FrontUQ19

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics

Pisa (Italy) – 11-13 September 2019

Book of Abstracts

Sponsors

Università di Pisa

ERCOFTAC

GAMM-UQ Activity Group

CNR-IMATI

Organizers

Maria Vittoria Salvetti – Università di Pisa, Italy
Lorenzo Tamellini – CNR-IMATI, Italy
Didier Lucor – CNRS-LIMSI, France
Oliver Ernst – Technische Universität Chemnitz, Germany
Claudia Schillings – Universität Mannheim, Germany
Alessandro Mariotti – Università di Pisa, Italy
frontuq19@imati.cnr.it

Organizing Secretariat

A.I.C. Asti Incentives & Congressi
P.zza San Uomobono, 30 - Pisa
tel. 050 598808 / 541402
frontUQ19@aicgroup.it

A.I.C.
ASTI INCENTIVES & CONGRESSI
PISA - ITALY

Keynote Lecture - G. Iaccarino - UQ & HPC: towards exascale ensemble simulations

Session Chair: M.V. Salvetti

Auditorium

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

UQ & HPC: towards exascale ensemble simulations

Gianluca Iaccarino

ICME - Institute for Computational & Mathematical Engineering
Mechanical Engineering Department
Stanford University - Stanford, CA USA – jops@stanford.edu

Key words: Uncertainty quantification, Multilevel Sampling, Exascale Computing, Multiphysics Simulations

In the framework of the Predictive Science Academic Alliance Program (PSAAP) the US Department of Energy is funding a Multidisciplinary Simulation Center at Stanford University to explore exascale computing strategies for multiphysics simulations. Stanford Center's research portfolio blends efforts in computer science, uncertainty quantification, and computational physics to tackle a challenging physical problem: the transfer of radiative energy to a turbulent mixture of air and solid particles. The context is provided by a relatively untested and poorly understood method of harvesting solar energy. The talk will describe the Center's effort to develop and validate a computational environment to simulate this challenging multi-physics problem emphasizing the strategies employed to carry out high-fidelity simulations and how uncertainty quantification techniques can be used to assess the overall performance of the system. A novel task-based programming system (Legion) is being deployed to tackle heterogeneous compute systems and retain portability and performance on next-generation computer architectures. Details of the implementation challenges and results obtained on various architectures will be discussed. The integration of large scale simulations and multi-level sampling for uncertainty analysis within the Legion framework will also be summarized.

[1] K. Duraisamy, G. Iaccarino, H. Xiao "Turbulence modeling in the age of data" Annual Review of Fluid Mechanics, Vol 51, pp. 357-377, 2019

[2] H. R Fairbanks, A. Doostan, C. Ketelsen, G. Iaccarino, "A low-rank control variate for multilevel Monte Carlo simulation of high-dimensional uncertain systems", J. of Computational Physics, Vol 341, pp 121-139, 2017

[3] L Jofre, G Geraci, HR Fairbanks, A Doostan, G Iaccarino "Multi-fidelity uncertainty quantification strategies for large-scale multiphysics applications: PSAAP II particle-based solar energy receiver", AIP Conference Proceedings 2018 (1), 140002

SW1 – Turbulence I

Session Chair: G. Iaccarino

Auditorium

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Bayesian field-inversion for turbulence anisotropy with informative priors

***Arent van Korlaar*[1] *and Richard P. Dwight*[1]**

[1] Aerodynamics Group, Faculty of Engineering, Delft University of Technology – r.p.dwight@tudelft.nl

Key words: Bayesian statistics, Reynolds-Averaged Navier-Stokes (RANS) equations, data-driven turbulence modelling, machine-learning, continuous adjoint

Reynolds-Averaged Navier-Stokes (RANS) and its associated turbulence closure models will continue to be necessary in order to perform computationally affordable flow simulations for the foreseeable future. The errors inherent in the semi-empirical turbulence closures, means that significant uncertainty is associated with the results [6, 2]. In this work we use data from expensive LES and DNS simulations to train new closure models for RANS, similar to previous deterministic work [5]. Our procedure is a two-step process, following [3]:

(a) First we find a local turbulence anisotropy correction to the RANS model, which causes the model to reproduce the given LES/DNS mean field.

(b) Secondly we regress the local correction discovered in part (a) as a function of the local mean-flow, using machine-learning techniques.

Step (a) is a field-inversion problem with a large space of valid solutions. Rather than using Tikhonov regularization, we introduce an informative prior on the correction derived using random matrix theory [7, 4]. This prior guarantees the positive-definiteness of the Reynolds stress tensor, and encourages physically reasonable corrections in the posterior. After doing this for several flows, in Step (b) we fit a stochastic regression model to the resulting data set [1]. The posterior covariance, approximated using the Hessian of the simulation code, is exploited to give the regression model realistic uncertainty. Unseen flows are then predicted with this model, which include now informed estimates of model uncertainty.

The framework is trained on channel flows, backward-facing steps, and the converging diverging duct. Predictions for the (unseen) periodic-hill are made (see Figure 1), demonstrating the ability of the framework to generalize beyond the training set.

References

[1] J.H.S. de Baar, R.P. Dwight, and H. Bijl. “Improvements to Gradient-Enhanced Kriging using a Bayesian Interpretation”. In: *International Journal for Uncertainty Quantification* 4.3 (2013), pp. 205–223.

[2] W.N. Edeling, P. Cinnella, and R.P. Dwight. “Predictive RANS simulations via Bayesian Model-Scenario Averaging”. In: *Journal of Computational Physics* 275 (2015), pp. 65–91.

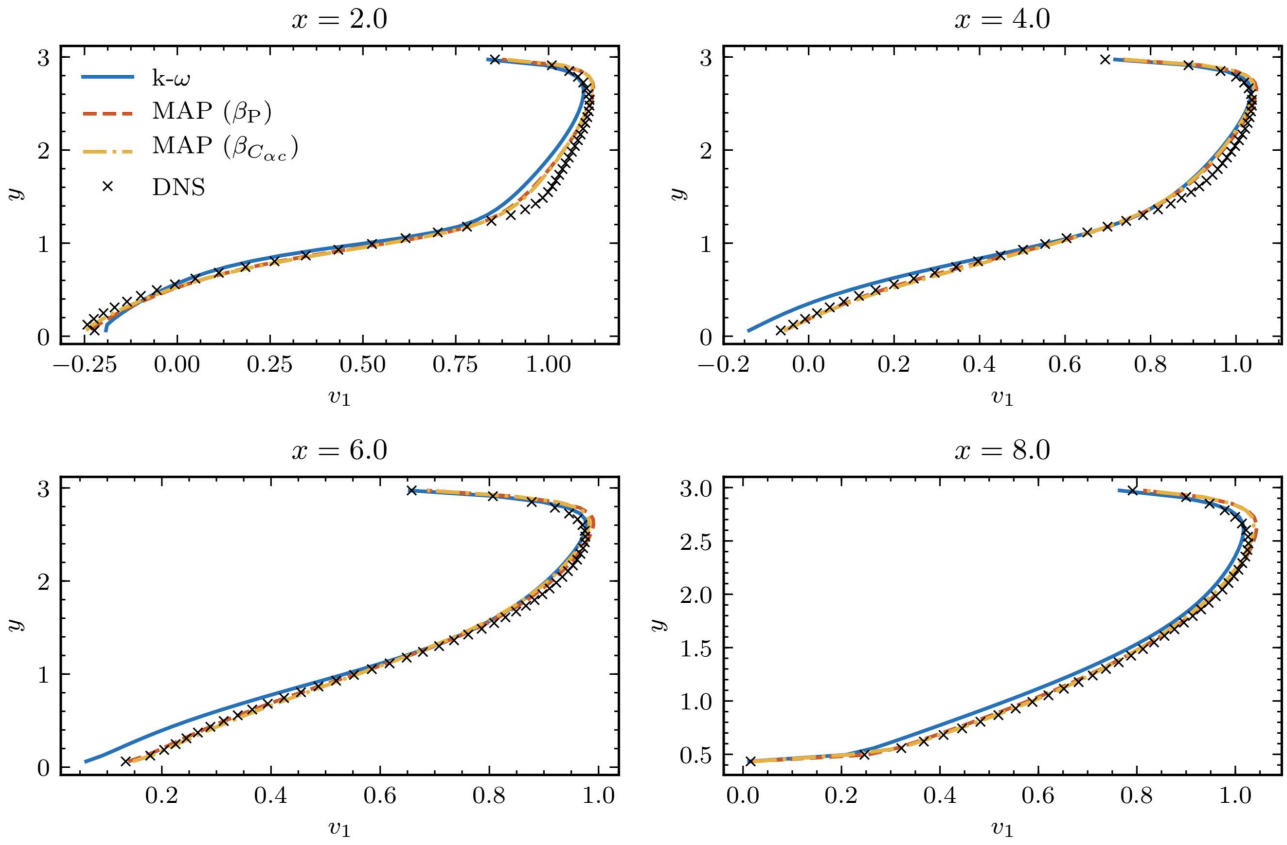
[3] Karthik Duraisamy Eric J. Parish. “A paradigm for data-driven predictive modeling using field inversion and machine learning”. In: *Journal of Computational Physics* 305 (2016), pp. 758–774.

[4] Roger G. Ghanem Heng Xiao Jian-Xun Wang. “A Random Matrix Approach for Quantifying Model-Form Uncertainties in Turbulence Modeling”. In: *arXiv* arXiv:1603.09656 [physics.flu-dyn] (2016).

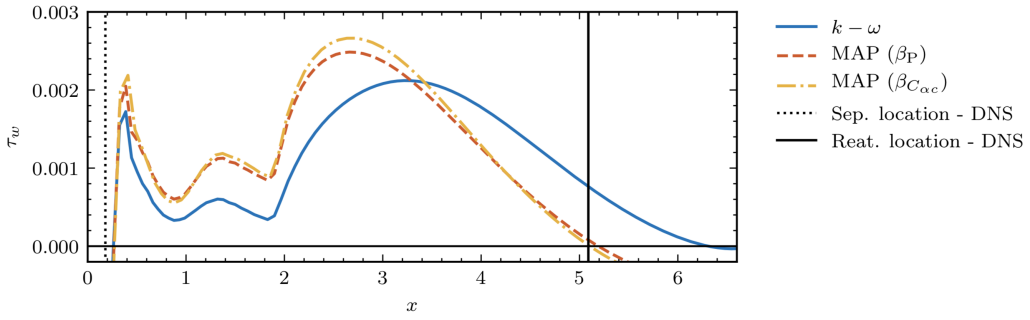
[5] Mikael L. A. Kaandorp and Richard P. Dwight. *Stochastic Random Forests with Invariance for RANS Turbulence Modelling*. 2018. eprint: `arXiv:1810.08794`.

[6] S.B. Pope. *Turbulent flows*. Cambridge Univ Pr, 2000.

[7] C. Soize. “Random matrix theory for modeling uncertainties in computational mechanics”. In: *Computer Methods in Applied Mechanics and Engineering* 194.12 (2005), pp. 1333–1366. ISSN: 0045-7825.



(a) Horizontal velocity profiles.



(b) Skin-friction on lower wall.

Figure 1: Prediction of periodic-hill mean-flow using RANS with baseline $k-\omega$, and two stochastic data-driven closure models. Model β_P learns a k-production correction; model $\beta_{C_{ac}}$ also learns an isotropy correction.

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Using Machine learning to predict and understand turbulence modelling uncertainties

Ashley Duncan Scillitoe[1]

[1]The Alan Turing Institute, London, UK – ascillitoe@turing.ac.uk

Key words: Epistemic uncertainty, Turbulence modelling, Sensitivity analysis, Machine learning.

Many industrial flows are turbulent in nature, and Reynolds-Averaged Navier-Stokes (RANS) based turbulence models play an important role in the prediction of such flows. Many simplifying assumptions are made in the development of a RANS model. These assumptions can lead to epistemic uncertainties which are still a major obstacle for the predictive capability of RANS models. If experimental measurements or higher fidelity simulation results are not available for comparison, it can be difficult to evaluate the accuracy of RANS predictions. Recently, data-driven strategies have been proposed to either quantify model uncertainty [2], or improve model accuracy [3]. Many of these strategies involve training supervised machine learning (ML) models on high fidelity CFD data, such as that from large eddy simulations [1].

Ling and Templeton [4] proposed a technique whereby a machine learning classifier is trained to detect whether a number of RANS modelling assumptions are broken. The classifier can then be used to predict regions of high and low uncertainty in RANS simulations where corresponding high fidelity data is not available. In the present work, the original technique is further refined, and applied to a number of flow configurations such as a recent family of bumps dataset [5]. The non-dimensional “features" used by Ling and Templeton to describe each flow to the ML model are revisited, with improvements made to ensure the ML classifier is more generalisable to other flows. New error metrics are also proposed to allow for other areas of RANS modelling uncertainty to be explored. Figure 1 shows a prediction made for one of the bump cases, with the region in red being a region where the Boussinesq hypothesis used by many RANS models would be invalid due to the high turbulent anisotropy.

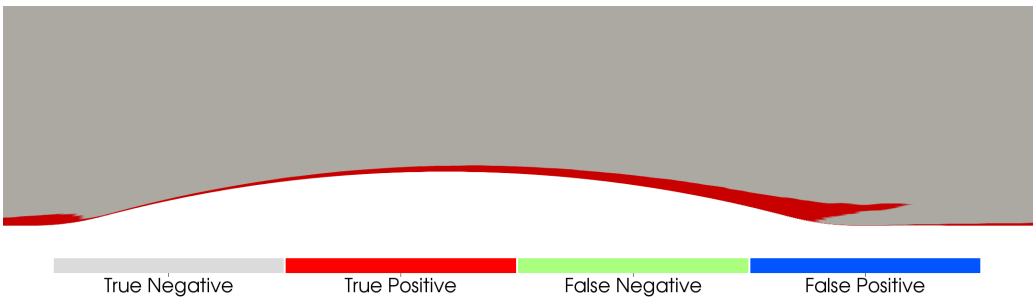


Figure 1: Regions in the flow over a bump [5] where the Boussinesq hypothesis is predicted to be invalid due to significant turbulent anisotropy, predicted by a random forest classifier.

Within the ML community there is an increasing interest in interpretability. Indeed, a common criticism of ML augmented RANS models is that they are a “black box", with the machine able to make accurate predictions but not explain why it has made them. The proposed RANS error classifier is examined using recently proposed ML interpretation methods such as individual conditional expectation [6] and Shapley additive explanations (SHAP) [7] plots. These novel techniques provide global and local explanations of model predictions. A SHAP summary plot, which summarises the global effect of each flow feature (the model inputs) on the turbulent

anisotropy metric (a model output), is shown in Figure 2. More detailed SHAP plots are discussed, such as SHAP dependence and local force plots. Now, the proposed classifier can not only be used to predict regions of uncertainty, but also to explain what physical flow features have caused this uncertainty. This brings with it the possibility of using the classifier to aid in the further understanding and development of turbulence models, in addition to its use as a tool in predicting “trust" regions in RANS simulations.

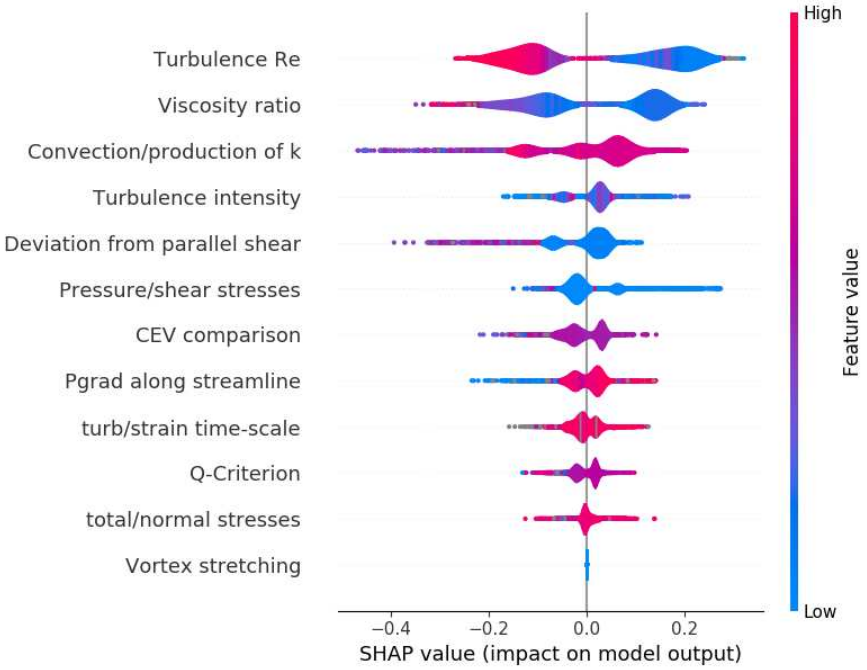


Figure 2: A SHAP summary plot showing the impact of flow features on the turbulent anisotropy error metric predicted in Figure 1.

[1] A. D. Scillitoe, P. G. Tucker and P. Adami, “Large eddy simulation of boundary layer transition mechanisms in a gas-turbine compressor cascade" Journal of Turbomachinery **141**, 6 (2019).

[2] W. Edeling, G. Iaccarino and P. Cinnella, “Data-Free and Data-Driven RANS Predictions with Quantified Uncertainty" Flow, Turbulence and Combustion **100**, 3 (2018).

[3] J. Wu, H. Xiao and E. Paterson, “Physics-informed machine learning approach for augmenting turbulence models: A comprehensive framework" Physical Review Fluids **7**, 3 (2018).

[4] J. Ling and J. Templeton, “Evaluation of machine learning algorithms for prediction of regions of high Reynolds averaged Navier Stokes uncertainty" Physics of Fluids **27**, 8 (2015).

[5] R. Matai and P. Durbin, “Large-eddy simulation of turbulent flow over a parametric set of bumps" Journal of Fluid Mechanics **866** (2019).

[6] A. Goldstein et al., “Peeking inside the black box: visualizing statistical learning with plots of individual conditional expectation" Journal of computational and graphical statistics **24**, 1 (2015).

[7] S. M. Lundberg and S. I. Lee, “A Unified approach to interpreting model predictions" Advances in neural information processing systems **30** (2017).

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

State Estimation for wall-bounded turbulent flows using the Immersed Boundary Method and Data Assimilation

Marcello Meldi[1,2]

[1]Institut Pprime, Department of Fluid Flow, Heat Transfer and Combustion CNRS - ENSMA - Université de Poitiers, UPR 3346, F86962 Futuroscope Chasseneuil Cedex, France

[2]Aix-Marseille Univ., CNRS, Centrale Marseille, M2P2 Marseille, France – marcello.meldi@ensma.fr

Key words: Immersed Boundary Method, Data Assimilation, Kalman Filter

The accurate prediction of numerous bulk flow features of unstationary flows such as aerodynamic forces is driven by the precise representation of localized near-wall dynamics, owing to the non-linear behavior of such configurations. This aspect is particularly relevant for the flow prediction around complex geometries. In this case classical body-fitted approaches may have to deal with high deformation of the mesh elements, usually providing poor numerical prediction. Additionally, the simulation of moving bodies may require prohibitively expensive mesh updates. In the last decades, the Immersed Boundary Method (IBM) [1, 2, 3, 4, 5] has emerged as one of the most popular strategies to handle these two problematic aspects. The main difficulty with IBM is the accurate representation of near wall flow features, which is a governing aspect in most engineering cases. The wall resolution required increases with the Reynolds number as finer structures are observed due to multi-scale interactions, leading to a faster rise of the resources demanded when compared with body-fitted methods.

The present work aims for the advancement of the IBM method recently developed by the Author via Data Assimilation (DA). DA includes a wide spectrum of tools which derive an optimized state integrating a model and available observation which are affected by uncertainties. Among these tools, the estimator recently proposed by the Author [6] is one of the very first tools which successfully provided an augmented state estimation integrating CFD and experimental data for the analysis of turbulent flows. Thus, the main objective is to improve the accuracy of the IBM method (model) integrating high-fidelity data (observation) via DA.

The study is performed for the flow around a circular cylinder for $Re_D = 3900$ [7, 8]. This flow configuration has been identified because the flow exhibits turbulent features in the wake but the boundary layer is laminar. This aspect allows to exclude the complex representation of wall turbulence effects in this initial analysis. In addition, this configuration does not exhibit a boundary layer separation driven by the geometry, allowing to perform a strong test of the capabilities of the IBM-DA approach to reconstruct essential physical features.

Table 1: Bulk flow quantities calculated with the numerical simulations of the database

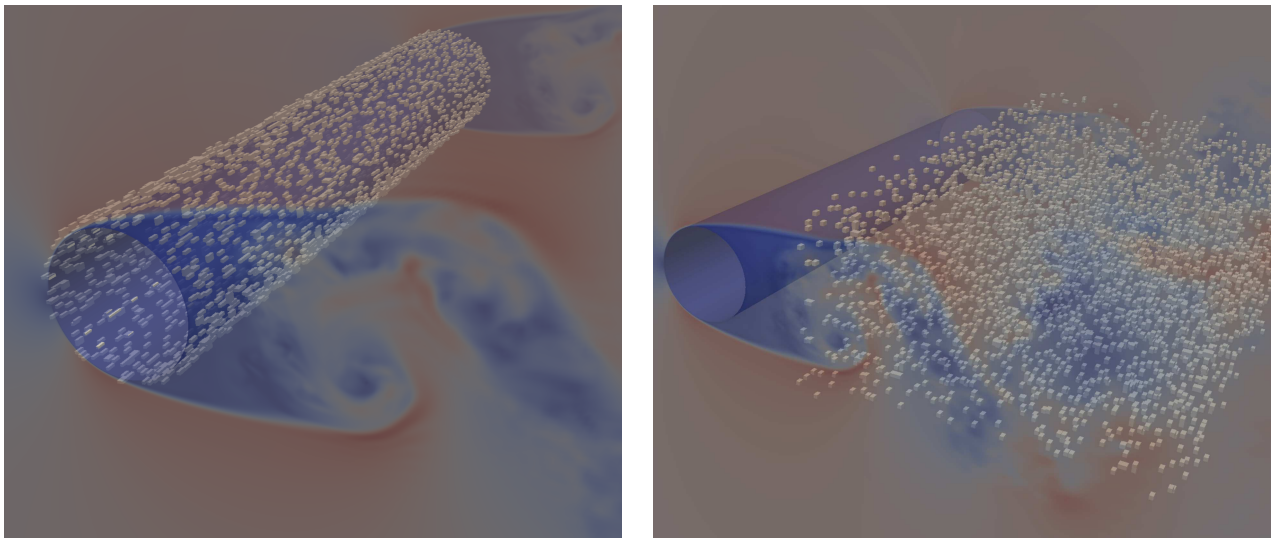
Simulation	C_D	C'_L	St	Rec. length
DNS	0.977	0.118	0.209	1.53
LES	1.093	0.25	0.2	1.15
IBM	1.225	0.101	0.2	1.7
IBM-DA-W	1.109	0.107	0.206	1.62
IBM-DA-K	1.233	0.117	0.207	1.52

Three classical simulations have been initially performed namely a body-fitted direct numerical simulation (DNS), a body-fitted large-eddy simulation (LES) and a classical, under-resolved IBM simulation (IBM). The predicted bulk flow quantities reported in Table 1 indicate that the lack of near-wall resolution is responsible

for a significant error in the prediction of the C_D when compared to the DNS. Thus, the IBM-DA strategy is used to improve the performance of IBM integrating the high precision DNS data. Formally, this means that the Kalman Filter strategy relies on:

- A continuous low-precision *model*, which is the IBM over the coarse mesh
- High confidence local observation, i.e. local, instantaneous velocity sampled from DNS data

The Kalman filter provides a precise state estimation which is used to calibrate the IBM volume forcing term introduced in the discretized equations. The performance of this strategy is tested estimating its sensitivity to the positions of the sensors. Two different distributions have been chosen for a cloud of 4000 sensors over which DNS data have been sampled (see fig. 1).



