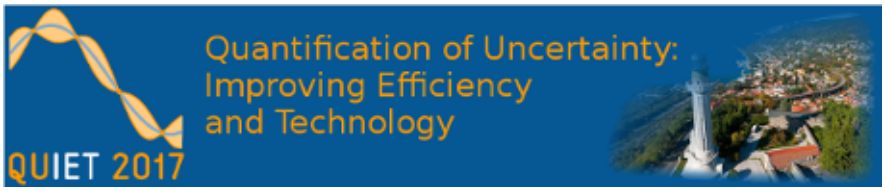


Identification of a Visco-plastic Model with Uncertain Parameters using Bayesian Methods

E. Adeli[1], B. Rosic[1], and H. G. Matthies[1]

[1]Technische Universität Braunschweig, Germany

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]

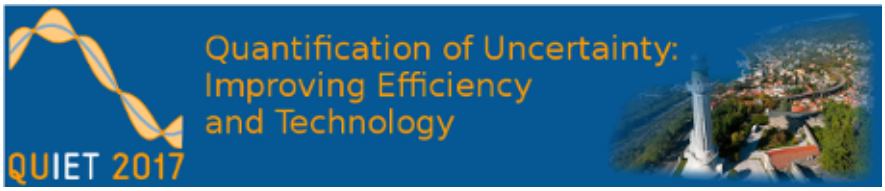
Once the forward model, which is a much more realistic model than the discrete model, is provided, in order to identify the model parameters, solving the inverse problem is studied. Employing some Bayesian approaches like Polynomial Chaos Expansion based update, leads us to update and identify the model 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

A. Anderlini[1], M. V. Salvetti[1], A. Agresta[2], and L. Matteucci[2]

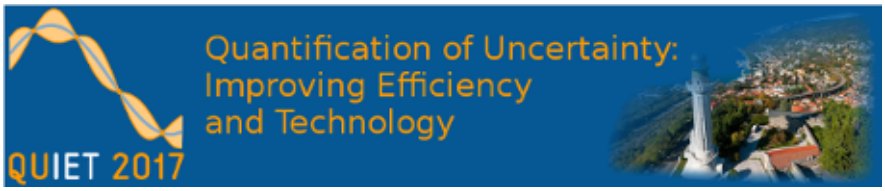
[1]University of Pisa, Italy
[2]Continental Automotive Italy S.p.A., Italy

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-ω 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.

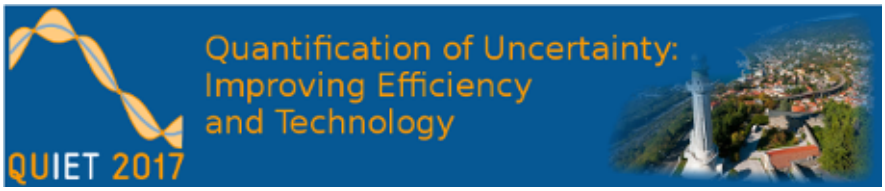


Adaptive Multi-Level Monte-Carlo method

E. Babushkina[1] and R. Kornhuber[1]

[1]Freie Universität Berlin, Germany

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 it's 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

A. Barone[1], A. Veneziani[1,2], H. Yang[3], and F. Fenton[1]

[1]Emory University, Atlanta, United States
[2]School of Advanced Studies IUSS, Pavia, Italy
[3]Florida State University, Tallahassee, United States

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.

This work has been supported by the NSF Project DMS 1412973/1413037 "Collaborative Research: Novel data assimilation techniques in mathematical cardiology - development, analysis and validation".

References

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

Quantification of Uncertainty: Improving Efficiency and Technology
QUIET 2017

Measure transport approaches to uncertainty quantification

D. Bigoni, A. Spantini, and Y. Marzouk

Massachusetts Institute of Technology, Cambridge, United States

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**

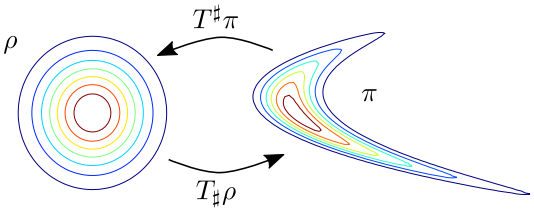


Figure 1: The transport T maps mass from the reference density ρ to the target density π.

