. Les fontaines Publiques de la Ville de Dijon. *Victor Dalmont, Paris*, 1856.
- [2] S. Pope. *Turbulent flows*. IOP Publishing, 2001.

# Data Assimilation for Cardiovascular Modeling with Applications to Optimal Flow Control

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Medical problems and mathematical modelling have always been co-related. Upgrading of medical imaging techniques has made way to model and numerically simulate the data, in a more efficient and effective manner. Data assimilation is therefore one of the key tools, required in order to detect, understand and treat serious ailments. Cardiovascular diseases, among many other, are a major cause of increase in death tolls across the world. The complex geometries of heart vessels add to the complications in simulating cardiovascular flows. These complications are highly amplified when considering the patient-specific problems. We present the on-going efforts to develop patient-specific cardiovascular models, starting from the reconstruction of the vessels of interest from the clinical data. An interesting application is the solution of optimal flow control problems, in order to predict fluid dynamics behaviour of cardiovascular parameters, patient-specifically, such as in cases of aortic coarctation or coronary artery disease. The aim is to obtain solution of these flow control problems in a real-time, many query and computationally inexpensive way combining finite-element with reduced-order modelling.

## References

- [1] F. Ballarin, E. Faggiano, S. Ippolito, A. Manzoni, A. Quarteroni, G. Rozza, and R. Scrofani. Fast simulations of patient-specific haemodynamics of coronary artery bypass grafts based on a POD-Galerkin method and a vascular shape parametrization. *Journal of Computational Physics*, 315:609–628, 2016.
- [2] F. Ballarin, E. Faggiano, A. Manzoni, A. Quarteroni, G. Rozza, S. Ippolito, C. Antona, and R. Scrofani. Numerical modeling of hemodynamics scenarios of patient-specific coronary artery bypass grafts. *Biomechanics and Modeling in Mechanobiology*, 2017.
- [3] Z. Chen, F. Ballarin, G. Rozza, A. M. Crean, L. Jimenez-Juan, and P. Triverio. Non-invasive assessment of aortic coarctation severity using computational fluid dynamics: a feasibility study. *20th Annual Scientific Sessions, Society for Cardiovascular Magnetic Resonance*, Washington, DC, Feb. 1-4 2017.
- [4] M. Gunzburger. *Perspectives in Flow Control and Optimization*, volume 5. SIAM, Philadelphia, 2003.

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# Additional information

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SISSA, the International School for Advanced Studies, was founded in 1978 and is a scientific center of excellence within the national and international academic scene. Located in Italy, in the city of Trieste, it features 80 professors, about 180 post-docs, 250 PhD students and 100 technical administrative staff. Situated on the scenic Karst upland, the School is surrounded by a 25 acre park, and offers a stunning view of the Gulf of Trieste.

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Websites:

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Wireless network access is provided within the SISSA campus. You can use your Eduroam credentials (from your institutions) or SISSA Guest Wi-fi. You should have received your credentials by email through the GRS system (SISSA Guests Registration) after providing requested data (ID copy) at the registration desk.

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Refreshments are served in the lobby (foyer) of the main lecture room. A cafeteria/restaurant is available in the main building A at the ground floor. On the opposite side, same floor, there is SISSA main scientific library. In the lobby of building A there is an ATM (Unicredit). In the same lobby two reserved rooms are available for small meetings and for group/individual work. Luggage storage and wardrobe is available in the main lecture room lobby. For further needs/requests: [quiet2017@sisssa.it](mailto:quiet2017@sisssa.it).

## Emergencies

Call 911 using SISSA telephones for first aid, call 555 SISSA emergency team for on campus emergencies. From cell phones numbers are +39 040 3787 911 and +39 040 3787 555, respectively. For emergency off campus call 112.

## Final Acknowledgements

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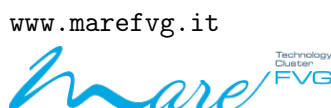


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# Quantification of Uncertainty: Improving Efficiency and Technology



July 18–21, 2017

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