(a) (b)

Figure 1: Positioning of the sensors for Data Assimilation

The performance of the IBM-DA simulations is assessed via observation of the computed bulk flow quantities, which are reported in table 1. Results for the simulation IBM-DA-W (sensors in the wall region) are remarkably good for all the physical quantities ($\approx 50\%$ improvement). On the other hand, the results for the simulation IBM-DA-K (sensors in the wake) are less satisfying. An excellent agreement is obtained for C_L', St and the recirculation length, which are quantities associated with the behavior of the wake. However, the drag coefficient C_D is mostly unchanged when compared to the classical IBM simulation. This implies that the accurate information obtained integrating the DNS data is not efficiently propagated upstream.

[1] C. S. Peskin, "Flow patterns around heart valves: A numerical method ," *Journal of Computational Physics*, vol. 10, no. 2, pp. 252 – 271, 1972.

[2] R. Mittal and G. Iaccarino, "Immersed boundary methods," *Annual Review of Fluid Mechanics*, vol. 37, pp. 239 – 261, 2005.

[3] M. Uhlmann, "An immersed boundary method with direct forcing for the simulation of particulate flows," *Journal of Computational Physics*, vol. 209, no. 2, pp. 448 – 476, 2005.

[4] A. Pinelli, I. Naqavi, U. Piomelli, and J. Favier, "Immersed-boundary methods for general finite-difference and finite-volume Navier–Stokes solvers ," *Journal of Computational Physics*, vol. 229, no. 24, pp. 9073 – 9091, 2010.

[5] H. Riahi, M. Meldi, J. Favier, E. Serre, and E. Goncalves, "A pressure-corrected immersed boundary method for the numerical simulation of compressible flows," *Journal of Computational Physics*, vol. 374, no. 1, pp. 361 – 383, 2018.

[6] M. Meldi and A. Poux, "A reduced order model based on Kalman Filtering for sequential Data Assimilation of turbulent flows," *Journal of Computational Physics*, vol. 347, pp. 207–234, 2017.

[7] M. Breuer, "Large eddy simulation of the subcritical flow past a circular cylinder: numerical and modeling aspects," *International Journal for Numerical Methods in Fluids*, vol. 28, pp. 1281–1302, 1998.

[8] P. Parnaudeau, J. Carlier, D. Heitz, and E. Lamballais, "Experimental and numerical studies of the flow over a circular cylinder at Reynolds number 3900," *Physics of Fluids*, vol. 20, no. 8, p. 085101, 2008.

SW2 – Turbulence II

Session Chair: R. Dwight

Auditorium

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Enhancing RANS with LES for Variable-Fidelity Optimization

Yu Zhang,[1,2] ***Richard P. Dwight,***[2] ***and Javier F. Gómez***[2]

[1]School of Aeronautics, Northwestern Polytechnical University, PRC – zhangyu91@mail.nwpu.edu.cn

[2]Aerodynamics Group, Aerospace Engineering, TU Delft – [r.p.dwight@tudelft.nl | jfatoug@gmail.com]

Key words: Uncertainty quantification, Reynolds-Averaged Navier-Stokes equations, Turbulence modeling, variable-fidelity optimization, LES

Reynolds-Averaged Navier-Stokes (RANS) based aerodynamic optimization is widely used in aerospace engineering due to its acceptable computational cost and turn-around time. However, in many important situations, such as friction-drag reducing surfaces (e.g. dimples) and designs where separation is critical, the physics demands scale-resolving simulations of turbulence such as large-eddy simulation (LES). LES is often useful for a final analysis, but its high computation cost precludes its use within a design loop.

Variable-fidelity methods with high-fidelity (hi-fi) model from LES and low-fidelity (low-fi) model from RANS are possible, but this class of methods rely for their efficiency on a high-correlation between the low-fi and hi-fi models, and still require a large number of hi-fi evaluations – whereas our target is $\sim$ 3 LES simulations per optimization. Furthermore variable-fidelity methods typically use only the (scalar) cost-function predictions, whereas LES contains a lot more information about the flow, potentially exploitable by RANS.

Therefore in this study, we propose an optimization procedure considering of two key steps:

1. Given $\simeq$ 3 LES simulations in the parameter space, we train a customized and stochastic RANS model which reproduces these LES mean-fields well, and provides estimates of remaining model error.
2. We use this enhanced RANS model to sample new locations in the parameter space, and build a variable-fidelity surrogate using co-Kriging, and the enhanced RANS error estimates.

The optimization is then performed on the surrogate using an EGO-like sampling procedure [1] [2].

The enhanced RANS model is obtained by using stochastic machine-learning methodologies to provide a prediction of the turbulence anisotropy tensor (b_{ij}), and the turbulence kinetic-energy (k), in terms of the mean-flow quantities resolved by RANS, in a manner analogous to algebraic Reynolds-stress models. We investigate stochastic versions of several machine-learning methods, in particular the Tensor Basis Random Forest (TBRF) [3], the Tensor Basis Neural Network (TBNN) [4], and a symbolic-regression method [5].

The variable-fidelity surrogate can not be a standard co-Kriging, as it must take into account the dependence of the accuracy of the low-fi model (enhanced-RANS), on the hi-fi model samples (from LES). In particular, the goal is that enhanced RANS is accurate on flows similar to the LES training cases; but errors increase far from the LES samples. A statistical model representing the structure of the errors is devised.

The framework is tested on a periodic hill case with parameters controlling the hills' shape [6]. All the methods are trained for a specific periodic hill [7], and then used for predicting the flow fields of periodic hills with different geometries to evaluate the statistic error. With the best-performed method, the variable-fidelity optimization using LES as the hi-fi analysis and enhanced RANS as low-fi analysis is tested. Comparison with single-fidelity optimization based on RANS and variable-fidelity optimization based on LES and standard RANS will be given.

[1] D. R. Jones, M. Schonlau, and W. J. Welch, "Efficient global optimization of expensive black-box functions," Journal of Global Optimization **13**(4), 455-492 (1998).

[2] Y. Zhang, Z. H. Han, and K. S. Zhang, "Variable-fidelity expected improvement method for efficient global optimization of expensive functions," Structural and Multidisciplinary Optimization **58**(4), 1431-1451 (2018).

[3] M. Kaandorp, *Machine learning for data-driven RANS turbulence modelling* (Master thesis, Delft University of Technology, 2018).

[4] J. Ling, A. Kurzawski, and J. Templeton, "Reynolds averaged turbulence modelling using deep neural networks with embedded invariance," Journal of Fluid Mechanics **807**, 155-166 (2016).

[5] M. Schmelzer, R. Dwight, and P. Cinnella, "Data-Driven Deterministic Symbolic Regression of Nonlinear Stress-Strain Relation for RANS Turbulence Modelling," In *Fluid Dynamic Conference*, 1-13 (AIAA, Atlanta, Georgia, 2018).

[6] J. F. Gómez, *Multi-fidelity Co-kriging optimization using hybrid injected RANS and LES* (Master thesis, Delft University of Technology, 2018).

[7] M. Breuer, N. Peller, Ch. Rapp, and M. Manhart, "Flow over periodic hills - Numerical and experimental study in a wide range of Reynolds numbers," Computers & Fluids **38**, 433-457 (2009).

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Stochastic analysis of the effect of modeling, numerical and geometrical parameters in large-eddy simulations of the flow around a 5:1 rectangular cylinder

Benedetto Rocchio,[1] ***Alessandro Mariotti,***[1] ***and Maria Vittoria Salvetti,***[1]

[1]DICI, University of Pisa, Italy – benedetto.rocchio@ing.unipi.it, alessandro.mariotti@unipi.it, mv.salvetti@ing.unipi.it

Key words: Rectangular 5:1 cylinder aerodynamics, upstream-corner rounding effect, polynomial chaos

The Benchmark on the Aerodynamics of a Rectangular Cylinder (BARC) having chord-to-depth ratio equal to 5 collects a large number of flow realizations obtained both in wind tunnel tests and in numerical simulations, part of them reviewed in [1]. This configuration (see Fig. 1a for a sketch) is often used in civil engineering, e.g. tall buildings and bridges, for which the Reynolds number are usually high and the flow is turbulent. Moreover, in spite of the simple geometry, the flow dynamics is complex, with flow separation at the upstream corners, reattachment on the cylinder side and vortex shedding in the wake. A significant dispersion was observed in numerical predictions, but also in experimental measurements, of the topology of the flow on the cylinder and of some related quantities of practical interest, such as the distribution of mean and fluctuating pressure on the cylinder sides. The wind tunnel tests in [2] indicated that the discrepancies observed between the different experiments may be mainly explained by different levels of freestream turbulence. On the other hand, the reasons of the discrepancies bewteen numerical predictions are not clear and different sensitivity studies carried out by the contributors were not conclusive. For instance, Bruno et al. [3] indicated that increasing the grid resolution in the spanwise direction in large-eddy simulations led to a significant reduction of the length of the mean recirculation zone present on the cylinder sides. Unexpectedly, this also deteriorated the agreement with the experiments. This gave the motivation to the stochastic analysis in [4], in which the sensitivity of LES results to grid resolution in the spanwise direction and to the amount of subgrid-scale (SGS) dissipation was investigated. We summarize herein the methodology and the main results; for more details we refer to [4].

The LES simulations are carried out for incompressible flow by using the open-source code Nek5000 that is based on a spectral-element method. The basis functions inside each element consist of Legendre polynomials, of the order N for velocity, and $N-2$ for pressure; $N = 6$ is adopted in the present study. The time discretization is based on the high-order splitting method, in which a third-order backward differentiation scheme is used for the time derivatives. The viscous terms are treated implicitly while an explicit scheme is considered for the non linear convective terms, with a third order forward extrapolation in time. The time step is such that approximately 3000 time steps are present in each vortex-shedding cycle. The computational domain is sketched in Fig. 1, in which its dimensions and the adopted boundary conditions are also reported. The spectral element sizes in the $xy-$plane are $\Delta x = \Delta y = 0.125D$.

As previously said, the sensitivity to the following parameters is investigated: the spanwise grid size, Δz (motivated by the previously cited study in [3]) and the weight of a low-pass explicit filter in the modal space, applied at the end of each step of the Navier-Stokes time integration, which can be considered as proportional to the amount of introduced SGS dissipation (see [4]).

Due to the large costs of each LES simulation, a systematic deterministic sensitivity analysis would not be affordable in practice. In order to obtain continuous response surfaces of the quantities of interest in the parameter space starting from a limited number of LES, the so-called gPC approach is adopted herein in its non-intrusive form. The input parameters are considered as random variables with a given PDF (assumed uniform herein) and the output quantities are directly projected over the orthogonal basis spanning the random

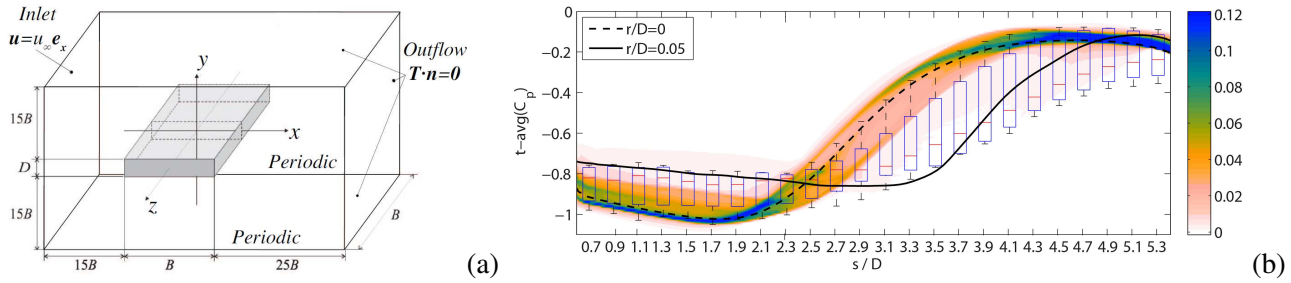


Figure 1: (a) Sketch of the computational domain and (a) mean pressure coefficient on the lateral sides of the cylinder obtained with sharp edges ($r/D = 0$) and roundings $r/D = 0.05$. A comparison is provided with the PDF of the stochastic analysis in [4] and with the ensemble statistics of the BARC experiments from [1]

space, without any modification of the deterministic solver. The polynomial expansion being truncated to the third order in each of the input parameter, 16 simulations were needed to compute the coefficients of the expansion. An example of the obtianed results is given in Figure 1b, in which the pdf of the mean pressure coefficient distribution on the cylinder side is shown. It can be seen that most of the occurrences cluster around a distribution which is significantly different from the experimental results (also reported in the figure). From a more detailed analysis of the results (see [4]), it is found that, both for a fine discretization in the spanwise direction or for a low SGS dissipation, numerical simulations tend to significantly under-predict the distance from the upstream corners at which the mean flow reattachment occurs and, thus, to have a shorter mean recirculation region aside the rectangular cylinder.

In principle, simulations with fine discretization and low SGS dissipation are expected to be the most reliable ones, since they are able to accurately take into account smaller scales. Thus, the fact that they give the largest disagreement with the experimental results is a sort of paradox. Since, this trend is consistent with that found in [3] with a completely different numerical method and SGS model, we concluded that the disagreement was most probably not due to the adopted numerics and modeling. A possible reason could be the presence of perfectly sharp corners in numerical simulations, while in experiments a small uncontrolled roundness is unavoidable. These perfectly sharp corners may generate some disturbances leading to a premature instability of the shear layers and hence to a too short mean recirculation zone on the cylinder sides. This hypothesis has been supported by the results of a LES simulations having a low subgrid-scale dissipation and highly refined grid but with rounded upstream corners ($r/D = 0.05$, r being the radius of the corner rounding). The mean pressure distribution obtained in this simulation is shown in Fig. 1b with a continuous line and can be compared to the one with the same set-up and sharp edges indicated by a dotted line. It can be seen that the presence of upstream corner roundings significantly improves the agreement with experimental results.

Therefore, we decided to carry out a stochastic sensitivity analysis to the rounding radius of the upstream corners. Continuous response surfaces in the parameter space are again obtained from a small number of LES simulations by using the generalized Polynomial Chaos (gPC) approach. The radius of the rounding is varied in the range $0 \leq r/D \leq 0.058$. The impact of the uncertainty in this parameter is evaluated on the quantities of interest in the BARC benchmark, in particular on the distribution on the cylinder of the mean and of the standard deviation of the pressure coefficient and the size of the main recirculation region on the cylinder lateral surface. The results will be shown in the final presentation.

[1] L. Bruno, M. V. Salvetti, and F. Ricciardelli, "Benchmark on the aerodynamics of a rectangular 5:1 cylinder: and overview after the first four years of activity," J. Wind Eng. Ind. Aerodyn. **126**, 87-106 (2014).

[2] C. Mannini, A. M. Marra, L. Pigolotti, and G. Bartoli, "The effects of free-stream turbulence and angle of attack on the aerodynamics of a cylinder with rectangular 5:1 cross section," J. Wind Eng. Ind. Aerodyn. **161**, 42-58 (2017).

[3] L. Bruno, N. Coste, and D. Fransos, "Simulated flow around a rectangular 5:1 cylinder: spanwise discretisation effects and emerging flow features," J. Wind Eng. Ind. Aerodyn. **104-106**, 203-215 (2012).

[4] A. Mariotti, L. Siconolfi, and M. V. Salvetti, "Stochastic sensitivity analysis of large-eddy simulation predictions of the flow around a 5:1 rectangular cylinder," Eur. J. Mech. B-Fluid **62**, 149-165 (2017).

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Numerical Uncertainties in Scale-Resolving Simulations of Wall Turbulence

Saleh Rezaeiravesh,[1] ***Ricardo Vinuesa,***[1,2] ***and Philipp Schlatter,***[1,2]

[1]Linné FLOW Centre, KTH Mechanics, Royal Institute of Technology, Sweden
[2]Swedish e-Science Research Centre (SeRC), Sweden
salehr@kth.se, rvinuesa@mech.kth.se, pschlatt@mech.kth.se

Key words: Uncertainty quantification, Wall-bounded turbulent flows, Nek5000, OpenFOAM

High-fidelity scale-resolving numerical approaches such as direct numerical simulation (DNS) and large eddy simulation (LES) are powerful tools to study the complex physics of wall-bounded turbulent flows. Two main challenges are encountered when using these approaches: the high computational costs at high Reynolds numbers (Re), and the accuracy of their predictions. The focus of the present study is on the latter. Using uncertainty quantification (UQ) techniques, the aim is to investigate how the accuracy of the quantities of interest (QoIs) of scale-resolving simulations is sensitive to various numerical parameters.

The numerical solutions of the Navier–Stokes equations for turbulent flows can be contaminated by some level of uncertainties and errors originating from different sources. Assume $\varphi_h(\mathbf{x}, t)$ represents a discrete flow quantity obtained by DNS/LES, where $\mathbf{x}$ is the position vector and t is time. The averaged value of this quantity over statistically homogeneous directions and finite time T is considered to be a QoI and represented by $\langle\varphi_h(\mathbf{x}, t)\rangle_T$. Given reference true data, $\langle\varphi_h^\circ(\mathbf{x}, t)\rangle$, we can write,

$$\|\langle\varphi_h(\mathbf{x}, t)\rangle_T - \langle\varphi_h^\circ(\mathbf{x}, t)\rangle\| \leq \|\langle\varphi_h(\mathbf{x}, t)\rangle - \langle\varphi_h(\mathbf{x}, t)\rangle_T\| + \|\langle\varphi_h(\mathbf{x}, t)\rangle - \langle\varphi_h^\circ(\mathbf{x}, t)\rangle\| .$$

On the right-hand side, the first and second terms represent the uncertainties due to finite time-averaging (sampling error), $\mathcal{E}_T$, and the combination of all other numerical and modeling errors (excluding the projection error), $\mathcal{E}_n$, respectively. Due to the dominant non-linearity of the Navier–Stokes equations and the fact that various numerical and modeling errors are intertwined, deriving accurate a-posteriori estimates for $\mathcal{E}_n$ in turbulent flows is not feasible. Here, the strategy is to study the sensitivity and behavior of the $\mathcal{E}_n$ of different QoIs with respect to several sources of uncertainty through systematic flow simulations. To this end, sufficient instantaneous samples are considered to ensure $\mathcal{E}_T \ll \mathcal{E}_n$. Further, the error in the profiles of QoIs is measured by $\epsilon_\infty[g] = \|g - g^\circ\|_\infty / \|g^\circ\|_\infty$, where $g(y) = \langle\varphi_h(y, t)\rangle_T$ and y denotes the wall-normal coordinate.

The wall-resolving simulations are performed using the open-source flow solvers `Nek5000` and `OpenFOAM`, which are respectively based on spectral-element and standard finite-volume methods. The focus is on canonical wall-bounded turbulent flows such as channel flow. For `Nek5000`, the impact of filtering, the order of the polynomial bases for velocity and pressure, the tolerance for iterative solutions for these quantities, and the grid resolution in different directions are investigated. These sets of factors are more detailed than what has been considered in previous studies, see *e.g.* Ref. [1]. For `OpenFOAM`, the study is focused on the effects of grid resolution and the discretization scheme for the non-linear convective term in the momentum equation, see [2].

In line with the described strategy, a UQ forward problem is formulated, in which the numerical parameters, such as grid resolution and filtering parameters, are considered to be uncertain. The associated uncertainties in these parameters (hereafter shown by $\mathbf{q}$) are propagated into the responses $\mathcal{R}$. The latter are defined to be the normalized deviation of the simulated flow QoIs from the reference DNS data. The parameters $\mathbf{q}$ are allowed to vary over the presumed admissible space $\mathbb{Q}$. Using polynomial chaos expansion (PCE) with stochastic collocation samples [3] in a non-intrusive way, surrogates are constructed for $\mathcal{R} = \tilde{f}(\mathbf{q})$. Employing the surrogates, the portraits of the errors in the QoIs are obtained over the whole space $\mathbb{Q}$. Moreover, the Sobol indices provide a quantitative basis to compare the global sensitivity of different errors with respect to variation of $\mathbf{q}$.

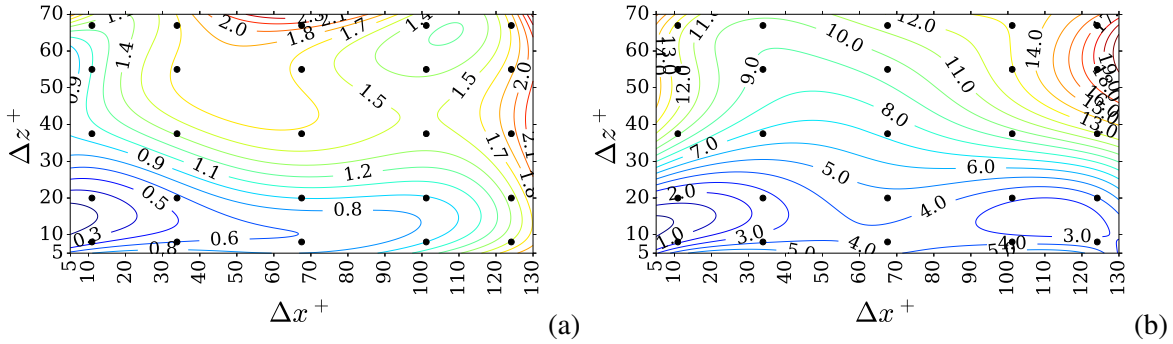


Figure 1: Isolines of (a) $\epsilon_\infty[\langle u \rangle]$ % and (b) $\epsilon_\infty[\mathcal{K}]$ % of turbulent channel flow in the admissible Δx^+-Δz^+ space, when using `Nek5000`. In all the simulations, $\mathrm{Re}_\tau = 300$ and $\Delta y_w^+ = 0.5$.