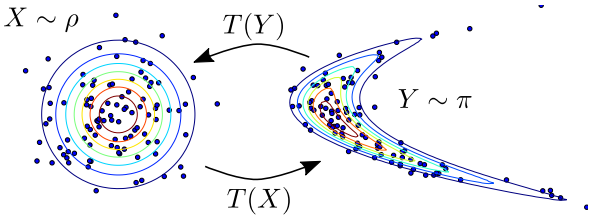


Figure 2: The transport T transforms quadratures for ρ to quadratures for π.

problem minimizing the Kullback-Leibler divergence between the approximate push-forward density $T_\sharp\rho$ and the target density π, over the set of Knothe-Rosenblatt rearrangements [2, 3]. This leads to an unconstrained optimization problem, whose convergence can be reliably monitored[1].

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

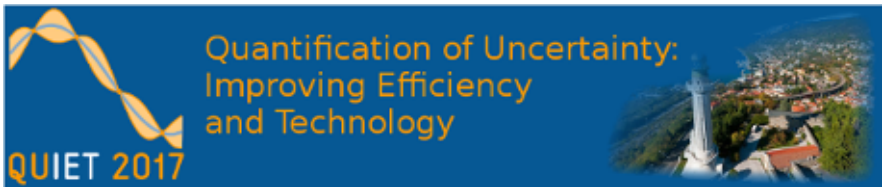
[1] D. Bigoni, A. Spantini, and Y. Marzouk. On the computation of monotone transports. *In preparation*, 2017.

[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.

[1] 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`.



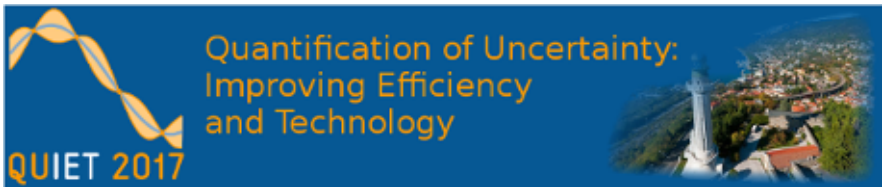
Effective Conductivity in Heterogeneous Composite Porous Media

C. Clark[1], C. L. Winter[1], and T. Corley[1]

[1]University of Arizona, Tucson, United States

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 hetereogeneity lead to incomplete information of the associated conductity 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 sumulation.

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.

A. Desai[1], M. Khalil[2], C. Pettit[3], D. Poirel[4], and A. Sarkar[1,2]

[1]Carleton University, Canada
[2]Sandia National Laboratories, United States
[3]United States Naval Academy, United States
[4]Royal Military Collage, Canada

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

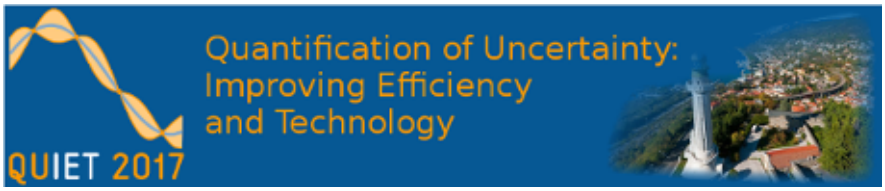
[1] S. Balay et al. PETSc users manual revision 3.6. Technical report, Argonne National Laboratory (ANL), 2016.

[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

N.C. Dexter[1], H. Tran[2], and C. G. Webster[1,2]

[1]University of Tennessee Knoxville
[2]Oak Ridge National Laboratory

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 ℓ_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

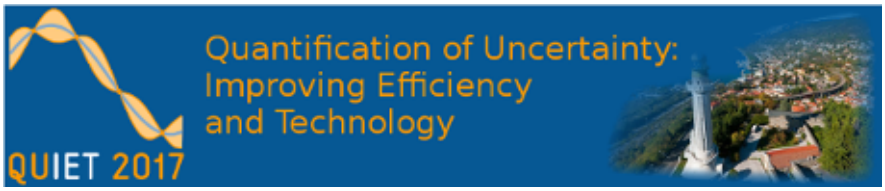
[1] A. Doostan and H. Owhadi. A non-adapted sparse approximation of pdes with stochastic inputs. *Journal of Computational Physics*, 230:3015–3034, 2011.