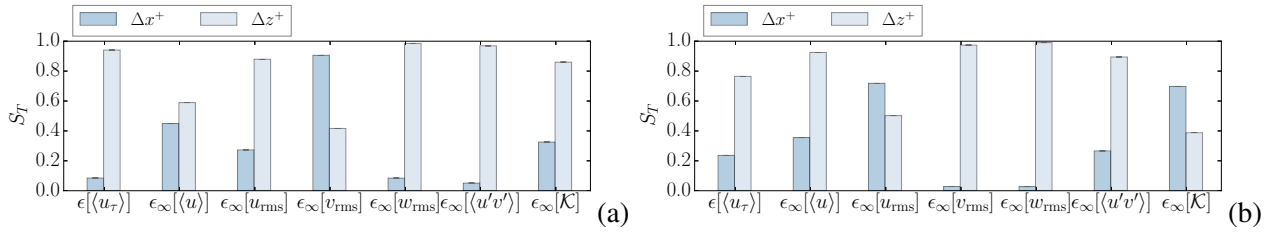


Figure 2: Total sensitivity indices of the error in different QoIs with respect to Δx^+ and Δz^+, when using (a) `Nek5000` and (b) `OpenFOAM`. In all the simulations, $\mathrm{Re}_\tau = 300$, $\Delta y_w^+ = 0.5$, $5 \leq \Delta x^+ \leq 45$, and $5 \leq \Delta z^+ \leq 30$.

When studying the impact of the grid resolution, $\mathbf{q}$ are taken to be the distance from the wall of the first off-wall grid point, Δy_w^+, and the grid cell spacings in the streamwise and spanwise directions, Δx^+ and Δz^+, respectively. Here, the superscript $^+$ denotes the viscous-unit based on the target reference friction Reynolds number Re_τ (based on friction velocity and channel half-height). Figure 1 illustrates the isolines of the error in the profiles of the mean velocity $\langle u \rangle$ and turbulent kinetic energy, $\mathcal{K}$, in the admissible Δx^+-Δz^+ space. Considering the results by `OpenFOAM`, see Ref. [2], the pattern of the error isolines clearly depends on the flow solver and the QoI, and it can be rather complex and unexpected. These reveal the intricacy that any theoretical error estimator has to deal with. Investigating the errors in other QoIs, it is concluded that at a similar resolution, `Nek5000` leads to more accurate results than `OpenFOAM`. For both solvers, the total Sobol indices in Figure 2 show that the errors in most of the QoIs are more sensitive to Δz^+ than Δx^+. The exceptions are the error in the wall-normal component of the root-mean-square (rms) velocity, v_{rms}, for `Nek5000`, and, the streamwise rms velocity u_{rms} and $\mathcal{K}$ for `OpenFOAM`. Taking into account the significance of having the same sensitivity for $\mathcal{K}$ as other QoIs, the appropriateness of `Nek5000` for simulating the wall turbulence is further confirmed.

In the next stage of the study, the predictions made by the derived guidelines and the PCE-based surrogates constructed based on the channel flow data will be validated for other wall-bounded turbulent flows such as pipe flow and also at higher Reynolds numbers. Then, the possibility of constructing surrogates using Gaussian processes (GP) is examined. The ultimate goal is to possibly exploit the GP-surrogates in an optimization problem. Such a problem aims at selecting an optimal combination of numerical parameters such that the QoIs of the channel flow, for instance, are within a given proximity of the target reference values. Besides constructing appropriate GP-surrogates, the success of the optimization depends on formulating the objective function as a combination of different error indicators.

[1] A. Mariotti, L. Siconolfi, and M. Salvetti, "Stochastic sensitivity analysis of large-eddy simulation predictions of the flow around a 5:1 rectangular cylinder," Eur. J. Mech. B/Fluids **62**, 149-165 (2017).

[2] S. Rezaeiravesh and M. Liefvendahl, "Effect of grid resolution on large eddy simulation of wall-bounded turbulence," Phys. Fluids **30**, 055106 (2018).

[3] D. Xiu, "Efficient collocational approach for parametric uncertainty analysis," Commun. Comput. Phys. **2(2)**, 293-309 (2007).

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Stochastic approach for the evaluation of aerodynamic flow over irregular rough walls

Federico Bernardoni, [1] ***Umberto Ciri,*** [1] ***Maria Vittoria Salvetti*** [2] ***and Stefano Leonardi,*** [1*]

[1] Department of Mechanical Engineering, University of Texas at Dallas, TX, USA
[2]DICI, University of Pisa, Italy
[1*]Stefano.Leonardi@utdallas.edu

Key words: Stochastic Analysis, Roughness

Despite increased attention over recent years, our knowledge of the flow over rough walls is far from complete. For example, for an irregular rough wall we cannot predict with good accuracy what is the drag coefficient. Due to the large number of geometrical parameters affecting the flow it has been challenging to develop parameterizations of rough walls. Given the high computational cost of performing deterministic numerical simulations for each different surface, several models have been developed to describe the aerodynamic flow field in terms of parameters such as the drag coefficient (C_d), the roughness length or the roughness function (see for example [1], [2], [3]). However, they all work well in the limited application sector for which they have been developed. The aim of the present study is to compute with a low computational cost the aerodynamic parameters for an irregular roughness using a stochastic surrogate model which relies on high fidelity data obtained from Direct Numerical Simulations (DNS). The streamwise and spanwise wavelengths of the roughness are assumed as uncertain features able to describe the geometry of the rough surface and a response model is then built in order to evaluate the drag coefficient, the roughness function and the velocity fluctuations by using the Polynomial Chaos Expansion (PCE). Then, given any Probability Density Function (PDF) describing a general rough surface, the aerodynamic properties of the overlying flow are evaluated using stochastic techniques avoiding the need of carrying out computationally expensive numerical simulations.

The roughness is modeled as a sinusoidal wavy-wall within a channel with x, y and z as the coordinates in the streamwise, vertical and spanwise directions, a as the amplitude of the roughness, λ_x and λ_z as respectively the streamwise and spanwise wavelengths. The spanwise wavelength is allowed to vary between $\lambda_z/2a = 10$ and $\lambda_z/2a = 100$ while the streamwise wavelength between $\lambda_x/2a = 1$ and $\lambda_x/2a = 20$; the amplitude is kept constant and equal to $a = 0.1h$, where h is the half height of the channel.

The response model able to efficiently evaluate each aerodynamic quantity of interest for each different uniform roughness is obtained using a 5^{th} order PCE for modelling of streamwise wavelength variability and a 3^{th} order polynomial for the spanwise wavelength. Gauss-Legendre polynomials were employed. Thus, in order to compute the coefficients of the polynomials, a total of 24 DNSs of a channel flow were carried out with regular roughness on the bottom wall, each of them characterized by different combinations of $\lambda_z/2a$ and $\lambda_x/2a$. All the simulations are performed at $Re_b = (U_b h)/\nu = 2,800$, where U_b is the bulk velocity h is the half height of the channel and ν is the kinematic viscosity. Periodic boundary conditions are applied in both streamwise and spanwise directions; the walls are modeled with the immersed boundary technique [4]. When an irregular rough surface is considered, the PDFs of the streamwise and spanwise wavelengths, chosen as representative parameters, are extracted by treating the shape of the rough surface as a signal and performing on it a time-frequency analysis using the Wavelet transform. Therefore, the ridges of the scalogram that is obtained represent at each location in space what are the most probable wavelengths in the considered roughness. Thus, the PDFs of both streamwise and spanwise wavelength across the entire domain are evaluated and taken as input for the stochastic analysis.

Using the Latin Hypercube Sampling method (LHS), the irregular roughness is represented in the stochastic

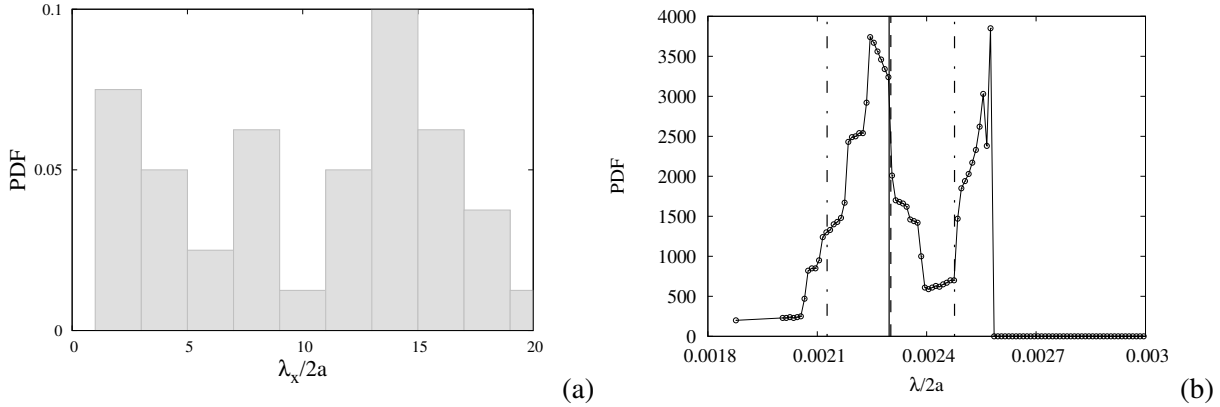


Figure 1: (a) PDF of the streamwise wavelength of the validation rough surface; (b) comparison of the C_d from the SA and from DNS: —— value of C_d from the DNS: $C_d = 2.30 \cdot 10^{-3}$; - - - - mean value from SA, $\mu(C_d) = 2.29 \cdot 10^{-}3$; —·— mean value ± standard deviation of C_d from SA; —— ∘ PDF of C_d from SA.

approach (SA) as a set of samples; each of them corresponds to a roughness with uniform streamwise and spanwise wavelength. The drag coefficient, the roughness function and the turbulence intensities are then easily evaluated by means of the PCE response model. Finally, all the responses are statistically analyzed in order to obtain the PDF and mean value of each aerodynamic quantity of interest over the considered irregular rough wall.

So far the proposed approach has been validated considering only a random variability of the streamwise wavelength of the roughness and keeping constant $\lambda_z/2a = 100$. Figure 1a) shows the PDF of the streamwise wavelengths of the surface considered for the validation process. The drag coefficient, the roughness function and the turbulence intensities over this irregular roughness have been evaluated with the proposed stochastic approach and compared with those obtained in a DNS carried out on the same surface. Figure 1b) shows, as an example, the PDF obtained from the SA of the drag coefficient. The comparison between the mean value (μ) of C_d from SA (dashed line) and the mean C_d from the DNS over the entire rough surface (solid line) is reported showing a good agreement. From the PDF it is also possible to obtain some information about the variability of C_d on the surface. For instance, it appears that there are two values of C_d which are highly probable to occur locally on different roughness elements: one is close to the mean value while the other one is significantly higher. From the available response surface, the value of $\lambda_x/2a$ leading to these high values of C_d and, thus contributing to the total drag, could be identified.

Summarizing, a stochastic approach based on PCE has been presented, which allows the aerodynamic quantities characterizing the flow over an irregular roughness distribution to be evaluated without the need of carrying out specific numerical simulations for each different roughness, largely reducing in this way the computational costs. Considering the variability of only the streamwise wavelength of the sinusoidal roughness, the comparison with DNS data has shown a very good agreement in terms of mean values over the rough surface of the quantities of interest. The validation of the proposed approach for irregular surface in both the streamwise and spanwise directions is ongoing and the results will be presented in the final paper.

[1] Flack K. A., Schultz M. P. : Review of Hydraulic Roughness Scales in the Fully Rough Regime, *J. Fluids Eng.*, **132**, 041203 (2010).

[2] Macdonald R.W., Griffiths R.F., Hall D.J. : An improved method for the estimation of surface roughness of obstacle arrays, *Atmos. Environ.*, **32**, 1857–1864 (1998).

[3] Zhu X., Iungo G. V., Leonardi S., Anderson W. : Parametric Study of Urban-Like Topographic Statistical Moments Relevant to a Priori Modelling of Bulk Aerodynamic Parameters, *Boundary-Layer Meteorol*, **162**, 231–253 (2017).

[4] Orlandi P., Leonardi S. : DNS of turbulent channel flows with two- and three-dimensional roughness, *J. Turbul.*, **7**, 1–22 (2006).

Keynote Lecture - S. Mishra - UQ for nonlinear hyperbolic PDEs with statistical solutions

Session Chair: L. Tamellini

Auditorium

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

UQ for nonlinear hyperbolic PDEs with statistical solutions

Siddhartha Mishra

ETH Zürich, Switzerland – siddhartha.mishra@sam.math.ethz.ch

Key words: Uncertainty Quantification, Non Linear Hyperbolic PDEs

Hyperbolic systems of conservation laws arise in a wide variety of problems in physics and engineering. Uncertainty quantification (UQ) is essential for these models on account of measurement errors for inputs and possible chaotic dynamics of the system. However, efficient UQ is very challenging due to the low regularity of underlying solutions, on account of shocks and turbulence as well as the need for possibly high dimensional description of the probability space. We present the recently proposed concept of statistical solutions as a suitable UQ framework for these PDEs. Statistical solutions are time-parameterized probability measures on integrable functions and we present a convergent Monte Carlo algorithm for computing them. Moreover, we will present several alternatives to accelerate the baseline Monte Carlo method. These include Multi-level Monte Carlo (MLMC), Quasi-Monte Carlo (QMC) and machine learning algorithms and we evaluate their applicability in this context.

SW3 – Methodology I

Session Chair: L. Tamellini

Auditorium

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Iterative construction of quadrature rules for Bayesian prediction

Laurent van den Bos[1] and Benjamin Sanderse[2]

[1] Centrum Wiskunde & Informatica, Amsterdam, The Netherlands – l.m.m.van.den.bos@cwi.nl

[2] Centrum Wiskunde & Informatica, Amsterdam, The Netherlands – b.sanderse@cwi.nl

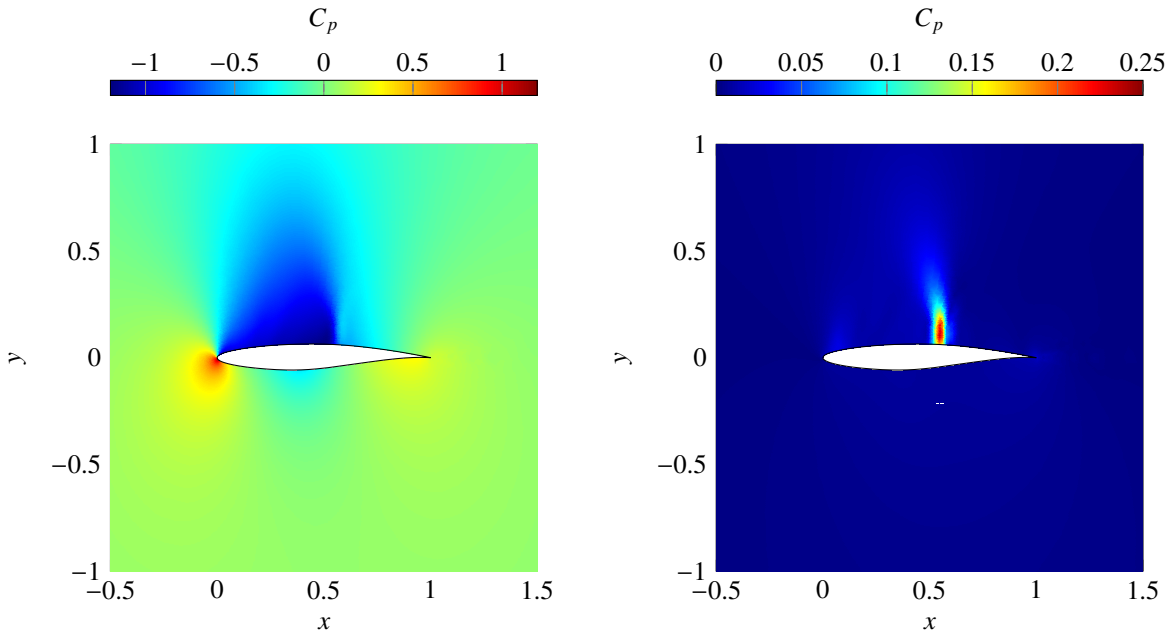
Key words: Numerical integration, Uncertainty Propagation, Bayesian prediction

A novel numerical integration framework for the purpose of uncertainty propagation in a Bayesian framework is proposed (this is also known as Bayesian prediction). The framework is based on quadrature rules, i.e. weighted averages of function evaluations, that are constructed as a subset of a large number of samples from the distribution [1, 2]. The goal is to determine integrals of the following form:

$$\mathbb{E}[u] = \int_{\Omega} u(\mathbf{x})\, q(\mathbf{x} \mid \mathbf{z})\, \mathrm{d}\mathbf{x}.$$

Here, $\mathbf{x}$ is a vector with uncertain parameters defined in the space $\Omega \subset \mathbb{R}^d$ ($d = 1, 2, 3, \ldots$) with probability distribution $q(\mathbf{x} \mid \mathbf{z})$. The function u describes a costly computational model and is typically the numerical solution of a system of partial differential equations that model fluid flow for given parameters $\mathbf{x}$.

The key challenge is that the distribution $q(\mathbf{x} \mid \mathbf{z})$ is a posterior. It follows from the statistical model that describes the relation between the model and measurement data [4]. The posterior is not known explicitly and depends directly on the computationally costly model u. The idea of the proposed approach is to iteratively add nodes to a quadrature rule such that it converges to a quadrature rule that determines weighted integrals



(a) Mean

(b) Standard deviation

Figure 1: Bayesian prediction of the pressure coefficient around the transonic RAE2822 airfoil. The calibrated parameters are the turbulence closure coefficients of the Spalart–Allmaras turbulence model.

with respect to the posterior. The nodes are nested, such that costly model evaluations are reused in subsequent iterations. The rules are constructed such that they have positive weights, which ensures that the quadrature rule estimations converge.

The efficiency and applicability of the integration framework is demonstrated by predicting the transonic flow over the RAE2822 airfoil, where the turbulence closure coefficients of the Spalart-Allmaras turbulence model are inferred from measurement data (see Figure 1). The results are comparable with existing literature on this topic [3], demonstrating that the proposed approach is a promising alternative to existing approaches for Bayesian model calibration and prediction.

[1] L. M. M. van den Bos, B. Koren, and R. P. Dwight. Non-intrusive uncertainty quantification using reduced cubature rules. *Journal of Computational Physics*, 332:418–445, 2017. 10.1016/j.jcp.2016.12.011.

[2] L. M. M. van den Bos, B. Sanderse, W. A. A. M. Bierbooms, and G. J. W. van Bussel. Generating nested quadrature rules with positive weights based on arbitrary sample sets. *ArXiV 1809.09842*, 2018.

[3] W. N. Edeling, P. Cinnella, R. P. Dwight, and H. Bijl. Bayesian estimates of parameter variability in the $k-\epsilon$ turbulence model. *Journal of Computational Physics*, 258:73–94, 2014. 10.1016/j.jcp.2013.10.027.

[4] M. C. Kennedy and A. O'Hagan. Bayesian calibration of computer models. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 63(3):425–464, 2001. 10.1111/1467-9868.00294.

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

A stochastic Galerkin reduced basis method for parametrized convection-diffusion-reaction equations based on adaptive snapshots

Christopher Müller,[1] ***and Jens Lang,***[1]

[1]Department of Mathematics , TU Darmstadt, Germany
cmueller@mathematik.tu-darmstadt.de

Key words: Stochastic Galerkin, Finite elements, Model order reduction, Adaptive methods, Convection-diffusion-reaction equations

We consider convection-diffusion-reaction equations with parametrized random and deterministic inputs. For a fixed value of the deterministic parameters, the problem reduces to a linear elliptic PDE with random input data and statistical moments of its solution such as mean and variance can be approximated by a stochastic Galerkin finite element (SGFE) method. There are scenarios, like robust optimization, where these statistical information must be computed for numerous different values of the deterministic parameter. In these particular cases, it can be computationally attractive to conduct a certain number of expensive preliminary computations in order to set up a reduced order model. The reduction of the overall computational costs than results from the fact that this reduced order model, here a so-called stochastic Galerkin reduced basis (SGRB) model [1], is low dimensional and can thus be evaluated cheaply for each deterministic parameter value. We construct the SGRB model using a proper orthogonal decomposition (POD) of SGFE snapshots. As a consequence, there is no need for an additional sampling procedure in order to evaluate the statistics of the solution of the reduced order model.

Computing the snapshots for the SGRB model means that several different SGFE problems have to be to solved, each associated with a large block-structured system of equations. When the costs of solving these systems are too high, adaptive methods can be applied to find favorable discrete spaces and lower the computational burden of the preliminary computations. Using an adaptive approach leads, however, to a setting where the snapshots belong to different SGFE subspaces. This fact interferes the standard POD procedure which relies on snapshots from the same static subspace. It is still possible to construct a reduced order model based on adaptive snapshots [2] but there are different theoretical and numerical issues that emerge. We address the issues that arise for the particular case of an SGRB model constructed with adaptively chosen SGFE snapshots and illustrate our findings based on a convection-diffusion-reaction test case where the convective velocity is the deterministic parameter and the parametrized reactivity field is the random input.

[1] S. Ullmann and J. Lang, “Stochastic Galerkin reduced basis methods for parametrized linear elliptic PDEs", arXiv: 1812.08519, (2018).

[2] S. Ullmann, M. Rotkovic and J. Lang, “POD-Galerkin reduced-order modeling with adaptive finite element snapshots”, J. Comput. Phys. **325**, (2016).

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Multiscale Uncertainty Quantification with Arbitrary Polynomial Chaos

Nick Pepper,[1] ***Francesco Montomoli,***[1] ***and Sanjiv Sharma*** [2]

[1]UQLab, Imperial College London, UK – nicholas.pepper16@imperial.ac.uk

[2]Airbus, UK

Key words: Uncertainty quantification; multiscale modelling; stochastic upscaling; polynomial chaos expansions; SAMBA; PDF matching

This work presents a methodology for upscaling uncertainty in multiscale models. The problem is relevant to aerospace applications where it is necessary to estimate the reliability of a complete part such as an aeroplane wing from scarce data of coupons. The upscaling equivalence is defined by a Probability Density Function (PDF) matching approach. By representing the inputs of the coarse model with a Polynomial Chaos Expansion (PCE) the stochastic upscaling problem can be recast as an optimisation problem. In order to define a data driven framework able to deal with scarce data a Sparse Approximation for Moment Based Arbitrary Polynomial Chaos is used. Sparsity allows the solution of this optimisation problem to be made less computationally intensive than upscaling methods relying on Monte Carlo sampling. Moreover this makes the PDF matching method more viable for industrial applications where individual simulation runs may be computationally expensive. Arbitrary Polynomial Chaos is used to allow the framework to use directly experimental data. Finally, the difference between the distributions is quantified using the Kolmogorov-Smirnov (KS) distance and the method of moments in the case of a multi-objective optimisation. It is shown that filtering of dynamical information contained in the fine scale by the coarse model may be avoided through the construction of a low fidelity, high order model.

SW4 – Methodology II

Session Chair: S. Mishra

Auditorium

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Intrusive Generalized Polynomial Chaos for the solution of the unsteady Navier-Stokes Equations

C. F. Silva,[1] ***P. Bonnaire***[1]***, S. Schuster***[1] ***and P. Pettersson,***[2]

[1] Technical University of Munich (TUM), Germany– silva@tfd.mw.tum.de

[2] Norwegian Research Center (NORCE), Norway

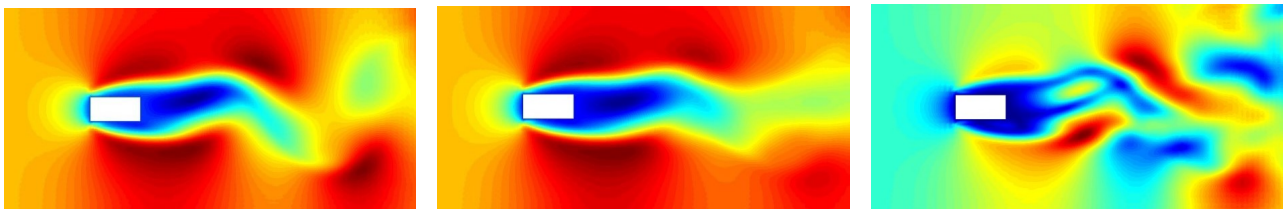
Key words: Uncertainty quantification, Computational Fluid Dynamics, generalized Polynomial Chaos.

Aiming at a robust design by means of Computational Fluid Dynamics (CFD) means not only aiming at precisely quantifying CFD output variables, but also at quantifying the sensitivity of the CFD outputs to input variations, and at evaluating probability density functions of the CFD outputs given input uncertainties. In other words, robust design means introducing rigorous Uncertainty Quantification (UQ) in the CFD design chain.

The present work is devoted to the study of (intrusive) generalized Polynomial Chaos (gPC) [1, 2] on unsteady CFD that exhibit limit cycles as solutions. Previous work on the long-time integration of oscillatory problems include the adaptive multi-element generalized polynomial chaos expansion [3], and Haar wavelet expansions [4]. Nevertheless, these approaches typically lead to very large number of basis functions. In the context of non-intrusive polynomial chaos, a time warping method was proposed in [5] to counteract that limitation. In this work we implement the asynchronous time integration proposed by [6], which is a method that shares the same time-scaling philosophy of [5]. By doing so, UQ is performed by solving only two simulations: one deterministic (reference) simulation and one computation on the set of extended equations that characterize the system with uncertainties.

The incompressible and compressible set of Navier-Stokes equations are discretized by finite volumes and finite differences, respectively. (i) The incompressible approach makes use of a Rhie-Chow interpolation. A quasi-implicit scheme for time discretization is implemented, where the convective part is linearized by a Crank-Nicolson approach. Additionally, the explicit Heun's method can be chosen as time advancing scheme. (ii) The compressible solver makes use of an adapted MacCormack method. This is an explicit finite difference method that utilizes a predictor-corrector time stepping scheme. The deterministic version of both solvers (incompressible and compressible) is validated against analytical flow solutions and experimental data. In particular, we focus on flows characterized by the Karman-vortex street, which develops due to flow separation around a bluff body.

A stochastic Galerkin projection is applied to both incompressible and compressible Navier-Stokes equations. Orthogonal polynomials are considered for the expansion and subsequent basis projection. Based on the work of [6], we additionally scale time at each time step for each realization. The goal here is to mimic an 'in phase' behaviour of the stochastic solutions. We study the Karman-Vortex street that is perturbed by an uncertain inlet velocity and laminar viscosity of the flow. We show that by introducing a 'local clock' in the stochastic domain it is possible to quantify the frequency of the limit cycles and the corresponding shift due to the aforementioned uncertainties . Additionally, we avoid the well-known problem (blow-up) of gPC when implemented in uncertain (long) time-dependent problems.



(a) Deterministic simulation (b) Expected value (igPC) (c) Standard deviation (igPC)

Figure 1: Deterministic and stochastic simulation for $Re = 100$ with uncertain inlet velocity of $u_1/u_0 = 0.2$.

Figure 1a shows one snapshot of the velocity field at time 3.87s, where no uncertainties are considered. Figures 1b and 1c show the expected value and standard deviation of this flow at the same instant of time, where uncertainty has been considered in the inlet velocity. By analyzing the field of standard deviation for several instants of time, it is possible to assess regions where the input uncertainties do not strongly affect the velocity field. This kind of study is of relevance since it suggests locations where measurements can be obtained that are not strongly affected by the uncertainties present in the system.

[1] R. G. Ghanem and P. D. Spanos. *Stochastic Finite Elements: A Spectral Approach*. Courier Corporation, 1991.

[2] D. Xiu and G. E. Karniadakis. The Wiener–Askey polynomial chaos for stochastic differential equations. *SIAM journal on scientific computing*, 24(2):619–644, 2002.

[3] X, Wan and G, E. Karniadakis. An adaptive multi-element generalized polynomial chaos method for stochastic differential equations. *Journal of Computational Physics* 209 (2):617-642, 2005

[4] O. P. Le Maıtre, O. M. Knio, H. N. Najm and R. G. Ghanem Uncertainty propagation using Wiener-Haar expansions *Journal of computational Physics* 197 (1):28-57, 2004.

[5] C. V. Mai and B. Sudret. Surrogate models for oscillatory systems using sparse polynomial chaos expansions and stochastic time warping *SIAM/ASA Journal on Uncertainty Quantification* 5 (1):540-571, 2017

[6] O. P. Le Maıtre, L. Mathelin, O. M. Knio and M. Y. Hussaini. Asynchronous time integration for polynomial chaos expansion of uncertain periodic dynamics *Discrete Contin. Dyn. Syst*, (28):199–226, 2010.

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

RBF-FD Meshless Solver to Investigate the Propagation of Geometric Uncertainty in Laminar Flows

Riccardo Zamolo[1] ***and Lucia Parussini***[2]

[1]DIA, University of Trieste, Italy – riccardo.zamolo@phd.units.it

[2]DIA, University of Trieste, Italy – lparussini@units.it

Key words: Polynomial Chaos, Meshless, RBF-FD, Spectral Element Method.

In this work we consider the uncertainty quantification in incompressible, laminar, 2D steady-state fluid dynamics problems where the domain geometries are described by stochastic variables. Such stochastic problems arise in practical applications where geometric uncertainties are due to manufacturing tolerances which lead to uncertainties in the performance of the product. The Non-Intrusive Polynomial Chaos method [1] is employed to estimate statistical quantities regarding the flow fields, i.e., velocity, pressure and temperature. The advantage of the non-intrusive formulation is that existing deterministic solvers can be employed as black boxes without any modification since the random response is based on a set of deterministic response evaluations.

An isothermal flow over a backward-facing step is initially considered, where the geometric uncertainty is given by the position of the step corner. The deterministic fluid-flow problems are solved by three different approaches: a Fictitious Domain/Least Squares Spectral Element Method [2], a Finite Volume Method and a Radial Basis Function-generated Finite Differences (RBF-FD) Meshless Method [3]. A comparison between the methods is then carried out, showing a very good agreement in terms of estimated statistical quantities.

Due to its geometric flexibility and its ability to easily deal with complex-shaped domains, the RBF-FD method is subsequently chosen and employed for the efficient prediction of geometric uncertainty effects in different fluid dynamics test case problems. Furthermore, the order of accuracy of the RBF-FD method can be easily increased by using larger stencils, i.e., more nodes in the local RBF expansion.

[1] S. Hosder, R. Walters and R. Perez, “A Non-Intrusive Polynomial Chaos Method for Uncertainty Propagation in CFD Simulations," In *Proceedings of 44th AIAA aerospace sciences meeting and exhibit*, 1-19 (AIAA, Reston, VA, 2006).

[2] L. Parussini, “Fictitious Domain Approach via Lagrange Multipliers with Least Squares Spectral Element Method," Journal of Scientific Computing **37**(3), 316-335 (2008).

[3] B. Fornberg and N. Flyer, “Solving PDEs with Radial Basis Functions" Acta Numerica **24**, 215-258 (2015).

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Wavelet-Assisted Multi-Element Polynomial Collocation Method

***Robert Sawko*[1], *Małgorzata J. Zimoń*[1] *and Alex Skillen*[2]**

[1]IBM Research, Daresbury Laboratory, UK – Corresponding author: RSawko@uk.ibm.com
[2]Science and Technology Facilities Council, Daresbury Laboratory, UK

Key words: polynomial chaos, polynomial annihilation, wavelet transform, surrogate modelling

Polynomial chaos (PC) is a widely used approach in uncertainty quantification (UQ) in computational fluid dynamics (CFD) studies. It represents the simulator output as a series expansion in the input parameters [5, 7] and has high rates of convergence for smooth quantities of interest. In its non-intrusive form, it treats the model as a *black box* and uses the results to estimate expansion coefficients either through *regression* or *spectral projection*.

Although very efficient for approximating low-order and smooth functions, the analysis becomes expensive or even infeasible if the response of the system is irregular, contains sharp transitions, steep gradients, or discontinuities. Using global basis may never lead to accurate approximations. To tackle this issue, a modification of PC for low-regular problems was proposed by Wan and Karniadakis [6]. Its non-intrusive formulation was later introduced by Foo et al. [2] and referred to as multi-element polynomial collocation method (ME-PCM). In following years, variations of this approach have been proposed, attempting to transform the problem into one that can be tackled with piecewise basis by first identifying the location of discontinuities (*edge tracking*) with the use of, e.g., polynomial annihilation [1, 3].

In this talk, we propose a two staged approach to tackle piecewise continuous or piecewise smooth functions. We first perform a random space decomposition coupled with local polynomial order estimation and then construct PC surrogates for each sub-domain. We use continuous wavelet transform (CWT) [4] to analyse local changes in power spectra and determine boundary separation by classifying the responses into related groups. The method is first demonstrated on model functions proposed in previous work on discontinuities and highly varying regions [1]. Example of such study is shown in Fig. 1. After dividing the parametric space, the points used for classification are re-used to generate local polynomial representation with determined number of terms.

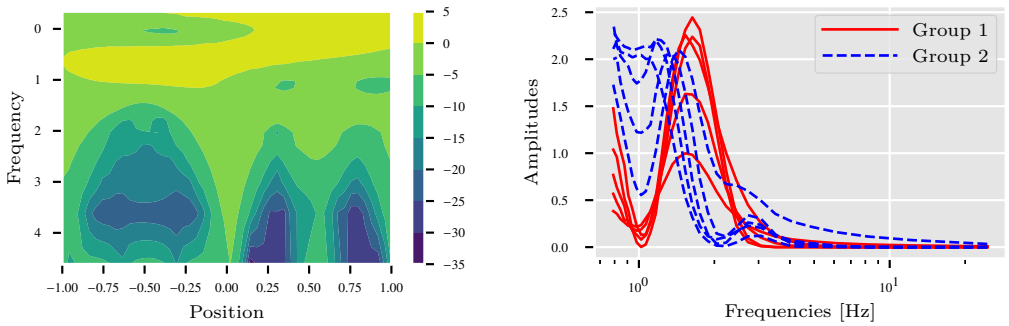


Figure 1: The scalogram (left) and classification (right) of functions based on an example in [1].

We then move to a quantity of interest from transient turbulent flow inside a U-bend pipe. A set of

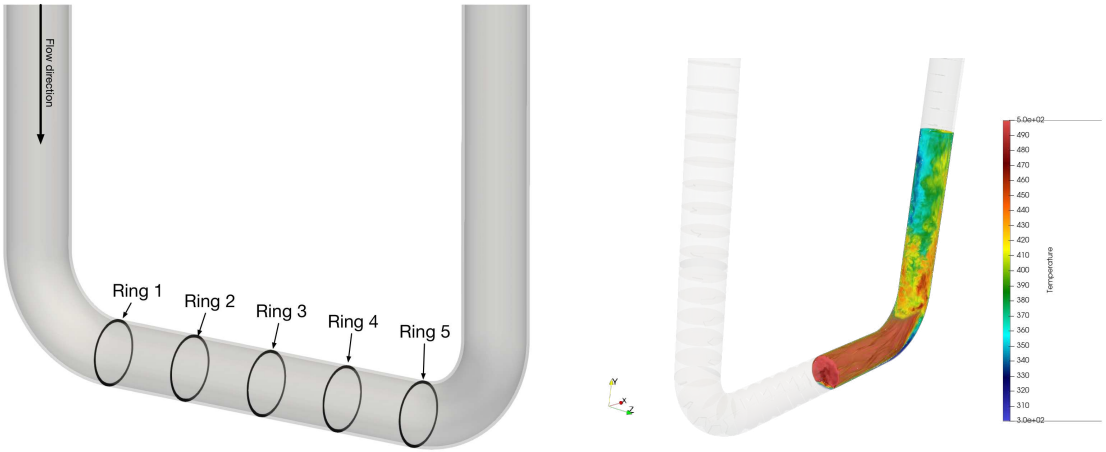


Figure 2: Right: wall temperature is collected for several rings along the streamwise dimension of the pipe. Left: a visualisation of turbulent flow.

Reynolds-averaged Navier–Stokes equations (RANS) of hot shock waves is solved with the uncertain input characterising the magnitude of the temperature jump. In the downstream of the pipe, the flow becomes unstably stratified leading to development of highly turbulent structures. We collect wall surface temperatures from rings as shown in Fig. 2. We then study the response temperature for each point using the method proposed above. The response exhibits piecewise smoothness and the wavelet-assisted approach described above performs well in cross-validation tests and small sample sizes.

Two primary features of the proposed method are an automatic detection of piecewise continuous or smooth regions and estimation of a maximum order required for the subsequent PC expansion. Detailed description of the adaptive method is presented. The results on model functions and simulated data are compared with other edge-detection analyses in terms of computational efficiency and accuracy of approximation for problems with low regularity. We show that application of wavelet-assisted approach for transient heat transfer simulations can result in cost-effective and accurate surrogate. At the end of the talk, we draw conclusions and suggests further improvements.

[1] R. Archibald, A. Gelb, and J. Yoon, *Polynomial fitting for edge detection in irregularly sampled signals and images*, SIAM Journal of Numerical Analaysis, 43 (2006), pp. 259–279.

[2] J. Foo, X. Wan, and G. E. Karniadakis, *The multi-element probabilistic collocation method (ME-PCM): Error analysis and applications*, Journal of Computational Physics, 227 (2008), pp. 9572–9595.

[3] J. D. Jakeman, R. Archibald, and D. Xiu, *Characterization of discontinuities in high-dimensional stochastic problems on adaptive sparse grids*, Journal of Computational Physics, 230 (2011), pp. 3977–3997.

[4] S. Mallat, *A wavelet tour of signal processing*, Elsevier, 1999.

[5] T. J. Sullivan, *Introduction to Uncertainty Quantification*, vol. 63, Springer, 2015.

[6] X. Wan and G. E. Karniadakis, *An adaptive multi-element generalized polynomial chaos method for stochastic differential equations*, Journal of Computational Physics, 209 (2005), pp. 617–642.

[7] D. Xiu, *Numerical Methods for Stochastic Computations: A Apectral Method Approach*, Princeton University Press, 2010.

SW5 – Poster short presentations

Session Chair: M.V. Salvetti

Auditorium

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Multi-continuum models for conjugate transport in random heterogeneous media and application to molecular communication

Federico Municchi, John Couch, and Matteo Icardi

School of Mathematical Sciences, University of Nottingham, UK – federico.municchi@nottingham.ac.uk

Key words: heterogeneous media, dual porosity, multi-rate mass transfer, conjugate transfer, subsurface flows

In fluid dynamics, conjugate heat/mass transfer refers to the problem of coupling a "mobile" fluid domain, where flow (Stokes or Navier-Stokes) and transport (advection-diffusion), with "immobile" inclusions, where diffusion dominates. This is therefore relevant to a wide range of problems in subsurface flows, porous media, and heat transfer applications. Fully resolved simulations are often unfeasible due to their complexity in capturing the possibly complicated, heterogeneous, and often uncertain micro-structures.

In this work, we derive a new upscaled (averaged) multi-continuum multi-rate transfer model [1] between a mobile phase and an immobile phase that does not require to resolve the interfaces between the regions, and implement it within the three-dimensional finite-volumes OpenFOAM(R) library. We show this is particularly suitable for Uncertainty Quantification studies where uncertainties in the material composition can be represented by uncertain parameters (rather than geometry) and propagate through the model.

We then focus on a simplification, leading to the so-called dual-porosity model, solve it analytically in one-dimension, and study the effects of uncertainties in the different parameters on specific quantities of interest for *molecular communication* applications. Molecular communication is a recently developed and very active field of research in communication theory, that deals with the design of low-energy communication strategies, based on the transport of particles and molecules. To design optimal and robust communication, we define a family of functionals of the fundamental solution of the PDE, representing communication-based optimality measures, and study their robustness on the input uncertainty.

[1] F. Municchi and M. Icardi, “Generalised Multi-Rate Models for conjugate transfer in heterogeneous materials," arXiv:1906.01316 [physics.comp-ph]

[2] Y. Fang, W. Guo, M. Icardi, A. Noel, and N. Yang, “Molecular Information Delivery in Porous Media," arXiv:1903.03738 [cs.IT]

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Enhancing the uncertainty quantification of pyroclastic density current dynamics in the Campi Flegrei caldera.

Andrea Bevilacqua,[1] ***Mattia de Michieli Vitturi,***[1] ***Tomaso Esposti Ongaro,***[1] ***and Augusto Neri,***[1]

[1]INGV, Sezione di Pisa, Italy – andrea.bevilacqua@ingv.it

Key words: Uncertainty quantification, Geophysical Flows, Volcanic Hazard Assessment

In this study we present a new effort to improve the uncertainty quantification (UQ) of pyroclastic density current dynamics in the Campi Flegrei caldera, thanks to the implementation of a new 2D depth-averaged granular flow model in the Monte Carlo simulation of key-controlling variables.

Campi Flegrei caldera is an active and densely populated volcanic area in the urban neighborhood of Napoli, characterized by the presence of many dispersed cones and craters, and by a caldera wall more than one hundred meters high, towards East. Basic mapping of pyroclastic density currents[1] (PDC) hazard at Campi Flegrei has been already reported in previous studies: some related to field reconstruction and numerical modeling of specific past eruptions or individual scenarios, while others endeavored to produce specific or integrated PDC hazard maps in which the variability of important parameters of the volcanic system was explicitly accounted for. In particular, [4, 2] obtained quantitative estimates of probabilistic PDC hazard, based on the implementation of a simplified kinematic invasion model able to represent main topographic effects. This model, called *box model*[2], was extensively run thousands of times in the Monte Carlo simulation varying vent location, eruptive scale, and time frequency of the future activity (see Fig. 1).

Figure 1: Temporal PDC invasion hazard map based on the box model integral equations, the vent opening map and the areal size distributions in [2], and the temporal estimates assuming that the volcano entered a new eruptive epoch in A.D. 1538 (see [1]). Contours and colors indicate the mean percentage probability of PDC invasion in the next 10 years.

In this study we build our effort upon the previous research started in [7, 5], and utilize the physical modeling approach of [6], with the efficient numerical solution of depth-averaged equations for the flow mass and momentum, considering the effects of basal and internal, velocity dependent, friction forces. The model describes the gas-particle mixture as a homogeneous flow, assuming a mechanism of particle deposition consistent with that previously implemented in the box model.

UQ is performed by assuming three different components in the input space: (i) rheology parameters, (ii)

[1]laterally moving, buoyantly expanding mixtures of hot gas and fragmental particles.

[2]a cylindrical box represents the current and changes in aspect ratio (i.e. stretches out) as the flow progresses.

volume scale, (iii) source location. Our statistical analysis focuses on the first two components, considering a relatively small number of source locations or an uncertain source location inside a subregion of the caldera. This is a first step before the exploration of the full spatial variability of the source location. The statistical inversion of box model equations, varying the vent location (x, y) and the value of inundated area A, can provide us with initial probability estimates for the volume scale of the PDC flow, either in terms of runout distance or volume extent of the multiphase mixture (see Fig. 2). Our depth averaged model relies on these estimates for setting up the volume scale of past flows. The calibration of rheology parameters is performed according to that. Thus, the rheology and volume components of the input space are conjointly explored by means of Latin Hypercube sampling, attempting a hierarchical conditioning on feasible inputs and plausible outputs [3].

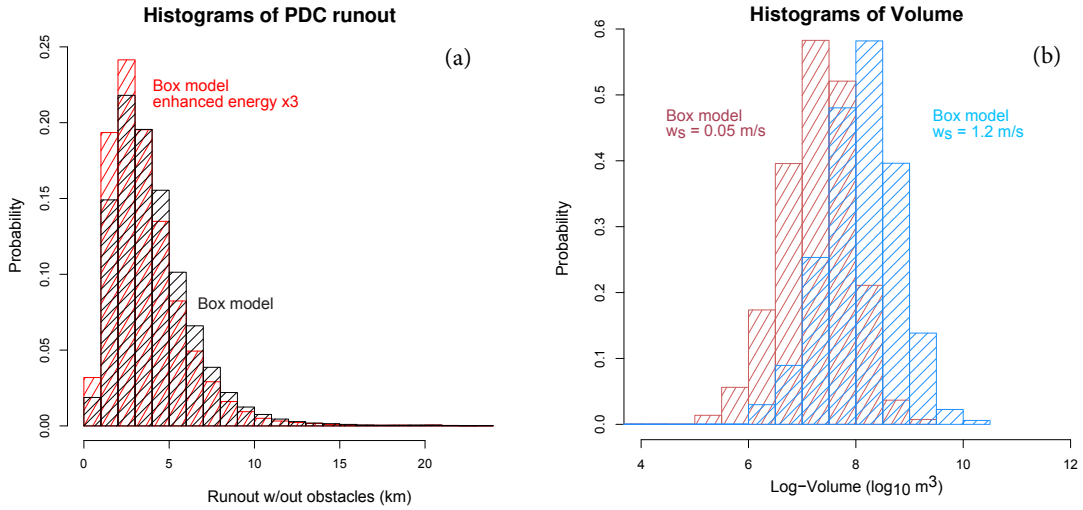


Figure 2: Results of Monte Carlo simulation varying the vent opening location (x, y) and the value of inundated area A, according to the probability models in [2]. Plot (a) shows the histograms of PDC runout obtained by probabilistic inversion of the box model integral equations. Red colored bars assume a hypothetical kinetic energy increase of three times in the flow front, due to the pressure rise before the obstacle [5]. Plot (b) shows the histograms of PDC log-volume of the multiphase mixture of solid and gas obtained by probabilistic inversion of the box model integral equations, with initial solid fraction of 1% volume. Different colors assume different values of velocity of settling, 1.2 m/s and 0.05 m/s. These values correspond to particle diameters of about $500\mu m$ and $25\mu m$, and solid densities of $1000kg/m^3$ and $2000kg/m^3$ respectively.