[2] E. Hale, W. Yin, and Y. Zhang. Fixed-point continuation for ℓ_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 ℓ_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 ℓ_1-minimization with applications to compressed sensing. *SIAM J. Imaging Sci.*, 1(1):143–168, 2008.

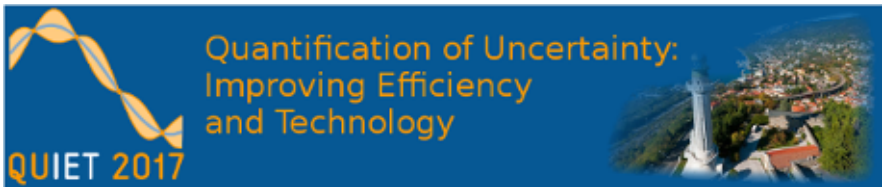


Parabolic PDEs with random coefficients on moving hypersurfaces

A. Djurdjevac[1], C. M. Elliott[2], R. Kornhuber[1], and T. Ranner[3]

[1]Freie Universität Berlin, Germany
[2]University of Warwick, United Kingdom
[3]University of Leeds, United Kingdom

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.



A Sparse Pseudo-Spectral Projection Method in Linear Gyrokinetics

I.-G. Farcas[1], T. Goerler[2], H.-J. Bungartz[1], and T. Neckel[1]

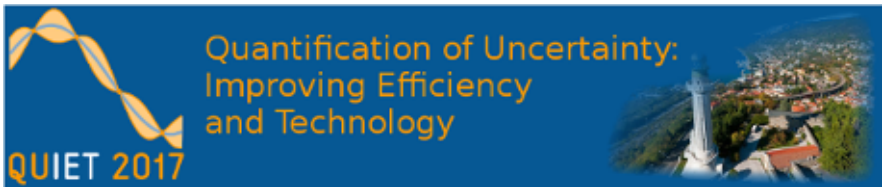
[1]Technische Universität München, Germany
[2]Max Planck Institute for Plasma Physics, München, Germany

The simulation of micro-turbulence in plasma fusion is essential for understanding the confinement properties 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 five dimensional phase spaces, taking into account electrons and deuterium ions. The outputs of interest are the growth rates and frequencies 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 simulations need be performed within the framework of uncertainty quantification. In this contribution, we consider two test cases. The first one is a modified version of an established benchmark. We initially consider the temperature gradients of ions and electrons to be uncertain, and, afterwards, we extend the number of uncertain parameters to seven. In the second test case, a real world scenario, we model the uncertainty in 11 input parameters, such as the two temperature gradients, the plasma β, or the collision frequency. We perform each simulation using 22 compute cores, each simulation runtime varying from a few minutes to several hours. Therefore, given the complexity of the underlying test cases, standard full grid-based stochastic approaches are computationally prohibitive. Thus, the underlying stochastic problem suffers from the curse of dimensionality.

To overcome the curse of dimensionality, we employ an adaptive sparse psuedo-spectral projection method. We construct sparse approximations of the outputs of interest based on tensorizations of one-dimensional pseudo-spectral projections. We choose the maximal degree of the projection basis and the quadrature rule to compute the projection's coefficients such that we have no so-called aliasing error. In addition, to keep the number of grid points and, hence, the computational cost small, we formulate our sparse approach in terms of Leja points. We also test an initial version of a dimension-adaptive algorithm in the two dimensional stochastic scenario. The underlying functionality is implemented in the sparse grid library `SG++` (`http://sgpp.sparsegrids.org/`). Finally, we exploit the non-intrusiveness of our approach and we simulate the underlying test cases using two layers of parallelism.

We compare our approach with a sparse grid-based interpolation method and a full grid based approach in the 2D stochastic scenario. The results show that our projection-based method behaves very similarly to the full grid approach, while being more accurate that the other sparse-based approach at the same computational cost. Furthermore, using Leja points and multiple layers of parallelism, we efficiently use the available resources, while minimizing the total number of runs in all test cases.



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

C. M. Fleeter[1], G. Geraci[2], M. S. Eldred[2], A. L. Mardsen[1], and D. E. Schiavazzi[3]

[1]Stanford University, United States
[2]Sandia National Laboratories, United States
[3]University of Notre Dame, United States

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.