[1] A. Bevilacqua, F. Flandoli, A. Neri, R. Isaia, S. Vitale, "Temporal models for the episodic volcanism of Campi Flegrei caldera (Italy) with uncertainty quantification," Journal of Geophysical Research: Solid Earth **121**, 11 (2016).

[2] A. Bevilacqua, A. Neri, M. Bisson, T. Esposti Ongaro, F. Flandoli, R. Isaia, M. Rosi, S. Vitale, "The effects of vent location, event scale, and time forecasts on pyroclastic density current hazard maps at Campi Flegrei caldera (Italy)," Frontiers in Earth Science **5**, 72 (2017).

[3] A. Bevilacqua, A.K. Patra, M.I. Bursik, E.B. Pitman, J.L. Macías, R. Saucedo, D. Hyman, "Probabilistic forecasting of plausible debris flows from Nevado de Colima (Mexico) using data from the Atenquique debris flow, 1955," Natural Hazards Earth System Science **19**, 791-820 (2019).

[4] A. Neri, A. Bevilacqua, T. Esposti Ongaro, R. Isaia, W.P. Aspinall, M. Bisson, F. Flandoli et al., "Quantifying volcanic hazard at Campi Flegrei caldera (Italy) with uncertainty assessment: 2. Pyroclastic density current invasion maps," Journal of Geophysical Research: Solid Earth **120**, 2330-2349 (2015).

[5] T. Esposti Ongaro, S. Orsucci and F. Cornolti, "A fast, calibrated model for pyroclastic density currents kinematics and hazard," Journal of Volcanology and Geothermal Research **327**, 257 - 272 (2016).

[6] M. de' Michieli Vitturi, T. Esposti Ongaro, G. Lari, and A. Aravena, "IMEXSfloW2D 1.0: a depth-averaged numerical flow model for pyroclastic avalanches," Geoscientific Model Development, **12**, 581-595 (2019).

[7] M. Todesco, A. Neri, T. Esposti Ongaro, P. Papale, and M. Rosi, "Pyroclastic flow dynamics and hazard in a caldera setting: Application to Phlegrean Fields (Italy)," Geochemistry Geophysics Geosystems, **7**, Q11003 (2006).

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Intrusive Polynomial Chaos for CFD using OpenFOAM

Jigar Parekh, **Roel Verstappen***

Bernoulli Institute, University of Groningen, Netherlands

* j.parekh@rug.nl

Key words: Intrusive Polynomial Chaos, OpenFOAM, Large Eddy Simulation

Computational Fluid Dynamics (CFD) involves simulating a physical system with a model. In such simulations, uncertainties may arise from various sources, namely, initial and boundary conditions, material properties, model parameters etc. It is therefore important to compute the confidence intervals in the predictions made using these CFD simulations. In order to reflect the uncertainty in the numerical solution, we need efficient Uncertainty Quantification (UQ) methods.

Monte Carlo (MC) sampling is one of the simplest approach to carry out UQ analysis. However, due to its requirement of large number of samples, MC method is computationally expensive for application in CFD. As an alternative, we can use Polynomial Chaos (PC) representations to propagate and quantify uncertainty in CFD. This approach is based on the spectral decomposition of the random variables in terms of basis polynomials containing randomness and the unknown deterministic expansion coefficients, $Y = f(x,q) = \sum_{i=0}^{n} f_i(x)\phi_i(q)$. There are two methods to determine these coefficients, namely, Intrusive Polynomial Chaos (IPC) and Non-intrusive Polynomial Chaos (NIPC). In NIPC, these coefficients are approximated using quadrature for numerical evaluation of the projection integrals, while in IPC, a reformulation of the original model is performed resulting in governing equations for the PC mode strengths of the model output.

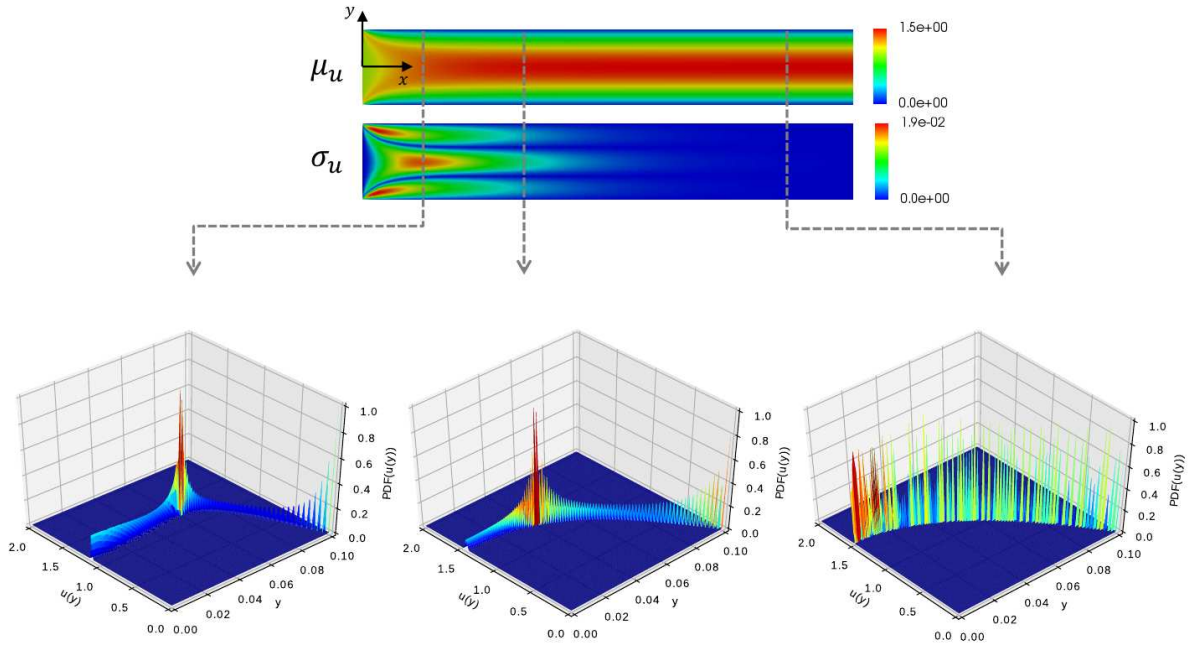


Figure 1: Probability distribution of the velocity in Poiseuille Flow with uncertain viscosity

Obviously, NIPC has an advantage that is uses the original model code without any modifications. However, Xiu [1] asserts that the NIPC, in general, requires the solution of much larger set of equations as compared to IPC, particularly for higher dimensional random space. Additionally, the aliasing error in NIPC can grow significantly with the number of random dimensions. This suggests that the IPC approach delivers most accurate solutions with least computational expense. Thus, in the present study, we focus on the IPC method for CFD – fundamentals, implementation and applications.

As the model code, we use OpenFOAM [2,3], which is a C++ toolbox to develop numerical solvers, and pre-/ post-processing utilities to solve continuum mechanics problems including CFD. OpenFOAM (a) is a highly templated code, enabling the users to customize the default libraries as needed for their applications, and, (b) gives access to most of the tensor operations (div, grad, laplaican etc.) directly at the top-level code. This avails enough flexibility to implement the IPC frame-work for uncertainty quantification in CFD. To obtain the inner products of polynomials, we use a python library called chaospy [4], as a pre-processing step to the actual OpenFOAM simulation.

To this end, we have tested the IPC implementation in OpenFOAM for specific laminar and turbulent flow problems in CFD. The results are in accordance with the analytical and MC approach. Currently, we are working on the quantification of uncertainties in turbulent flows which are highly sensitive towards model parameters. As a future work, we look forward to make detailed comparisons with the non-intrusive counterpart.

[1] D. Xiu "Fast Numerical Methods for Stochastic Computations:A Review," Communications in Cmoputational Physics, 5 (2008).

[2] H. G. Weller, G. Tabor, H. Jasak, and C. Fureby, "A tensorial approach to computational continuum mechanics using object-oriented techniques," Computers in Physics 12 (1998)

[3] ESI-OpenCFD, "OpenCFD Release OpenFOAMv1806," 2018

[4] J.Feinberg and H. P. Langtangenac, "Chaospy: An open source tool for designing methods of uncertainty quantification," The Journal of Computational Science 11 (2015)

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

`PolyChaos.jl` – Toward an Open Source Julia Package for Polynomial Chaos Expansion

Tillmann Mühlpfordt, Veit Hagenmeyer, Timm Faulwasser

Institute for Automation and Applied Informatics, Karlsruhe Institute of Technology, Germany
tillmann.muehlpfordt@kit.edu, veit.hagenmeyer@kit.edu, timm.faulwasser@ieee.org

Key words: Uncertainty quantification, polynomial chaos, orthogonal polynomials, quadrature

The theoretical foundations of uncertainty quantification (UQ) constitute an amalgamation of several research areas. Among those are statistics, applied mathematics, and numerical optimization. To apply UQ to practical applications—such as fluid dynamics—means to have a deep understanding of the real problem at hand, how it can be posed mathematically, and how it can be solved numerically. Nowadays, the approach to solving UQ problems numerically involves to a large extent programming and making use of numerical software tailored to UQ purposes. Hence, the successful application of UQ methods to real-world applications hinges on fast, reliable, easy-to-use software. Furthermore, it is desirable to make this software accessible to the public by publishing it as a transparent, open source software. Not only can potential errors be spotted and corrected in open source software, but researchers across the globe are empowered to add features or contribute otherwise, for instance by improving the documentation. Another advantage of open source UQ software is that the very people who develop UQ methods can implement their methods. Arguably, the researchers who develop UQ methods are the prime candidates to implement their UQ methods—a setting for which open source UQ software provides an ideal setting. In light of this, our contribution to the UQ community is `PolyChaos.jl`, an open source software package for polynomial chaos expansion written in the Julia programming language [1].

Polynomial chaos expansion (PCE) is a Hilbert space technique for random variables of finite variance. It is widely applied in UQ with use cases ranging from fluid dynamics [2], geosciences [3], electrical engineering [4] and power systems [5]. Polynomial chaos dates back to Norbert Wiener [6] and has had its renaissance around the turn of the century [7, 8]. Mathematically, PCE is a spectral decomposition of random variables of finite variance in terms of polynomials that are orthogonal relative to the probability density of the random variable. Loosely speaking, PCE is to a random variable what a Fourier series is to a periodic signal, namely a representation of an infinite-dimensional mathematical object in terms of finitely many real-valued coefficients—which also raises the question of truncation errors [9]. Polynomial chaos allows for efficient uncertainty propagation by employing intrusive or non-intrusive Galerkin projection for instance. Also, PCE provides stochastic moments of random variables without having to sample, and PCE is by construction not restricted to a single particular distribution such as Gaussian random variables.

As a numerical method PCE combines algorithms from orthogonal polynomials and Gauss quadrature. There exist mature software tools that provide implementations of several orthogonal polynomials that can be used in the context of PCE. For example, UQLab [10] offers a dedicated module for PCE in Matlab with a wide range of functionalities: sparse and basis-adaptive PCE, least-angle regression, several truncation schemes for orthogonal bases to name a few. While UQLab provides a rich suite of functionalities and an excellent documentation it requires Matlab, which is in conflict with the idea of open source software. Another bundle of software tools is the UQ Toolkit [11], which is written in C++, also offering a Python front end. The PCE functionality in the UQ Toolkit comprises: construction of orthogonal bases, numerical quadrature, operations for both intrusive and non-intrusive Galerkin projection. Unfortunately, UQ Toolkit is restricted to a pre-defined set of orthogonal polynomials, not allowing for custom probability density functions. `PolyChaos.jl` now aims to make a step toward an open source software package for polynomial chaos expansion that is applicable to

arbitrary probability densities, written in the Julia programming language.

Julia is a scientific programming language [12] that combines the readability of scripting languages such as Matlab or Python with the computational speed of compiled languages such as C/C++. Doing so, it solves the two-language problem where researchers rapid-prototype in one (usually scripting) language, and then have to turn to a second (usually compiled) language to obtain fast code. To solve this problem Julia has an intricate type inference system for variables, embedded in a just-in-time compilation. This allows researchers for scripting-like development of code, at the same time they can enforce type stability, i.e. enforcing that an integer variable has to remain an integer at run time. Finally, Julia is free to use and every software package is publicly available.

Currently, the functionality of `PolyChaos.jl` includes: construction of orthogonal bases for standard probability densities by analytic formulae, construction of orthogonal bases arbitrary for probability density functions based on the Stieltjes or Lanczos procedure [13], Gauss-type quadrature rules by means of the Golub-Welsch algorithm [13], multivariate basis construction by total-order truncation, computation of univariate and/or multivariate scalar products of basis polynomials. Arguably, the functionality of `PolyChaos.jl` represents just a small subset of established tools such as UQLab or UQ Toolkit, hence `PolyChaos.jl` should currently be treated as a complement to existing packages. However, we believe that `PolyChaos.jl` in its current state is nevertheless a useful contribution to the UQ community for several reasons: it provides the core functionality for intrusive PCE; it helps publicize the capabilities of Julia for UQ; it strictly adheres to the open source idea; its code architecture is simple, hence allowing for rapid addition of other PCE features such as basis-adaptive PCE.

[1] T. Mühlpfordt, F. Zahn, F. Becker, T. Faulwasser, and V. Hagenmeyer. *github.com/timueh/PolyChaos.jl: v0.1.2*. Mar. 2019.

[2] H. N. Najm. "Uncertainty Quantification and Polynomial Chaos Techniques in Computational Fluid Dynamics". In: *Annual Review of Fluid Mechanics* 41.1 (2009), pp. 35–52.

[3] S. Oladyshkin, H. Class, and W. Nowak. "Bayesian updating via bootstrap filtering combined with data-driven polynomial chaos expansions: methodology and application to history matching for carbon dioxide storage in geological formations". In: *Computational Geosciences* 17.4 (2013), pp. 671–687.

[4] A. Monti, F. Ponci, and T. Lovett. "A polynomial chaos theory approach to the control design of a power converter". In: *2004 IEEE 35th Annual Power Electronics Specialists Conference (IEEE Cat. No.04CH37551)*. Vol. 6. 2004, 4809–4813 Vol.6.

[5] T. Mühlpfordt, T. Faulwasser, and V. Hagenmeyer. "Solving Stochastic AC Power Flow via Polynomial Chaos Expansion". In: *IEEE International Conference on Control Applications*. 2016, pp. 70–76.

[6] N. Wiener. "The homogeneous chaos". In: *American Journal of Mathematics* (1938), pp. 897–936.

[7] R. G. Ghanem and P. D. Spanos. *Stochastic Finite Elements: A Spectral Approach*. Springer, 1991.

[8] D. Xiu and George E. M. Karniadakis. "The Wiener-Askey polynomial chaos for stochastic differential equations". In: *SIAM Journal on Scientific Computing* 24.2 (2002), pp. 619–644.

[9] T. Mühlpfordt, R. Findeisen, V. Hagenmeyer, and T. Faulwasser. "Comments on Truncation Errors for Polynomial Chaos Expansions". In: *IEEE Control Systems Letters* 2.1 (2018), pp. 169–174.

[10] S. Marelli and B. Sudret. "UQLab: A Framework for Uncertainty Quantification in Matlab". In: *Vulnerability, Uncertainty, and Risk*, pp. 2554–2563.

[11] B. Debusschere, K. Sargsyan, C. Safta, and K. Chowdhary. "Uncertainty Quantification Toolkit (UQTk)". In: *Handbook of Uncertainty Quantification*. Ed. by Roger, David Higdon, and Houman Owhadi. Cham: Springer International Publishing, 2017, pp. 1807–1827.

[12] J. Bezanson, A. Edelman, S. Karpinski, and V. Shah. "Julia: A Fresh Approach to Numerical Computing". In: *SIAM Review* 59.1 (2017), pp. 65–98.

[13] W. Gautschi. *Orthogonal Polynomials: Computation and Approximation*. Oxford: Oxford University Press, 2004.

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Stochastic fluid flow model to quantify the contribution of small-scale inhomogeneity to large-scale flow structuration.

Pranav Chandramouli,[1] ***and Etienne Memin,***[1]

[1]INRIA Rennes Bretagne Atlantique, Rennes, France – pranav.chandramouli@inria.fr

Key words: Stochastic Large Eddy Simulation, Fluid Dynamics, Flow Structuration

A stochastic framework is developed for the simulation of fluid flows by decomposing the velocity ($\boldsymbol{U}$) into a large scale smooth component ($\boldsymbol{u}$) and a small-scale fluctuating noise denoted by a brownian term ($\boldsymbol{\sigma}\dot{\boldsymbol{B}}_t$) [4]:

$$\boldsymbol{U}(\boldsymbol{X}_t, t) = \boldsymbol{u}(\boldsymbol{X}_t, t) + \boldsymbol{\sigma}(\boldsymbol{X}_t, t)\,\dot{\boldsymbol{B}}_t \tag{1}$$

This decomposition facilitates the rigorous development of the stochastic conservation equations from a stochastic Reynolds Transport Theorem [4, 5]. The derived stochastic momentum conservation equation is given as:

$$d_t\boldsymbol{u} + \Big(\big(\underbrace{\boldsymbol{u} - \frac{1}{2}\nabla\cdot\boldsymbol{a}}_{\text{advection bias } (\boldsymbol{u}^*)}\big)dt + \boldsymbol{\sigma}d\boldsymbol{B}_t\Big)\cdot\boldsymbol{\nabla}\Big)\boldsymbol{u} - \underbrace{\frac{1}{2}\boldsymbol{\nabla}\cdot\Big((\boldsymbol{a}\nabla)\boldsymbol{u}\Big)dt}_{\text{Dissipation}} = -\nabla p + \nu\Delta\boldsymbol{u}dt + \nu\Delta\boldsymbol{\sigma}d\boldsymbol{B}_t \tag{2}$$

The derivation intrinsically introduces terms denoting the contribution of the small-scales, i.e. the dissipation and advection due to $\boldsymbol{\sigma}d\boldsymbol{B}_t$. Additionally we see two terms unique to this decomposition: an added dissipation term similar to the "sub-grid scale dissipation" seen in the filtered Navier-Stokes equations and a modification of the large-scale advection, both characterised by the inhomogeneity at the small noisy scales. This inhomogeneity is represented by the tensor $\boldsymbol{a} = \boldsymbol{\sigma}\boldsymbol{\sigma}^T$ which is henceforth referred to as the variance tensor. The advection bias is similar to the "turbophoresis" phenomena that tends to drive fluid particles outside regions of high fluctuation variance [1] (see also [2] for an analysis on a turbulent wake flow of this modified advection)

Applying a change of variable from $\boldsymbol{u}$ to $\boldsymbol{u}^*$ and rearranging, under a quasi-harmonic assumption on the advection modifier ($(\frac{1}{2}\nabla\cdot\boldsymbol{a})$, allows a direct parallel to be drawn between these stochastic conservation equations and the Craik-Leibovich equations [3] for Langmuir turbulence. Within such a parallel, the advection modifier plays the role of Stokes drift. This term quantifies the small-scale contribution to large-scale instabilities and flow structuration by inducing a "vortex" force. Thus, a numerical simulation with this stochastic model including the advection bias, defined by a well-characterised noise, should better structure the flow. This is indeed observed in a stochastic simulation of flow through a channel at Re_τ 590. As in Langmuir circulation where wind driven surface waves lead to a Stokes drift induced vortex forces, the inhomogeneity at the scale of the noise, characterised through the advection bias, in our stochastic LES induces vortex forces in a channel. This vortex flows leads to flow structuration in the form of streaks, as is observed for Langmuir circulation. Such numerically observed streaks with the stochastic LES framework for channel flow, both quantitatively and qualitatively, match better with the reference data-set than a classical deterministic LES framework (see Figure 1). The streak sizes observed with the stochastic model are of comparable size to the direct numerical simulation data-set especially at larger distances from the wall. The classical LES, performed using the dynamic Smagorinsky model, is seen to mis-predict the size and energy of the streaks at all distances from the wall.

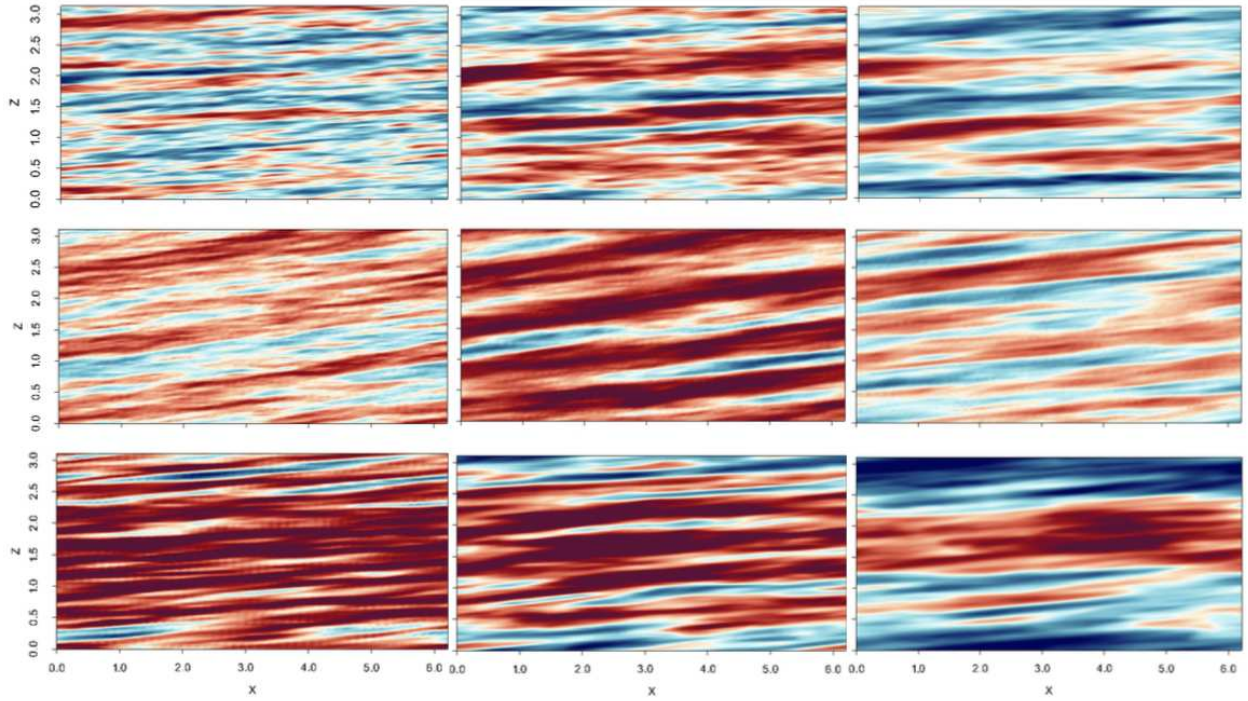


Figure 1: 2D time-averaged streamwise velocity fluctuation (< u'u' >) contours at three different heights from wall (y+ = 50 (left), 100 (middle), and 200 (right)). From top to bottom, reference direct numerical simulation data-set, stochastic simulation, and classical LES. Blue indicates low-speed streaks and red indicates high-speed streaks.

[1] M. Caporaloni, F. Tampieri, F. Trombetti, and O. Vittori. Transfer of particles in non-isotropic air turbulence. J. Atmos. Sci. , **32**, 565-568 (1975).

[2] P. Chandramouli, E. Memin, D. Heitz, S. Laizet. Coarse large-eddy simulations in a transitional wake flow with flow models under location uncertainty. Comput. Fluids. **168**, 170-189 (2018)

[3] A. D. D. Craik, S. Leibovich. A rational model for Langmuir circulations. J. Fluid Mech. **73**, 401-426 (1976)

[4] E. Memin. Fluid flow dynamics under location uncertainty. Geophys. Astro. Fluid. **108**, 119-146 (2014).

[5] V . Resseguier, E. Memin, B. Chapron. Geophysical flows under location uncertainty, Part I Random transport and general models. Geophys. Astro. Fluid. **111**, 149-176 (2017).

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Embedded Ridge Approximation: Ideas and Algorithms in Vector-valued Dimension Reduction

Chun Yui Wong,[1] ***Pranay Seshadri,***[2] ***and Geoffrey Parks,***[3]

[1]Department of Engineering, University of Cambridge – cyw28@cam.ac.uk

[2]Department of Engineering, University of Cambridge; The Alan Turing Institute, London – pseshadri@turing.ac.uk

[3]Department of Engineering, University of Cambridge – gtp10@cam.ac.uk

Key words: Ridge Approximation, Dimension Reduction

Physical quantities of interest (qois) encountered in uncertainty quantification can often be expressed as a function of primal quantities, such as the pressure field in a computational fluid dynamics solution. Usually, a primal quantity at a certain point in the output domain will only be weakly affected by perturbations far from it, which manifests as strongly anisotropic dependence on the input variables. By exploiting this fact, we establish that these primal quantities often admit a stronger ridge structure than conventional qois, such as the lift and drag coefficients of an airfoil, or the total deflection of an elastic structure. Thus, we can reduce the quantity of simulation data required for the low-dimensional approximation of qois by considering them as a function of primal quantities. We call this approach *embedded ridge approximation*. In this talk, we quantify the improvement in accuracy that can be achieved via embedded ridge approximation compared to that of conventional subspace-based dimension reduction.

Moreover, the dependence structure of primal quantities on the input variables is often smooth. That is, neighbouring primal quantities often depend on a similar set of input variables. Motivated by this observation, we propose sparse storage algorithms for PDE solution fields using a few ridge directions. Using an example pertaining to the shape design of the NACA0012 airfoil, we demonstrate the efficacy of the ideas presented in this talk. For example, in figure 1 we show the improvement in mean squared approximation error of the drag coefficient of this airfoil by using embedded methods over direct methods given a limited amount of simulation data.

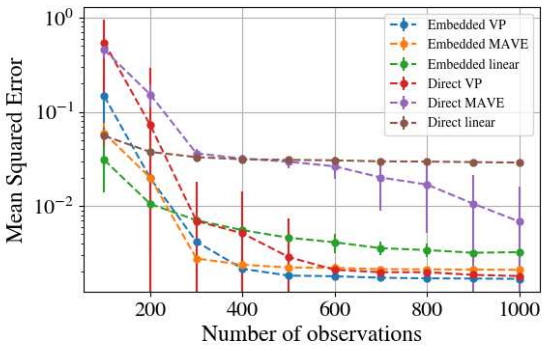


Figure 1: Mean squared approximation error of embedded and direct dimension reduction methods for approximating the drag coefficient of the NACA0012 airfoil (VP = Variable Projection, MAVE = Minimum Average Variance Estimation).

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Experimental investigation of the accuracy of the modelled frictional pressure loss for annular pipe flow based on rheological characterization of a non-Newtonian drilling fluid

Solveig Riisøen,[1] ***and Fionn Iversen,***[2]

[1] NORCE - Norwegian Research Centre, Bergen – Solveig.Riisøen@norceresearch.no
[2] NORCE - Norwegian Research Centre, Bergen – Fionn.Iversen@norceresearch.no

Key words: Uncertainty Quantification, Fluid Dynamics, Experimental, Bayesian Regression, Drilling Fluid

During drilling operations, it is important to accurately model the pressure profile in the well in order to control the drilling process and achieve a more efficient drilling program. The frictional pressure loss is the component with the highest uncertainty compared to the hydrostatic component. It is therefore important to get a better understanding of the uncertainties related to the modelling of this pressure loss. The pressure gradient is calculated amongst others with the fluid rheological properties as input.

This study compares the modelled frictional pressure loss using the rheological characterization of a drilling fluid as measured with a high-precision rheometer with the actual pressure loss measured in a flow loop experiment at the University of Stavanger (UoS). The rheometer measurement is carried out with shear rate as control parameter, while in pipeline flow the readily available control parameter is the pressure gradient. An important difference lies in uncertainties in the relation between shear rate and pressure gradient in pipelines. The main contributors to the uncertainties are further investigated with focus on experimental errors and bias with regards to the model used. The drilling fluid used in this study is the aqueous solution of Poly-Anionic Cellulose (PAC) with viscoelastic shear thinning behaviour. The method of uncertainty quantification has been performed in several steps:

1. First the uncertainty related to the experimental data were quantified. This uncertainty has been evaluated by statistical methods based on a series of experiments.
2. Then the curve fitting of the experimental data and the propagation of the uncertainties of the estimated regression parameters were handled. Bayesian regression and Monte Carlo simulations have been applied for this purpose.
3. Finally, the propagation of uncertainty from the regression parameters to the frictional pressure loss of fluid flow in pipe, based on functional relationship, is handled by the GUM theory (The Evaluation of Measurement Data - Guide to the Expression of Uncertainty in Measurement).

Through finding a reliable method of identifying and quantifying the main sources of uncertainties for pressure loss modelling, this work shall contribute to optimize the drilling process with respect to efficiency and safety. The results are of importance also for other industries dealing with non-Newtonian fluid flow in pipes.

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Convective Heat Enhancement Uncertainties of Pressure and Temperature Data Acquisition in Rectangular Channel

Aasa S.A.,[1] ***Jen T.C.***[1] ***and Romeo Fono-Tamo,***[1]

[1]University of Johannesburg, aasagangan@yahoo.com

Key words: Uncertainty Analysis, Temperature, and pressure drop, heat Exchanger

Convective analysis in passive heat exchanger techniques is fast becoming a major solution to vast growing modern technology that is saddled with high energy dispensing capacity. In this study, the uncertainty analysis is carried out in a rectangular end-wall dimple channel for both the pressure and temperature of the end-wall. This is based on the expected values and variances associated with deterministic errors of upper and lower bias limits at 95 percent confidence level interval of the true measured data. These data are acquired using the DAQTM instrument through pressure tube and T-type thermocouples attached to dimple end-wall. The uncertainty details of the instrument the error in the data are analysis using Monte Carlo data procedures. The data are repeated three consecutive times, for the first case (pressure drop); the velocity and the channel pressure are kept constant and in the second case (Surface Temperature); Velocity and the temperature are kept constant. The velocity of 10 ms-1 is used for each test time and this is equivalent to pressure variation of 12 to 34 Pa and 28 to 63 degree Celsius respectively. The data were validated using the Kalma Nikuradse method for the channel pressure drops. From the results the uncertainties of pressure drop were found to be in range of 2 -4.5 percent from the inlet to the exit of the test section and the uncertainties of the temperature were 1 – 2 percent from the inlet to the exit of the test section.

[1] R. J. Moffat, “Using Uncertainty Analysis in the Planning of an Experiment," Journal of Fluids Engineeringl **107(2)**, 173 (1985).

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Uncertainty Characteristic of Friction Factors and Nusselt Number in Heat Enhancement Rectangular Channel

Jen T.C.,[1] ***Aasa S.A.***[1] ***and Romeo Fono-Tamo,***[1]

[1]University of Johannesburg, 218104165@student.uj.ac.za

Key words: Uncertainty Analysis, Friction factor, Nusselt Number and pressure drop, Convective heat Enhancement

Burden of enormous energy dispenses heat exchanger, in a vastly growing modern technology, has turned over affects on the design life span of the system. One way of improving this effect is through effective heat enhancement, this is found in passive techniques, hence, the need for an accurate data acquisition system. Uncertainty analysis is a major way to ensure accurate data acquisition, for this study, a rectangular dimple end-wall channel uncertainty of friction factor and Nusselt number are analysed. This is based on the expected values and variances associated with deterministic errors of upper and lower bias limits at 95 percent confidence level interval of the true measured data. These data are acquired using the DAQTM instrument through pressure tube and T-type thermocouples attached to dimple end-wall. The uncertainty details of the instrument errors in the data are analysis using Monte Carlo procedures. The data are repeated three consecutive times, for the first case (pressure drop); the velocity and the channel pressure are kept constant and in the second case (Surface Temperature); velocity and the heat source are kept constant; constant velocity 7 ms-1 used for each test time. The data were validated using the Kalma Nikuradse method for the channel pressure drops and Dittus Boetler for Nusselt number. From the results the uncertainties of friction factors and Nusselt number were found to be in range of 2 – 7 percent and 3 – 5.5 percent from the inlet to the exit of the test section.

[1] R. J. Moffat, “Using Uncertainty Analysis in the Planning of an Experiment," Journal of Fluids Engineeringl **107(2)**, 173 (1985).

Keynote Lecture - G. Karniadakis - Physics-informed neural networks (PINNs) with uncertainty quantification
Session Chair: D. Lucor
Auditorium

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Physics-Informed Neural Networks (PINNs) with Uncertainty Quantification

George Em Karniadakis

Brown University, United States – George_Karniadakis@Brown.edu

Key words: Physics-Informed Neural Networks, Uncertainty Quantification

We will present a new approach to develop a data-driven, learning-based framework for predicting outcomes of physical and biological systems and for discovering hidden physics from noisy data. We will introduce a deep learning approach based on neural networks (NNs) and generative adversarial networks (GANs). Unlike other approaches that rely on big data, here we 'learn' from small data by exploiting the information provided by the physical conservation laws, which are used to obtain informative priors or regularize the neural networks. We will also make connections between Gauss Process Regression and NNs and discuss the new powerful concept of meta-learning. We will demonstrate the power of PINNs for several inverse problems in fluid mechanics, solid mechanics and biomedicine including wake flows, shock tube problems, material characterization, brain aneurysms, etc, where traditional methods fail due to lack of boundary and initial conditions or material properties. We will address the issue of total uncertainty quantification, namely the uncertainty associated with the network separately from the uncertainty in the parameters, data and models. We will present different methods, including dropout, Vadam, GANs and polynomial chaos variants for neural network implementations.

ST1 – Methodology III *Session Chair: G. Karniadakis* *Auditorium*	ST2 – Applications I *Session Chair: A. Mariotti* *Room B*

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Adaptive, Reinforcement Learning based, Model Management for Multifidelity Monte-Carlo

Ludger Paehler,[1] ***and Nikolaus A. Adams,***[2]

[1]Institute of Aerodynamics and Fluid Mechanics, Technical University of Munich, Germany – ludger.paehler@tum.de

[2]Institute of Aerodynamics and Fluid Mechanics, Technical University of Munich, Germany – nikolaus.adams@tum.de

Key words: Uncertainty quantification, Fluid Dynamics, Turbulent Flows, Reinforcement Learning

The quantification of uncertainties in turbulent flows poses a myriad of challenges for established approaches. While intrusive approaches are out of the question due to highly complex code libraries, traditional non-intrusive, sampling-based approaches require too many samples to be feasible. As turbulent flows depend on solving the finescale turbulent structures they must ideally be simulated in a direct approach, where the finescale structures are resolved up to the Kolmogorov scale [2]. This poses a significant computational burden with a single simulation costing $\gg$100k CPU hours.

However, in most applications we have access to other models and surrogates, which encapsulate subaspects of the process. Multifidelity Monte-Carlo allows us to relate lower-resolution models, different modelling approaches and surrogate models to the "true", high-fidelity model. This is done by linking the different fidelities through correlation coefficients for the calculation of the Monte-Carlo estimator. Paramount to such an approach is an efficient model management strategy, which allows for the limitation of the computational cost to, in this case, less than 30 high-fidelity models.

State-of-the-art model management techniques either rely on the calculation of error and cost rates [3] or posing model management for Multifidelity Monte Carlo as optimization problems [4], where the right balance between high-fidelity model evaluations and surrogate models has to be struck. But as the first approach requires up front calculation of the model's properties and the second approach scales poorly to larger model ensembles both are ill-suited for the herein envisioned application to generic model ensembles with adaptive models.

Using Reinforcement learning [1] we propose a fully adaptive, intelligent model management routine which has the ability to adapt to changes in arbitrarily large model ensemble or fidelity hierarchies. Moreover, it also allows for the full incorporation of adaptive low-fidelity models. By applying a hierarchical approach the algorithm is equipped with two overarching objectives; a variance threshold and unbiasedness. The "workers" controlling the allocation to each sample then aim to satisfy the set objectives. In this task the workers are free to decide on their respective actions, but are being evaluated and rewarded for meeting the assigned objectives. The hierarchical construction of the proposed algorithm scales to arbitrarily many objectives and achieves close to optimal computational ressource allocation for the computation of Monte-Carlo estimators with a specified tolerance for variance.

[1] P. Dayan, and G. E. Hinton, "Feudal reinforcement learning," In *Advances in Neural Information Processing System 6*, pp. 271-278 (1993).

[2] F. Diegelmann, V. Tritschler, S. Hickel, and N. A. Adams, "On the pressure dependence of ignition and mixing in two-dimensional reactive shock-bubble interaction," Combustion and Flame **163**, (2016).

[3] M. B. Giles, "Multilevel monte carlo path simulation," Operations Research **56**, 3 (2008).

[4] B. Peherstorfer, K. Willcox, and M. Gunzburger, "Optimal model management for multifidelity Monte Carlo estimation," SIAM Journal on Scientific Computing **38**, 5 (2016).

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Interpretability Within a Level-Set Data Assimilation Framework

***Hans Yu*[1], *Matthew P. Juniper*[1], *Luca Magri*[1,2]**

[1]Department of Engineering, University of Cambridge

[2]Institute for Advanced Study, Technical University of Munich

Key words: Uncertainty quantification, forward propagation, inverse problem, data assimilation, level-set method, reduced-order model, combustion

The advent of statistical learning in fluid mechanics is in various aspects reminiscent of the revolution brought about by Computational Fluid Dynamics (CFD). One of these aspects pertains to the issue of trust: While the rise of CFD happened in lockstep with the rapid developments in hardware and software at that time, the a-priori fidelity of the results is best understood in terms of numerical analysis, i.e. the roles of numerical dissipation and dispersion as well as the importance of numerical formulations that respect the conservative nature of the governing equations. Statistical learning techniques such as deep learning have repeatedly proven their worth in tasks previously considered inaccessible to machines [1, 2]. Nevertheless, their black-box nature is the greatest obstacle to establishing the degree of trust necessary for wide-spread acceptance and application to critical fluid mechanics problems [3].

This paper focuses on the issue of interpretability for data assimilation, a particular statistical learning technique, which is here applied to interface problems solved by so-called level-set methods [4]. Data assimilation gives the statistically optimal estimate based on model predictions and experimental observations. On a spectrum of purely physics-driven methods (e.g. direct numerical simulations) on one end and purely data-driven methods (e.g. deep neural networks) on the other end, data assimilation is a hybrid method. Level-set methods are of interest to the fluid mechanics community because many physical phenomena are governed by interface kinematics, e.g. shock waves, premixed flames and multi-phase flows. Despite the specific choice of statistical learning technique and governing equations here, the considerations regarding interpretability are generic, and thus relevant to statistical learning in fluid mechanics in general.

To verify the fidelity of a CFD code, one can use either a canonical testcase or the method of manufactured solutions [5]. For statistical learning in fluid mechanics, there is no unified approach to interpretability yet. In this paper, we highlight a number of interpretability features present in our level-set data assimilation framework, which should be of general interest to statistical learning frameworks in fluid mechanics:

The role of representation. In deep learning, it has long been recognized that the performance of a neural network heavily depends on the representation of the data [6]. Similarly, different formulations are available for interface problems. We verify various formulations in one and two dimensions. Moreover, we discuss how we combine data assimilation with an efficient level-set method in an encoder-decoder type of architecture. Note how many of the so-called physics-informed machine learning frameworks boil down to the question of representation, e.g. in turbulence closure models [7, 8, 9].

The role of information. It is notoriously impossible to gain insight into a neural network from only looking at the nodes in each layer and their assigned weights. The situation is different for data assimilation, where climatology in the form of covariance matrices gives us valuable insight into the interaction between model and data. We look at both the limiting cases of sparse and complete data.

Uncertainty quantification. In our level-set data assimilation framework, we follow a Bayesian approach, where the learning outcomes are probability distributions. The language of probability theory allows for the precise statement of the inference performed, e.g. filtering, smoothing and prediction. We demon-

strate how careful manipulation of joint and marginal distributions yields conditional distributions suitable for visualization and parameter estimation.

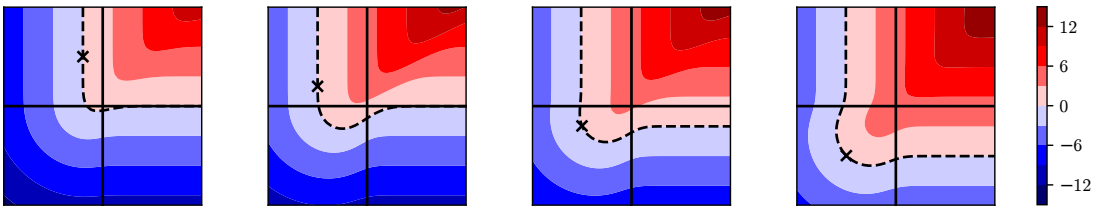


Figure 1: Sensitivity of two-dimensional level sets (black dashed lines) to assimilation of individual data points (black crosses).

This paper concludes with an example taken from combustion where our level-set data assimilation framework is applied to the dynamics of a ducted premixed flame [10]. We demonstrate a Bayesian approach to forward propagation, parameter estimation and uncertainty quantification.

[1] Alex Krizhevsky, Ilya Sutskever, and Geoffrey E. Hinton. ImageNet Classification with Deep Convolutional Neural Networks. In *Advances in Neural Information Processing Systems 25*, pages 1097–1105. Curran Associates, Inc., 2012.

[2] David Silver, Aja Huang, Chris J. Maddison, Arthur Guez, Laurent Sifre, George van den Driessche, Julian Schrittwieser, Ioannis Antonoglou, Veda Panneershelvam, Marc Lanctot, Sander Dieleman, Dominik Grewe, John Nham, Nal Kalchbrenner, Ilya Sutskever, Timothy Lillicrap, Madeleine Leach, Koray Kavukcuoglu, Thore Graepel, and Demis Hassabis. Mastering the game of Go with deep neural networks and tree search. *Nature*, 529(7587):484–489, January 2016.

[3] Been Kim, Rajiv Khanna, and Oluwasanmi O. Koyejo. Examples are not enough, learn to criticize! Criticism for Interpretability. In *Advances in Neural Information Processing Systems 29*, pages 2280–2288. Curran Associates, Inc., 2016.

[4] Hans Yu, Matthew P. Juniper, and Luca Magri. Combined State and Parameter Estimation in Level-Set Methods. *arXiv:1903.00321 [physics]*, March 2019. arXiv: 1903.00321.

[5] Lee Shunn, Frank Ham, and Parviz Moin. Verification of variable-density flow solvers using manufactured solutions. *Journal of Computational Physics*, 231(9):3801–3827, May 2012.

[6] Ian Goodfellow, Yoshua Bengio, and Aaron Courville. *Deep learning*. Adaptive computation and machine learning. The MIT Press, Cambridge, Massachusetts, 2016.

[7] Eric J. Parish and Karthik Duraisamy. A paradigm for data-driven predictive modeling using field inversion and machine learning. *Journal of Computational Physics*, 305:758–774, January 2016.

[8] Julia Ling, Andrew Kurzawski, and Jeremy Templeton. Reynolds averaged turbulence modelling using deep neural networks with embedded invariance. *Journal of Fluid Mechanics*, 807:155–166, November 2016.

[9] Gianluca Iaccarino, Aashwin Ananda Mishra, and Saman Ghili. Eigenspace perturbations for uncertainty estimation of single-point turbulence closures. *Physical Review Fluids*, 2(2), February 2017.

[10] Hans Yu, Thomas Jaravel, Jeffrey W. Labahn, Matthias Ihme, Matthew P. Juniper, and Luca Magri. Physics-informed data-driven prediction of premixed flame dynamics with data assimilation. Technical report, Center for Turbulence Research, 2018.

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Investigation of PDE-constrained deep neural networks for efficient flow field assimilation

Atul Agrawal,[1] ***Anne Sergent,***[1,2] ***Yann Fraigneau,***[1] ***and Didier Lucor***[1]

[1]LIMSI, CNRS, Université Paris-Saclay, Campus universitaire bât 508 Rue John von Neumann, F - 91405 Orsay cedex, France – didier.lucor@limsi.fr

[2]Sorbonne Université, UFR d'Ingénierie, F-75005, Paris, France – anne.sergent@limsi.fr

Key words: physics-informed machine learning, deep neural network, data assimilation.

The development of data-driven surrogate models for the prediction of complex fluid phenomena, in place of more standard numerical simulations, is an ongoing challenge in various fields and may help when many-query and/or real-time simulations (e.g. uncertainty quantification, data assimilation, control...) are required. Here, we decide to investigate the potential of integrating deep neural networks (DNN), which are known to be performant in capturing transient and intermittent phenomenon with the possibility of handling translations, rotations and other invariances, in more classical numerical methods for computational fluid mechanics [1]. Inspired by recent works [2, 3], the strategy retained in this study is the one of training a DNN by leveraging some underlying physical laws of the system. The idea is to incorporate prior scientific knowledge to be used as a guideline for designing efficient deep learning models. In particular, a natural approach is to incorporate (some of) the governing partial differential equations (PDEs) of the physical model (e.g. mass/momentum/energy conservation) at the core of the DNN, i.e. in the loss/likelihood functions. We propose to investigate how this additional information effectively regularizes the minimization procedure in the training of DNN for fluid flows, and enables them to generalize well with fewer training samples. More specifically, we will report on the influence of the choice and the dimensionality of the domain of interest for data acquisition as well as subsequent training and predictions, in relation to the problem geometry, initial/boundary conditions and flow regimes. Finally, we will report on the DNNs training attempt on large direct numerical simulations database acquired for turbulent convective flow in rectangular cavity with buoyant effects.