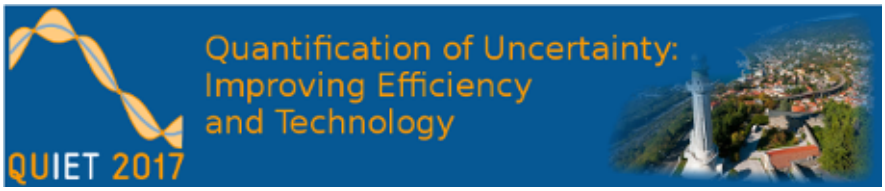
In this work we explore the possibility to leverage the automated pipeline [1] implemented in SimVascular [3], which is able to generate a cascade of model fidelities for cardiovascular models, into the multilevel-multifidelity [2] framework for UQ analysis in presence of large number of uncertainty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

S. Hijazi[1], G. Stabile[1], A. Mola[1], and G. Rozza[1]

[1]International School for Advanced Studies, Trieste, Italy

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

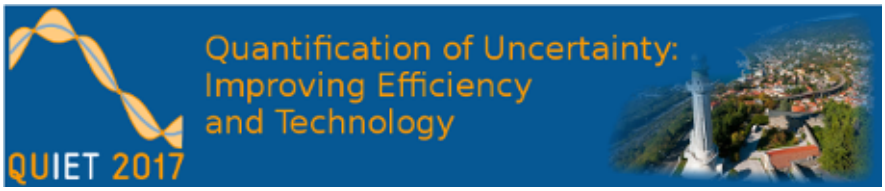
[1] J. S. Hesthaven, G. Rozza, and B. Stamm. Certified reduced basis methods for parametrized partial differential equations. *SpringerBriefs in Mathematics*, 2015.

[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.

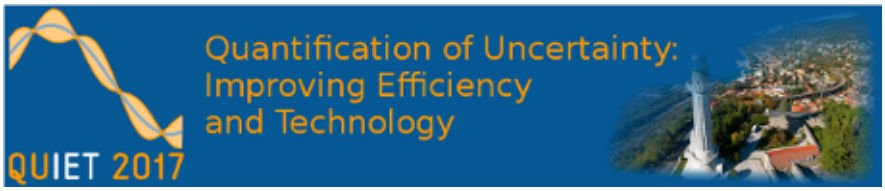


Techniques for reducing computational complexity of sparse grid stochastic collocation methods

P. Jantsch[1] and C. G. Webster[1,2]

[1]University of Tennessee, Knoxville, United States
[2]Oak Ridge National Laboratory, United States

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

K. Lee[1] and H. Elman[2]

[1]Department of Computer Science, University of Maryland
[2]University of Maryland, College Park

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 $u(\boldsymbol{x}, \xi) : \bar{D} \times \Gamma \to \mathbb{R}$ that satisfies

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

where $\mathcal{L}$ is a linear elliptic operator and $a(\boldsymbol{x}, \xi)$ is a positive random field parameterized by a set of random variables $\xi = \{\xi_1, \ldots, \xi_M\}$. 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 $a(\boldsymbol{x}, \xi)$ 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,

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

where $\otimes$ is the Kronecker product, κ_u is the rank of the solution u (i.e., $\kappa_u = \mathrm{rank}(U)$), $\mathrm{mat}(\cdot)$ 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 $O(\mathrm{nnz}(G_k)+\mathrm{nnz}(K_k)))$, 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.

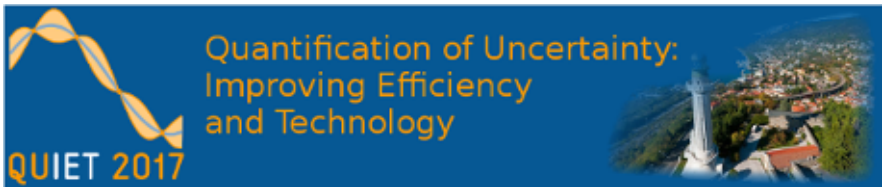
In particular, it has been shown that the solution of (2) can be approximated by a tensor of low rank (i.e., $U \approx \sum_{l=1}^{\tilde{\kappa}_u} v_l w_l^T$ with $\tilde{\kappa}_u \ll \kappa_u$), which further reduces computational effort [2]. To compute a low-rank approximation of the solution efficiently, 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 spectroscope

K. Liegeois[1], R. Boman[1], Ph. Mertens[2], A. Panin[2], E. T. Phipps[3], and M. Arnst[1]

[1]Université de Liège, Belgium
[2]Institute of Energy and Climate Research - Plasma Physics, Jülich, Germany
[3]Sandia National Laboratories, Albuquerque, United States

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].

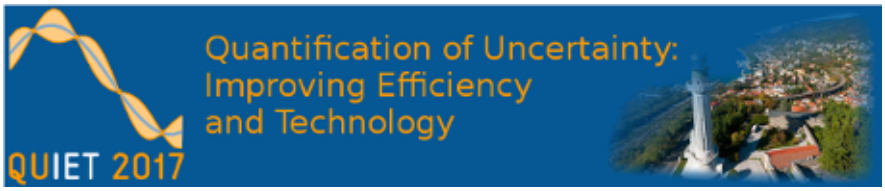
The present work addresses the embedded approach through its application to a thermomechanical analysis of the front mirror of the Charge eXchange Recombination Spectroscopy system of the ITER tokamak [1]. This thermomechanical analysis involves the prediction of the heat-induced optical distortion of 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

M. Martin[1], F. Nobile[1], and S. Krumscheid[1]

[1]École Polytechnique Fédérale de Lausanne, Switzerland

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.

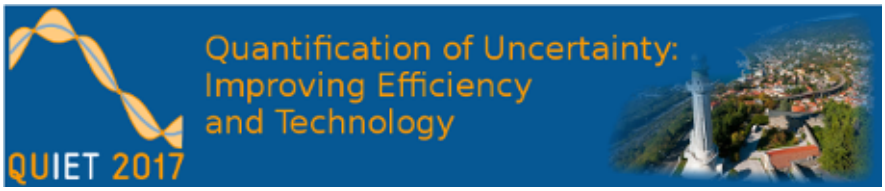
[5] D. Kouri. *Optimization Governed by Stochastic Partial Differential Equations*. 2011.

[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. Ruszczynski. Lectures on stochastic programming: Modeling and theory. 2009.



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

C. Müller[1], S. Ullmann[1], and J. Lang[1]

[1]Technische Universität Darmstadt, Germany

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.

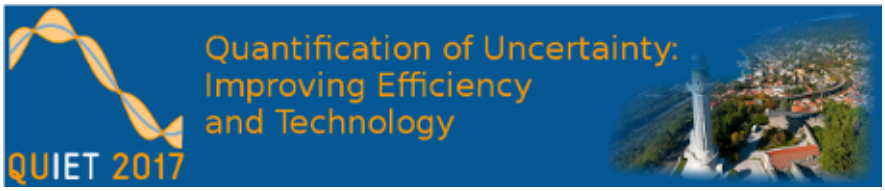
References

[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.

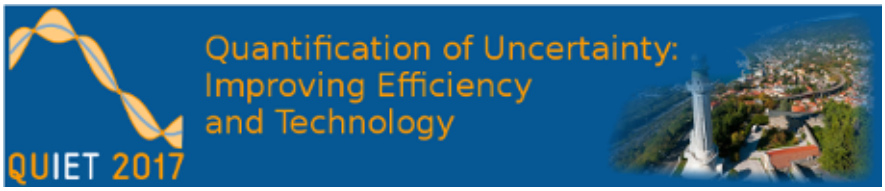


Reduced basis methods for groundwater flow

C. J. Newsum[1] and C. E. Powell[1]

[1]The University of Manchester, United Kingdom

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.

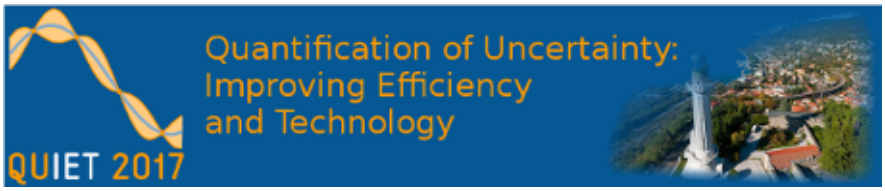


Towards Uncertainty Analysis for Multi-scale Models

A. Nikishova[1] and A. Hoekstra[1]

[1]University of Amsterdam, Netherlands

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.