Figs. (1-2) present some preliminary results for an incompressible, laminar, time-dependent 2D flow past a stationary cylinder with an imposed fixed wall temperature (Reynolds and Peclet numbers: Re=100 and Pec=71). Only the simulated temperature field within the domain depicted by the $[2, 10] \times [-3, 3]$ yellow rectangle, cf. Fig. (1), is collected for several shedding cycles and used for the DNN training. In addition, numerical constraints corresponding to the advection-diffusion temperature transport equation, conservation of mass and momentum equations of the fluid are imposed to the DNN-predicted quantities during the training. Results presented at a particular instant of the time-window, cf. Fig. (2), show that hidden quantities, here, $[u, v, p]_{(t,x,y)}$, are correctly learned and predicted through the implicit encoding of the underlying PDEs.

[1] J.N. Kutz. Deep learning in fluid dynamics. *J Fluid Mech.*, 814:1-4, 2017.

[2] M. Raissi, P. Perdikaris, and G.E. Karniadakis. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *J. Comp. Phys.*, 378:686-707, 2019.

[3] Y. Zhu, N. Zabaras, P. Koutsourelakis, and P. Perdikaris. Physics-constrained deep learning for high-dimensional surrogate modeling and uncertainty quantification without labeled data. *arXiv:1901.06314*, 2019.

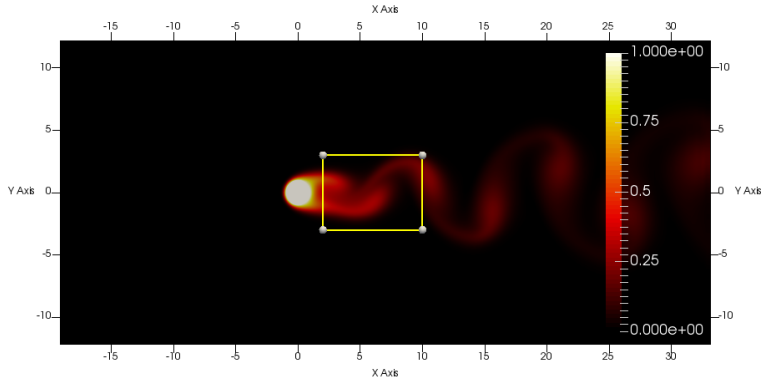


Figure 1: System considered: DNS-simulated two-dimensional flow past a heated cylinder. The simulated temperature field within the domain depicted by a $[2, 10] \times [-3, 3]$ yellow rectangle is collected for several shedding cycles and used for the DNN training.

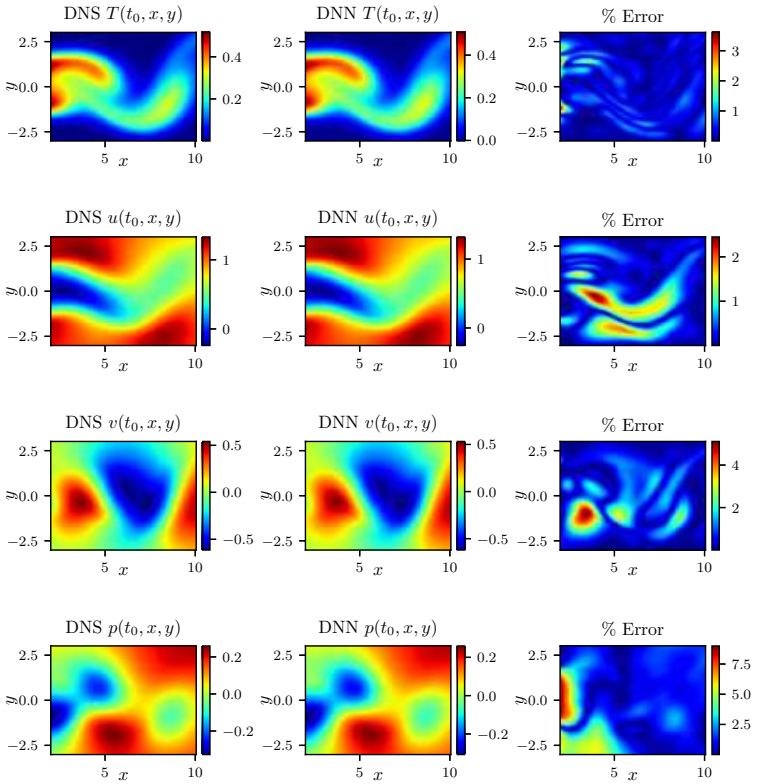


Figure 2: System predicted: reference DNS-simulated (left column) and DNN-predicted (middle column) snapshots of temperature (1st row), streamwise (2nd row) and crossflow (3rd row) velocities and pressure (last row) fields at a particular time instant t_0. The right column represents the relative error (in percentage) normalized with the maximum value of the simulated field at that time. *Only the simulated temperature field data is used to train the DNN, which is capable of reconstructing the hidden fields with satisfactory accuracy.*

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Uncertainty Quantification of Time–Averaged Quantities and their Sensitivities in Chaotic Systems

Kyriakos Dimitrios Kantarakias,[1]***, Karim Shawki,***[1] ***and George Papadakis,***[1]

[1]Imperial College London, Department of Aeronautics, United Kingdom – k.kantarakias@imperial.ac.uk

Key words: Uncertainty Quantification, Sensitivity Analysis, Least Squares Shooting Shadowing, Polynomial Chaos Expansion

This paper focuses on quantifying the statistical behaviour of sensitivities of time-averaged quantities of chaotic systems. Such systems, written in the general form

$$\frac{d\boldsymbol{u}}{dt} = \boldsymbol{f}(\boldsymbol{u}, \boldsymbol{s}), \tag{1}$$

where $\boldsymbol{u}$ are the field variables and $\boldsymbol{s}$ denotes the design parameters vector, have at least one positive Lyapunov exponent. For many practical problems that involve turbulent flows, for example in aerodynamics, it is of interest to compute cost functions that are time–averaged quantities of the flow field, i.e.

$$\overline{J}_\infty = \lim_{T\to\infty} \frac{1}{T} \int_0^T J(\boldsymbol{u}, \boldsymbol{s}) dt \tag{2}$$

as well as their sensitivities $\frac{d\overline{J}_\infty}{ds}$, that can be used in gradient–based optimization. As shown in many publications in the literature ([5] is just one example), quantifying uncertainties in chaotic systems in the form of equation (1) with the Polynomial Chaos Expansion (PCE) requires a large number of PCE coefficients in order to compute accurately the statistical moments of an objective at a certain time instant, as the system evolves further and further away from the initial condition. For large systems, this can make the computational demands of the PCE prohibitive.

In this work, we focus on time-average objectives $\left(\overline{J}_\infty\right)$, and their sensitivities $\left(\frac{d\overline{J}_\infty}{ds}\right)$, for uniformly hyperbolic and ergodic systems. To that end, an approach for applying the PCE to chaotic dynamical systems is discussed. Applications are made to the Lorenz attractor and the Kuramoto–Sivashinsky (KS) system, which are ergodic and their time–averages vary smoothly with respect to s. It is shown that, at least for these systems and the range of parameters examined, PCE can predict the statistical behavior of time-averaged objectives with a low number of spectral PCE coefficients.

Results for the Lorenz system,

$$\frac{dx}{dt} = \sigma(y - x), \frac{dy}{dt} = x(\rho - z) - y, \frac{dz}{dt} = xy - \beta z \tag{3}$$

with the the time–averaged objective function is

$$\overline{J} = \frac{1}{T} \int_0^T z\, dt \tag{4}$$

can be seen in table 1. Notice that results from non-intrusive PCE are in good agreement with the Monte–Carlo simulations, ever for a low chaos order.

This approach is subsequently applied to the sensitivities with respect to some design parameters. It has been shown by Ruelle [6] that such sensitivities exist and are smooth with respect to variations in the design

Stochastic Input	Moment	PCE $C = 1$	PCE $C = 2$	PCE $C = 3$	Monte Carlo
$\rho \sim N(32, 1.5)$	μ_J	27.816	27.809	27.822	27.821
$\beta \sim U(2.4, 2.6)$	σ_J	1.533	1.523	1.553	1.549
$\rho \sim N(32, 1.5)$	μ_J	27.786	27.774	27.788	27.779
$\beta \sim U(2.0, 3.0)$	σ_J	1.593	1.593	1.593	1.595
$\rho \sim N(32, 0.5)$	μ_J	27.809	27.779	27.785	27.780
$\beta \sim U(2.0, 3.0)$	σ_J	0.713	0.720	0.723	0.721

Table 1: UQ of objective (4) in the Lorenz system for $T = 1000$ and $m = 2$ uncertain variables. Comparison between PCE for 3 orders of chaos ($C = 1, 2, 3$) and the Monte Carlo for N = 5000 samples. The initial conditions are random.

parameters for uniformly hyperbolic systems. However, conventional methods for computing the gradient of time-average quantities, such as the adjoint method, fail when the system under investigation has at least one positive Lyapunov exponent (refer to [3]).

To address this challenge, Wang et al [1] successfully introduced the Least Squares Shadowing (LSS) algorithm based on the shadowing lemma for uniformly hyperbolic and ergodic systems. We employ a modification of the LSS algorithm, the preconditioned version of the Multiple Shooting Shadowing(MSS) algorithm (proposed in [4]) to compute the sensitivities of time–averaged quantities that emerge from the Kuramoto–Sivashinsky (KS) system and the Lorenz attractor. The MSS method is coupled with non-intrusive PCE to quantify the effects of real–world uncertainties to the statistical moments of such sensitivities. It is shown that this coupling can lead to an accurate computation of the statistics of such sensitivities, again for a low chaos order. Such sensitivities have been shown to be continuous and smooth, provided that the conditions for the shadowing lemma hold up. Some results can be seen for the sensitivity of objective 4 with respect to β, for the Lorenz system. Notice that the results are in good agreement with the Monte–Carlo simulation.

An efficient coupling approach is introduced, that takes advantage of the shadowing properties of such systems

Uncertain Input		$C = 1$	$C = 2$	MC MSS	MC FD
$\beta \sim N(0.5, 0.1)$	μ_{dJ_β}	-1.5834	-1.5793	-1.5796	-1.5801
	σ_{dJ_β}	0.0579	0.0573	0.0596	0.0601

Table 2: UQ of the sensitivity of the objective (4) with respect to β in the Lorenz system for $T = 200s$. Uncertainty is introduced through β. Comparison between non-intrusive PCE for $C = 1$, $C = 2$, the Monte Carlo for N = 5000 samples of the MSS solver and the Monte Carlo for N = 5000 with Finite Differences.

to reduce the computational cost of doing UQ with non-intrusive PCE in chaotic systems. This new method is called the shadowing PCE (sPCE).

[1] Qiqi Wang , Rui Hu and Patrick Blonigan, "Least Squares Shadowing sensitivity analysis of chaotic limit cycle oscillations," Journal of Computational Physics, (2014).

[2] Qiqi Wang and Patrick Blonigan, "Multiple shooting shadowing for sensitivity analysis of chaotic dynamical systems," Journal of Computational Physics, (2018).

[3] G L Eyink, T W N Haine and D J Lea, "Ruelle's linear response formula, ensemble adjoint schemes and Levy flights," Nonlinearity, (2004).

[4] Karim Shawki, George Papadakis, "A Preconditioned Multiple Shooting Shadowing Algorithm for the Sensitivity Analysis of Chaotic Systems" Journal of Computational Physics (under review, 2019, https://arxiv.org/abs/1810.12222).

[5] Michal Branicki and Andrew J. Majda, "Fundamental limitations of polynomial chaos for uncertainty quantification in systems with intermittent instabilities," Communications in Mathematical Sciences, (2013).

[6] David Ruelle, " A review of linear response theory for general differentiable dynamical systems," Nonlinearity, (2009).

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Bayesian Network PDEs for Flow and Transport in Energy Materials

Eric Joseph Hall,[1] ***Kimoon Um,***[2] ***Markos Katsoulakis,***[3] ***and Daniel Tartakovsky***[2]

[1]Chair of Mathematics for Uncertainty Quantification, RWTH Aachen University, Germany – hall@uq.rwth-aachen.de

[2]Energy Resources Engineering, Stanford University, USA – kimoon.um@gmail.com, tartakovsky@stanford.edu

[3]Mathematics and Statistics, University of Massachusetts Amherst, USA – markos@math.umass.edu

Key words: Bayesian networks, domain knowledge, multiscale modeling, energy storage, uncertainty quantification, global sensitivity analysis, mutual information

Microscopic (pore-scale) properties of porous media affect and often determine their macroscopic (Darcy- or continuum-scale) counterparts. Understanding the relationship between processes on these two scales is essential to both the derivation of macroscopic models of, e.g., transport phenomena in natural porous media, and the design of novel materials, e.g., for energy storage. Most microscopic properties exhibit complex statistical correlations and geometric constraints, which presents challenges for the estimation of macroscopic quantities of interest (QoIs), e.g., in the context of global sensitivity analysis (GSA) of macroscopic QoIs with respect to microscopic material properties. We present a systematic way of building correlations into stochastic multiscale models through Bayesian networks. The proposed framework allows us to construct the joint probability density function (PDF) of model parameters through causal relationships that are informed by domain knowledge and emulate engineering processes, e.g., the design of hierarchical nanoporous materials. These PDFs also serve as input for the forward propagation of parametric uncertainty. To assess the impact of correlations and causal relationships between microscopic parameters on macroscopic material properties, we use a moment-independent GSA based on the differential mutual information that leverages the structure of the Bayesian network and accounts for both correlated inputs and complex non-Gaussian QoIs. The global sensitivity indices are used to rank the effect of uncertainty in microscopic parameters on macroscopic QoIs and to quantify the impact of causality on the multiscale model's predictions. Our findings from numerical experiments in [1] indicate two practical outcomes. Firstly, that the inclusion of correlations through structured priors based on causal relationships impacts predictions of QoIs which has important implications for decisions support, engineering design, etc. Secondly, we observe the inclusion of structured priors with non-trivial correlations yields different effect rankings than independent priors and moreover these rankings are more consistent with the anticipated physics of a model problem.

[1] K. Um, E. J. Hall, M. A. Katsoulakis, and D. M. Tartakovsky, "Causality and Bayesian network PDEs for multiscale representations of porous materials," arXiv: 1901.01604 (2018).

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Uncertainty propagation through a simplified car Model

Fabien Taghon,[1] ***Rémi Pradeau,***[2] ***and Antoine Dumas***[3]

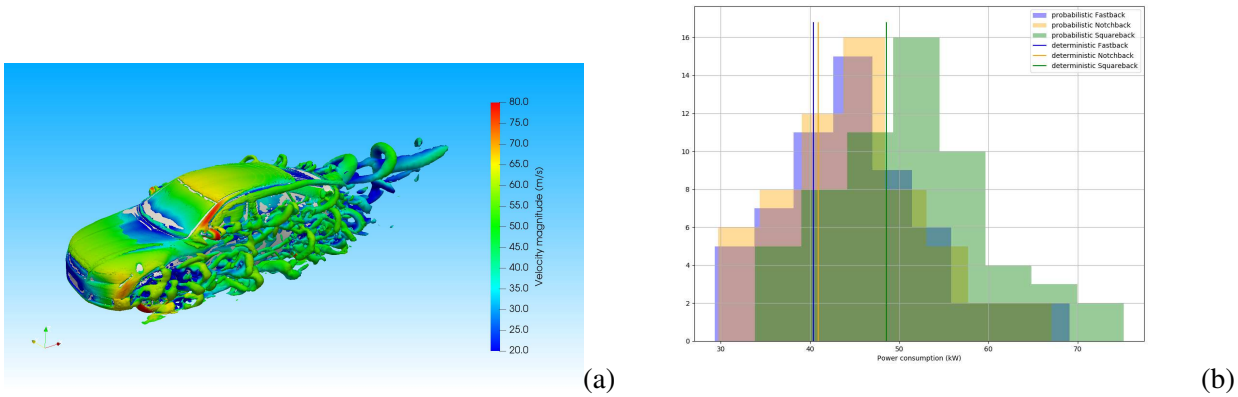
[1]Phimeca, France – taghon@phimeca.com

[2]Phimeca, France – pradeau@phimeca.com

[3]Phimeca, France – dumas@phimeca.com

Key words: Uncertainty propagation, DrivAer, OpenFOAM, openturns, natural wind, drag, lift

After the Volkswagen fraud scandal, the actual car fuel consumption began to raise more and more concerns. This fuel consumption is directly driven by the aerodynamics performance of the car. In addition, the flow seen by a car is defined by car speed and natural wind, the last one being usually less studied. Therefore, we aimed at defining the role played by the natural wind in car fuel consumption. As wind is intrinsically a stochastic process, we dealt with its influence in a probabilistic framework. To do this, we used openturns, an opensource library dedicated to uncertainty engineering, and OpenFOAM to compute aerodynamics performance of the three designs of the DrivAer simplified car model. Probability distributions have been chosen for natural wind speed and direction and different designs of experiment have been tested, like quasi Monte-Carlo and Latin Hypercube Sampling. As a result, it appeared that mean consumption over time was quite different than the deterministic one, computed without natural wind. Moreover, it appeared that the variability of the lift applied on the rear wheels was not the same for fastback, notchback and squareback designs.



(a) (b)

Figure 1: Q-criterion coloured with speed (a) and probability distribution of power consumption (b)

[1] R. Yazdani, *Steady and Unsteady Numerical Analysis of the DrivAer Model* (Department of Applied Mechanics, Chalmers university of technology, Göteborg, 2015).

[2] G. Shinde, A. Joshi and K. Nikam, *Numerical Investigations of the DrivAer Car Model using Opensource CFD Solver OpenFOAM,* In *OSCIC 13*, (Hamburg, 2013).

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Multi-Δt approach for peak-locking error correction and uncertainty quantification in PIV

Sagar Adatrao and Andrea Sciacchitano

Department of Aerospace Engineering, Delft University of Technology, Delft, The Netherlands
[s.adatrao@tudelft.nl; a.sciacchitano@tudelft.nl]

Key words: particle image velocimetry, uncertainty quantification, peak locking, multi-Δt, linear regression

Peak-locking is a well-known error source in digital particle image velocimetry (PIV), which is mainly ascribed to particle image diameters small with respect to the sensor's pixel size [1], [2]. Such error source is particularly relevant in high-speed PIV measurements with CMOS cameras, whose large pixel size (of the order of 10 to 20 μm) yields particle image diameters often smaller than one pixel. Several approaches have been proposed to quantify and reduce the peak-locking errors ([3], [4] among others). Approaches based on multi-Δt image acquisition have shown high potential and are considered in the present work. The recent work of Legrand et al. [5] offers a 1-D analytical modelling of the peak-locking errors and allows for measurement correction. However, the method is iterative and computationally expensive to estimate calibration coefficients mentioned in the algorithm. Also, selection of two Δt's is not trivial in presence of turbulence in the flow and Δt values should be adjusted for different levels of turbulence. In the present work, a simple approach based on linear regression of the measured displacements from multiple Δt acquisitions is proposed to correct the peak-locking errors and quantify the uncertainty on the measured displacement.

The methodology considers a stationary process, where the local flow statistics are constant in time. Indicating with u_{true} the local time-average true velocity, the true particle image displacement is proportional to the time interval Δt (provided that Δt is sufficiently small, so that truncation errors can be neglected):

$$\Delta x_{true} = u_{true} \cdot \Delta t \tag{1}$$

In presence of peak locking, the measured particle image displacement is equal to the true displacement (which increases linearly with Δt) plus a measurement error, which is a non-linear function of the sub-pixel particle image displacement. In the proposed approach, the image acquisition is conducted with multiple Δt's, and for each Δt the time-average particle image displacement $\overline{\Delta x}(\Delta t)$ is evaluated. Then, a linear regression is carried out among the measured time-average displacements at different Δt's, yielding a regression displacement $\Delta x_{regr}(\Delta t)$. When the Δt's are selected properly, the latter represents a correction to the measured displacement where systematic errors due to peak locking are removed.

The uncertainty on the time-average particle image displacement at each Δt can be expressed as:

$$U_{\overline{\Delta x}}(\Delta t) = \sqrt{U_p^2(\Delta t) + U_{regr}^2} \tag{2}$$

where, U_p and U_{regr} are the precision uncertainty from randomness in the measurements and regression uncertainty, respectively [6]:

$$U_p(\Delta t) = \frac{t_{C.I.,\nu}}{\sqrt{N}} \sqrt{\frac{1}{N-1} \sum_{i=1}^{N} [\Delta x_i(\Delta t) - \overline{\Delta x}(\Delta t)]^2} \tag{3}$$

$$U_{regr} = t_{C.I.,\nu} \sqrt{\frac{1}{n-2} \sum_{i=1}^{n} [\overline{\Delta x}(\Delta t_i) - \Delta x_{regr}(\Delta t_i)]^2} \tag{4}$$

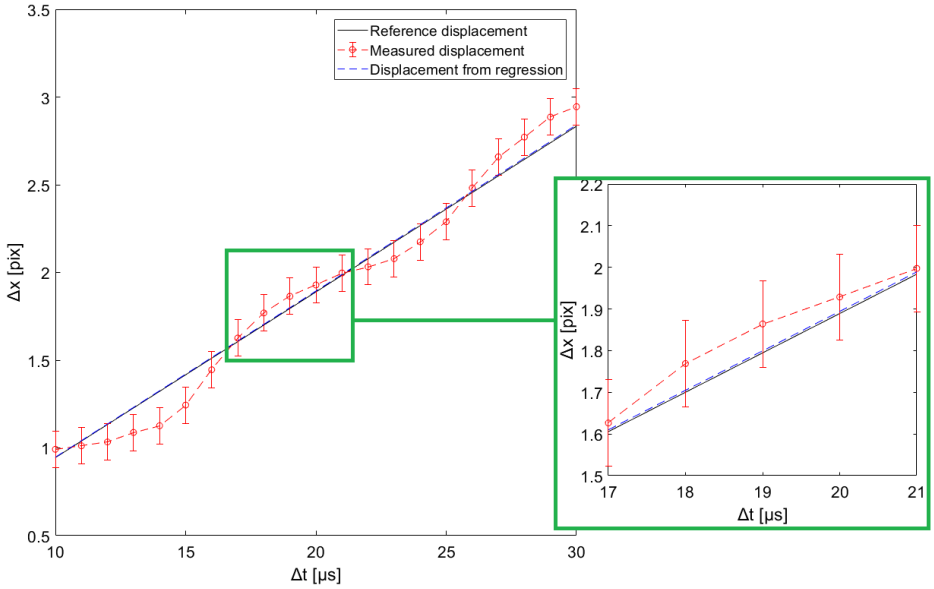


Figure 1: Plots of reference, measured and regression displacements with uncertainty levels on measured displacements for multiple Δt acquisitions

Here, $t_{C.I.,\nu}$ is the t-statistic describing the desired confidence interval, N is the number of instantaneous measured displacements at each Δt acquisitions and n is the number of Δt acquisitions.