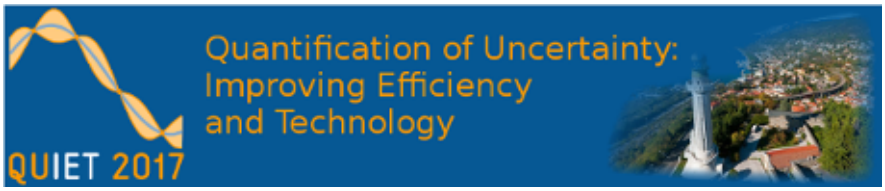


Statistically optimal weights for distributed Tikhonov-regularization

K. Pieper[1] and M. Gunzburger[1]

[1]Florida State University, Tallahassee, United States

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'

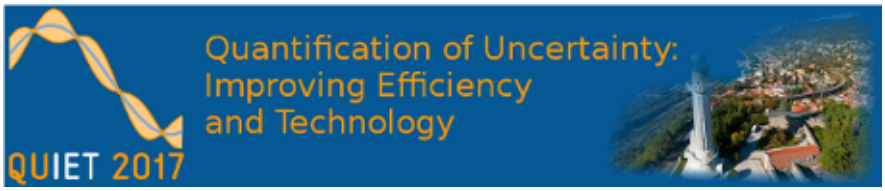
Pranjal[1] and D. Silvester[1]

[1]The University of Manchester, United Kingdom

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(ℓ) 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(ℓ) 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

A. Quaglino[1], S. Pezzuto[1], P.-S. Koutsourelakis[2], and R. Krause[1]

[1]Universitá della Svizzera Italiana, Switzerland
[2]Technische Universität München, Germany

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 hardwares, 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.

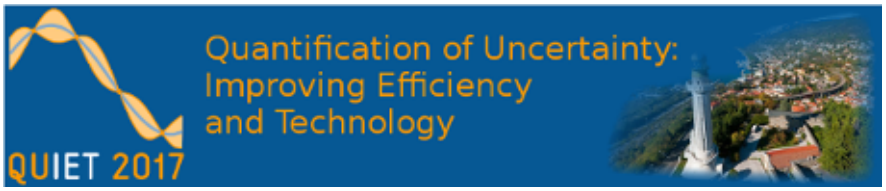
References

[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.



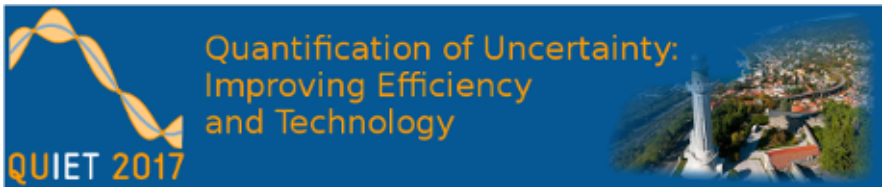
Multilevel Monte Carlo for transmission problems with geometric uncertainties

L. Scarabosio[1]

[1]Technische Universität München, Germany

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^∞-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 aproach also for other problems lacking smoothness with respect to the stochastic parameter.

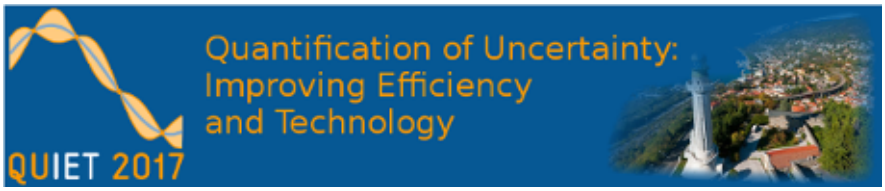


Reduced Basis Methods and Their Application to Ensemble Methods for the Navier-Stokes Equations

M. Schneier[1] and M. Gunzburger[1]

[1]Florida State University, Tallahassee, United States

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

C. Spannring[1], S. Ullmann[1], and J. Lang[1]

[1]Technische Universität Darmstadt, Germany

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

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

The uncertain input ξ 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

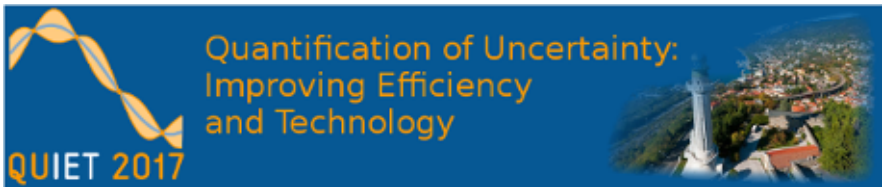
$$s(\xi) = l(u(T; \xi)).$$

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. Ohlberger. Reduced basis method for finite volume approximations of parametrized linear evolution equations. *ESAIM Math. Model. Numer. Anal.*, 42:277–302, 2008.



Stabilization techniques for pressure recovery applied to POD-Galerkin methods for the incompressible Navier-Stokes equations

G. Stabile[1] and G. Rozza[1]

[1] International School for Advanced Studies, Trieste, Italy

In the field of model reduction is crucial to create reduced order models (ROMs) that preserve the stability properties of the original system. Several methods are available in literature for the stability enforcement of reduced order methods.

One promising approach, known as supremizer stabilization [2, 1], is based onto the enrichment of the reduced basis space, with the solution of a supremizer problem, in order to fulfil the well known inf-sup condition. The efficiency and applicability of this stabilization technique has already been verified in the framework of reduced order methods based on high fidelity finite element solvers and recently has been applied also in a finite volume context [4].

In this contribution a comparison between the supremizer stabilization and a Poisson equation for pressure stabilization [3] is presented and discussed.

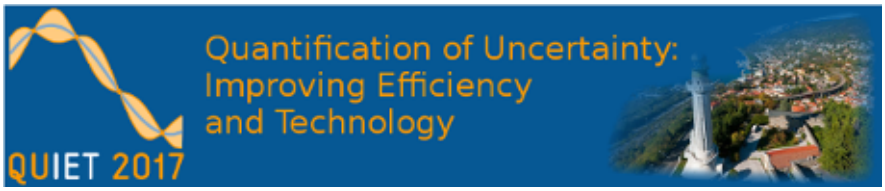
References

[1] F. Ballarin, A. Manzoni, A. Quarteroni, and G. Rozza. Supremizer stabilization of POD-Galerkin approximation of parametrized steady incompressible Navier–Stokes equations. *International Journal for Numerical Methods in Engineering*, 102(5):1136–1161, 2015.

[2] G. Rozza, D. B. P. Huynh, and A. Manzoni. Reduced basis approximation and a posteriori error estimation for Stokes flows in parametrized geometries: Roles of the inf-sup stability constants. *Numerische Mathematik*, 125(1):115–152, 2013.

[3] G. Stabile, S. Hijazi, A. Mola, S. Lorenzi, and G. Rozza. POD-Galerkin reduced order methods for CFD using Finite Volume Discretisation: vortex shedding around a circular cylinder. *Communications in Applied and Industrial Mathematics*, 2017.

[4] G. Stabile and G. Rozza. Stabilized Reduced order POD-Galerkin techniques for finite volume approximation of the parametrized Navier–Stokes equations. *submitted*, 2017.



Deterministic Risk Prediction with Reduced Basis Methods

J. Stemick[1] and W. Dahmen[1]

[1]RWTH Aachen University, Germany

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 predicition 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 aleviate the high evaluation cost several model reduction techniques have already been applied (see e.g. [1], [3]).

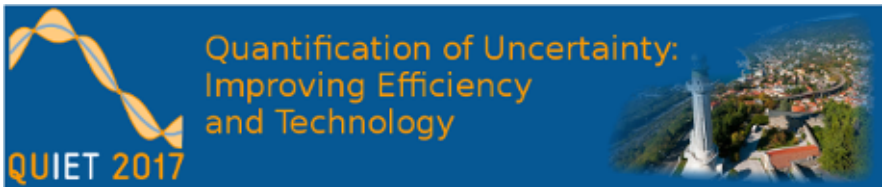
In this work we are looking at deterministic approaches to the problem. Such approaches naturally hinge on sampling the parameter domain and thus suffer greatly from high parameter dimensions. Under which circumstances can the curse of dimensioninality be broken? Guided by the Karhunen-Loeve decomposition 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

M. Strazzullo[1], F. Ballarin[1], R. Mosetti[2], and G. Rozza[1]

[1]International School for Advanced Studies, Trieste, Italy
[2]National Institute of Oceanography and Experimental Geophysics, Trieste, Italy

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.

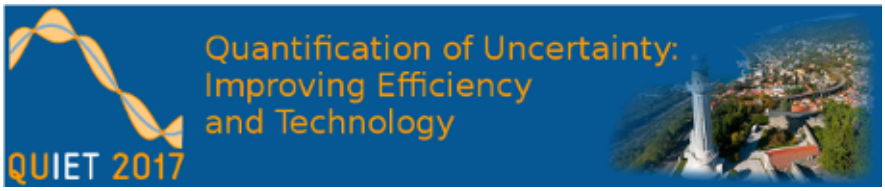
[2] R. Mosetti, C. Fanara, M. Spoto, and E. Vinzi. Innovative strategies for marine protected areas monitoring: the experience of the Istituto Nazionale di Oceanografia e di Geofisica Sperimentale in the Natural Marine Reserve of Miramare, Trieste-Italy. In *OCEANS, 2005. Proceedings of MTS/IEEE*, pages 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

M. Tezzele[1], F. Salmoiraghi[1], A. Mola[1], and G. Rozza[1]

[1]International School for Advanced Studies, Trieste, Italy

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 tyipically 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

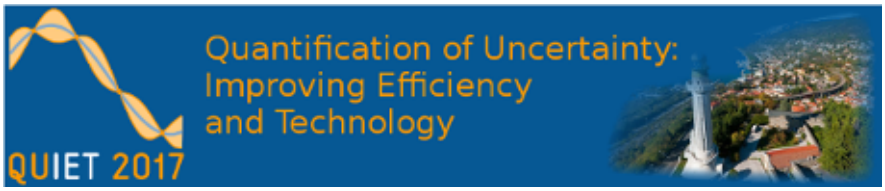
[1] PyGeM: Python Geometrical Morphing. `https://github.com/mathlab/pygem`.

[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.

J.-F. Gerbeau[1,2], D. Lombardi[1,2], and E. Tixier[1,2]

[1]INRIA de Paris, France
[2]UPMC Sorbonne Universités, France

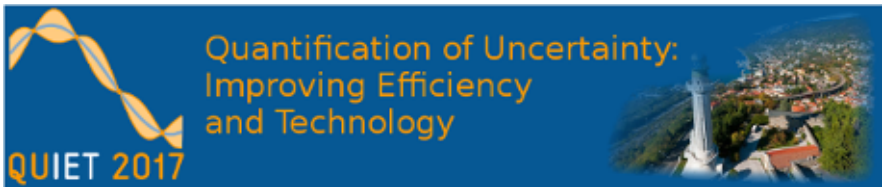
Computational models based on ODEs or PDEs provide a large number of outputs (or features). However, for several tasks such as classification, regression or parameter estimation, a large number of features generally leads to an ill-posed and computationally challenging problem. Therefore, a strategy 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 $\boldsymbol{\vartheta} = (\vartheta_1, \ldots, \vartheta_p)$ is the vector of parameters of interest. Let $\mathbf{v}(\mathbf{u};\boldsymbol{\vartheta})$ denote the vector of model ouputs. First, a dictionary of features $\{f_1, \ldots, f_{N_f}\}$ 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 pof 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 ϑ_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 ϑ_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:

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

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

M. Vohra[1], D. McDougall[1], T. Oliver[1], and R.D. Moser[1]

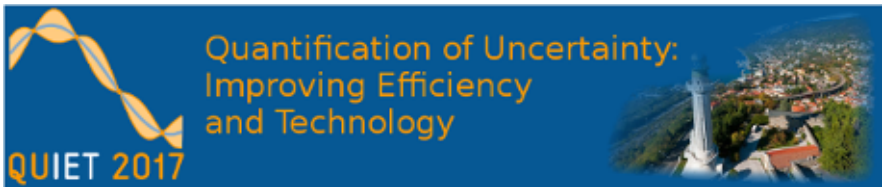
[1]The University of Texas at Austin, United States

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

Z. Zainib[1], Z. Chen[2], F. Ballarin[1], P. Triverio[2], L. Jimenez-Juan[3], A. Crean[4], and G. Rozza[1]

[1]International School for Advanced Studies, Trieste, Italy
[2]University of Toronto, Canada
[3]Sunnybrook Health Sciences Centre, Toronto, Canada
[4]University Health Network, Toronto, Canada

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.