The methodology is applied and assessed for PIV experiment with a uniform flow. Following Kislaya and Sciacchitano [7], the measured particle image displacement at time separation Δt is compared with the true or reference particle image displacement (Δx_{ref}). The latter is evaluated from the displacement Δx_{aux} occurring during an auxiliary (much larger) time separation Δt_{aux}, such that peak locking errors can be considered negligible:

$$\Delta x_{ref} = \Delta x_{aux}(\Delta t / \Delta t_{aux}) \tag{5}$$

It is clear from Fig. 1 that the measured displacements vary non-linearly with the time separation Δt, whereas the displacements from the regression analysis follow closely the reference ones. The uncertainty on the measured time-average displacement computed by equation (2) exhibits a coverage of 66.67% at 68% confidence level considering the measurements at different Δt acquisitions, which proves the validity of the multi-Δt for uncertainty quantification.

The work proceeds with the uncertainty quantification of higher order statistics (Reynolds normal and shear stresses), and with an application of the methodology to the wake flow of a NACA0012 wing at 15 degrees angle of attack. Also, the optimum number of acquisitions (Δt's) and the separation between two consecutive Δt's is discussed.

[1] R. J. Adrian and J. Westerweel *Particle Image Velocimetry* (Cambridge University Press, Cambridge, United Kingdom, 2011).

[2] M. Raffel, C. E. Willert, F. Scarano, C. J. Kaehler, S. T. Wereley and J. Kompenhans, *Particle Image Velocimetry - A practical guide* (Springer, 3rd edition, Town, 2018).

[3] K. T. Christensen, "The influence of peak-locking errors on turbulence statistics computed from PIV ensembles," Experiments in Fluids **36**, 484-497 (2004).

[4] M. R. Cholemari, "Modeling and correction of peak-locking in digital PIV," Experiments in Fluids **42**, 913-922 (2007).

[5] M. Legrand,J. Nogueira, R. Jimenez, A. Lecuona and F. De Gregorio, "Full characterization of the peak-locking error by means of orthogonal functions and application to the flow around a helicopter fuselage model," In *19th International Symposium on the Laser and Imaging Techniques to Fluid Mechanics*, page (Publisher, Lisbon, Portugal, 2018).

[6] H. W. Coleman HW and W. G. Steele, *Experimentation, Validation, and Uncertainty Analysis for Engineers* (Hoboken, N.J: Wiley, 3rd edition, 2009).

[7] A. Kislaya and A. Sciacchitano, "Peak-locking error reduction by birefringent optical diffusers," Meas. Sci. Technol. **29**, 025202 (2018).

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

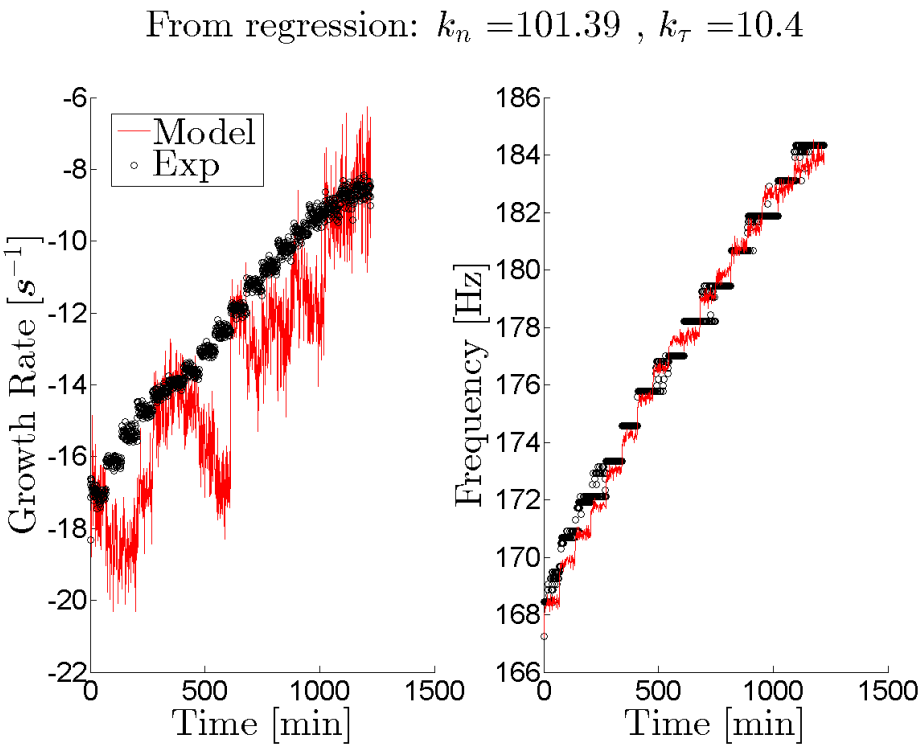
A Bayesian Approach for Predicting Thermoacoustic Oscillations in a Rijke Tube

Francesco Garita, [1] ***Hans Yu*** [1] ***, and Matthew Juniper*** [1]

[1]Department of Engineering, University of Cambridge

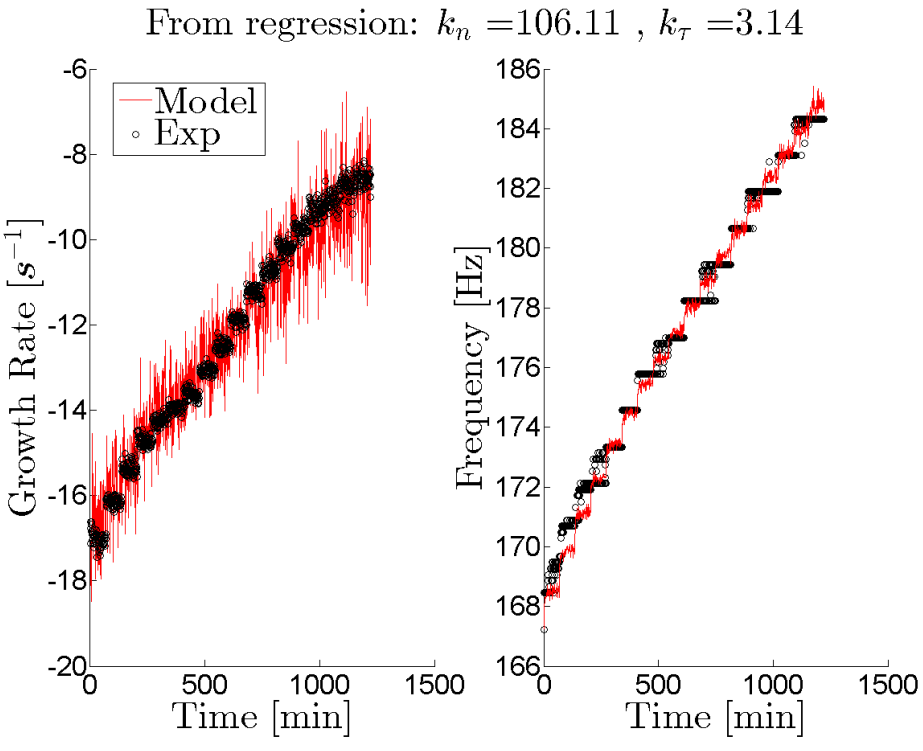
Key words: Thermoacoustics, Data Assimilation, Ensemble Kalman Filter

Predicting and eliminating thermoacoustic oscillations is a significant challenge in gas turbine design. Here we combine a thermoacoustic experiment with a thermoacoustic model and use data assimilation to infer the parameters of the model, rendering it predictive. The experimental apparatus consists of a vertical Rijke tube containing an electric heater (up to 300 Watts). The heater drives a base flow via natural convection, and thermoacoustic oscillations via velocity-driven heat release fluctuations. The growth/decay rates and frequencies of these oscillations are measured every few seconds. There are two models: one for the base flow and one for the acoustics. Both are unsteady. The parameters of the base flow model (Nusselt numbers and pressure loss coefficient) are estimated from many thousand measurements using an ensemble Kalman filter that accounts for both experimental and state and parameter errors. The parameters of the acoustic model are inferred by regression. Figure 1 shows a comparison between experimental observations and model predictions of growth rate and frequency of the thermoacoustic oscillations. As time progresses, the heater power is increased by 10 Watts, approximately every hour. In this case, no information is assimilated into the base flow model, and as a result predictions are fairly poor. On the other hand, results significantly improve when data assimilation is performed, as depicted in Figure 2. This study shows that, with thorough Bayesian inference, a simple model with a few parameters can become a predictive model. The process reveals deficiencies in the model and, when combined with physical insight, shows how to improve it. This work proves the concept for small systems and prepares the ground for complex systems.



(a)

Figure 1: Experimental observations and model predictions of growth rate (left) and frequency (right) of the oscillations, obtained without performing data assimilation in the base flow model



(b)

Figure 2: Experimental observations and model predictions of growth rate (left) and frequency (right) of the oscillations, obtained performing data assimilation in the base flow model

ST3 – Applications II *Session Chair: M. Diez* *Auditorium*	ST4 – Environmental I *Session Chair: O. Knio* *Room B*

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Stochastic calibration of cavitation model parameters for simulations of 3-phase injector internal flows

Alessandro Anderlini,[1] ***Maria Vittoria Salvetti,***[1] ***Antonio Agresta,***[2] ***and Luca Matteucci***[2]

[1]DICI, University of Pisa, Italy – alessandro.anderlini@ing.unipi.it, mv.salvetti@ing.unipi.it
[2]Continental Automotive Italy S.p.A., Italy – Antonio.Agresta@continental-corporation.com, Luca2.Matteucci@continental-corporation.com

Key words: Injector flow, hydraulic flip, cavitation, generalized Polynomial Chaos

This work focuses on numerical simulations of injector internal flows for automotive applications. It has been widely demonstrated in the literature that the vehicle emission level is strictly related to the properties of the spray exiting the injector which, in turn, is deeply influenced by the flow behavior inside the nozzle; the study of this type of flow is thus of practical interest. The flow inside injectors is complex and characterized by the interaction of turbulence and cavitation in channels of very small size and of very complicated geometry (see Fig.1*a* containing a zoom of a realistic injector tip), and this makes simulations and experiments very challenging. Moreover, in realistic applications, the fuel pumped inside the nozzle is injected in a domain filled by a third gaseous phase (typically air). Depending on the injector geometry and the pressure difference between inlet and outlet, indeed, the flow may go into the so-called "hydraulic flip" condition, i.e. a back flow of air from outside the injector to the inlet corner, that replaces cavitation. The presence of hydraulic flip leads to bad spray characteristics and, therefore, it must be avoided in practice.

From a numerical point of view, an accurate modeling of all the previously listed physical phenomena is crucial for the reliability of the simulations. As for the multiphase model, we adopted an approach widely used for this type of flow, i.e. a single set of equations for a fluid whose properties are weighted by the volume fractions of the pure phases, using additional transport equations for the volume fractions of air and vapor, the second of which has a source term containing the Scherr-Sauer cavitation model [2]. This model contains four free-parameters that must be a-priori assigned, and it is reasonable to suppose that their uncertain values may influence the simulation results. Regarding turbulence, we adopted an Unsteady Reynolds-Averaged-Navier-Stokes (URANS) approach; this choice is motivated by the fact that, in an industrial context, the compromise

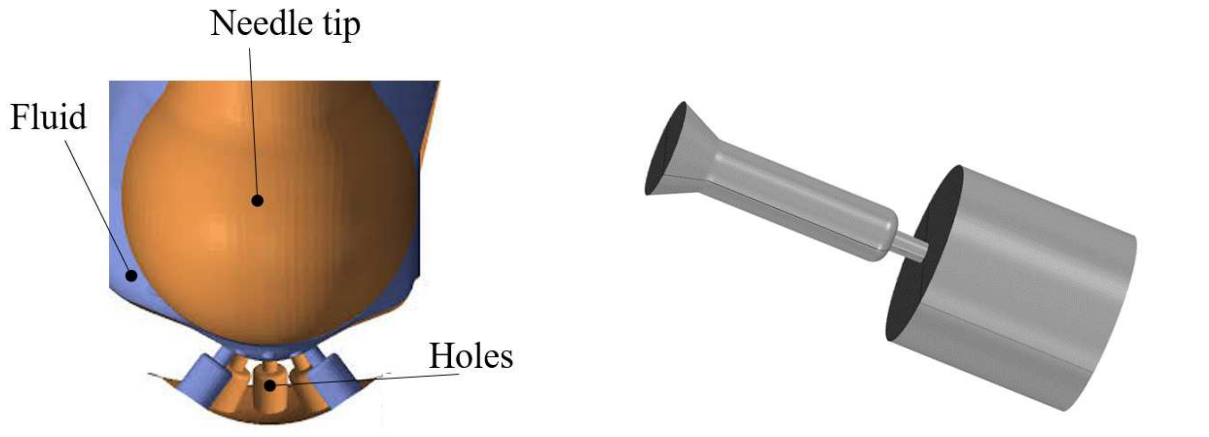


Figure 1: Realistic multi-hole injector (a) and one-hole simplified (b) geometries

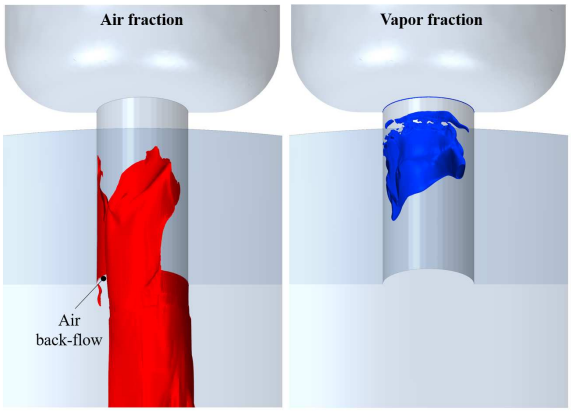


Figure 2: Instantaneous iso-surfaces of air and vapor fraction under unsteady hydraulic flip condition

between accuracy and computational cost can not be avoided, making the "cheap" URANS of practical interest.

In the present work, we want to quantify the impact of the cavitation model parameters on the numerical predictions for a test-case geometry, i.e an axisymmetric real-size channel, for which experimental data are available (see Fig.1*b*). In spite of the simplified geometry, this flow configuration is representative of a real injectors and contains most of the aforementioned flow features. In a previous work [1], through stochastic techniques such as generalized polynomial chaos and stochastic collocation, we showed that two parameters among the four are the most important, so we decided to focus only on these two, namely the vaporization and condensation factors.

Since a fully deterministic analysis would imply prohibitive computational costs also for this simplified axisymmetric problem, we used a stochastic methodology, based on generalized polynomial chaos, in order to obtain continuous response surfaces in the parameter space starting from a limited number of deterministic simulations. The response surfaces has been thus used to carry out a parameter calibration against experimental data. The quantities of interest taken into consideration are the critical cavitation point (CCP), i.e. the value of the outlet pressure at which the flow inside the injector can be considered choked (for a fixed inlet pressure), and the mass-flow-rate (MFR) at the CCP. In more details, we searched for the minimum percent difference of MFR inside a parameter sub-domain in which the absolute difference of CCP was lower than 0.5 bar. An 'optimal' set up of the cavitation model is thus found and is a-posteriori validated in the real 3D geometry showing significant improvements respect to the default parameter set-up; then, we carry out a deeper analysis in hydraulic flip conditions (see Fig.2) in order to give an accurate description of this phenomenon.

Moreover, this set-up has been applied to a complex one-hole injector geometry, as e.g. a sector of a real geometry, containing all the difficulties encountered in real applications, and the results will be included in the final presentation.

[1] A. Anderlini, M.V. Salvetti, A. Agresta and L. Matteucci, "Stochastic sensitivity analysis of numerical simulations of injector internal flows to cavitation modeling parameters," Computers & Fluids **183**, pages 130–147 (2019).

[2] J. Sauer and G.H. Schnerr, "Unsteady cavitating flow - a new cavitation model based on a modified front capturing method and bubble dynamics," In *Proceedings of the 2000 ASME Fluid Engineering Summer Conference*, pages 1073–1079 (2000).

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Comparison of uncertainty propagation methods applied to industrial turbomachinery design with operational, geometrical and manufacturing uncertainties

Dirk Wunsch,[1]***, Charles Hirsch,***[1]***, Simon Abraham,***[2]***, Francesco Contino,***[2]***, Pieterjan Robbe,***[3]***, and Stefan Vandewalle,***[3]

[1]Numeca International, Brussels, Belgium – dirk.wunsch@numeca.be

[2]Vrije Universiteit Brussel (VUB), Brussels, Belgium

[3]KU Leuven, Department of Computer Science, Leuven, Belgium

Key words: Uncertainty Quantification, Probabilistic Collocation, Stepwise Regression, Multi-Level Monte-Carlo, Turbomachinery Design

Significant research and development effort has been dedicated over the past few years to the improvement of uncertainty propagation techniques. A variety of uncertainty propagation methods spanning from advanced sampling methods like Multi-Level Monte-Carlo, over various Stochastic Collocation and Polynomial Chaos based methods to perturbation techniques were significantly advanced. They are now ready to address in the order of ten uncertainties in industrial applications [3].

The current research work compares three of these methods. First, the Non-Intrusive Probabilistic Collocation Method (NIPColM) [5], [7], which relies on Lagrange interpolating polynomials, second, a stepwise regression method for sparse polynomial chaos expansions [1] and third, Multi-Level (MLMC) and Multi-Index Monte-Carlo methods (MIMC) [2].

All three methods are benchmarked against the same industrial scale test case, which is the transonic NASA rotor 37. This test case was defined in its original form with 5 simultaneous operational and geometrical uncertainties [4] and all methods are run on this low dimensional configuration. In a second step, the number of uncertainties is increased to demonstrate the potential of the respective methods. The stepwise regression method is run in a configuration with 27 simultaneous operational and geometrical uncertainties, while 2007 uncertainties are accounted for the MLMC and Multi-Level Quasi Monte-Carlo (MLQMC). These 2007 uncertainties replicate the manufacturing variability of the compressor blade surface.

In order to concentrate on the comparison of the uncertainty propagation methods applied to simultaneous operational, geometrical and manufacturing uncertainties, the exact same simulation chain [6] from geometry modification, mesh generation and flow simulation is used for all three methods. This workflow is fully automated.

The results include a comparison of the NIPColM with the stepwise regression method. This comparison shows that the NIPColM is very efficient in estimating the mean value and standard deviation of various quantities of interest, like the mass flow rate, isentropic efficiency, or total pressure ratio. Table 1 shows that for 5 simultaneous uncertainties the mean value is converged with 11 runs of CFD solver, while the stepwise regression methods requires 20 CFD runs. Predicting higher moments, like skewness and kurtosis, the stepwise regression method shows its potential as seen in table 1. For comparable values of these moments, the NIPColM requires 71 and 341, while 30 and 50 CFD runs are sufficient for the stepwise regression method.

A second advantage of the stepwise regression method is that it does not rely on all samples run to be valid. For example, a sample can be invalid if one of the points to evaluate lies in physically unfeasible regions. In the medium dimensional case with 27 simultaneous uncertainties the NIPColM could predict values only for a

	Stochastic collocation method			Sparse regression method		
	Level 1 (11 runs)	Level 2 (71 runs)	Level 3 (341 runs)	20 runs	30 runs	50 runs
Mean	0.855	0.855	0.855	0.855	0.855	0.855
Variance	2.5×10^{-5}	2.7×10^{-5}	2.6×10^{-5}	2.8×10^{-5}	2.6×10^{-5}	2.6×10^{-5}
Skewness	-5.6×10^{-8}	-7.1×10^{-8}	-7.5×10^{-8}	-5.0×10^{-8}	-6.8×10^{-8}	-7.6×10^{-8}
Kurtosis	1.2×10^{-9}	2.0×10^{-9}	1.9×10^{-9}	2.2×10^{-9}	1.8×10^{-9}	1.9×10^{-9}

Figure 1: Predicted statistical moments for isentropic efficiency

Level 1, while the Level 2 that requires roughly 1000 CFD runs could not predict a result because of around ten failed samples. The stepwise regression method simply omits potentially failed samples and is in this respect more robust.

The MLMC, MLQMC and MIMC methods, which are used in this study, are not competitive in terms of computational cost for low dimensional problems, but this was not expected. Its true potential lies in addressing very high dimensional problems, which are unfeasible for both the NIPColM and stepwise regression method. In addition to comparison with the other two methods, the speed-up resulting from these multi-level or multi-index formulations is given with respect to standard Monte-Carlo methods. On the high dimensional case with 2007 uncertainties it reaches speed-up of a factor of 5 for MLMC and 15 for MLQMC, while significantly larger speed-ups of up to 180 for MLQMC can be expected if the mesh strategy is tuned for the MLMC.

[1] Abraham, S., Raisee, M., Ghorbaniasl, G., Contino, F., and Lacor, C., "A robust and efficient stepwise regression method for building sparse polynomial chaos expansions," J. Comput. Phys., Vol. 332, pp. 461-74 (2017).

[2] Blondeel P, Robbe P, Van hoorickx C, Lombaert C,Vandewalle S., "Multilevel Monte Carlo for uncertainty quantification in structural engineering," arXiv:1808.10680v1 (2018).

[3] Hirsch C, Wunsch D, Szumbarski J, Laniewski-Wolk L, Pons-Prats J, Editors, *Uncertainty Management for Robust Industrial Design in Aeronautics,* Notes on Numerical Fluid Mechanics and Multidisciplinary Design 140, Springer, 2019.

[4] Klostermann S, "UMRIDA test case database with prescribed uncertainties," Notes on Numerical Fluid Mechanics and Multidisciplinary Design 140, pp. 15-32 (2019).

[5] Loeven GJA, Witteveen JAS, Bijl H, "Probabilistic collocation: an efficient non-intrusive approach for arbitrarily distributed parametric uncertainties," Proc. of the 45th AIAA Aerospace Sciences Meeting and Exhibit, AIAA paper 2007-314 (2007).

[6] Numeca, "FINE/Design3D User manual version 13.2," (2019).

[7] Wunsch D, Nigro R, Coussement G, Hirsch C, "Quantification of combined operational and geometrical uncertainties in turbomachinery design," In *Proceedings of the ASME TurboExpo GT2015*, GT2015-43399, Montreal, (2015).

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Sensitivity analysis on a CFD model for prediction of a gear pump leakages

Serena Morselli[1], Cristian Ferrari[1], Nicolò Beccati[1], Pietro Marani[1]

[1]C.N.R. IMAMOTER

Keywords: CFD, gear pump, sensitivity analysis, dynamic mesh

In the field of modern fluid mechanical problems, the evolution of numerical simulation codes and the availability of high-computational-power platforms allowed the spread of Computational Fluid Dynamics (CFD) techniques with the aim of predicting complex fluid-flow phenomena. CFD is frequently used on applications where the object needs a detailed analytic study in spite of the lack of parameters. A typical example is represented by the clearances inside a volumetric pump during his functioning. This uncertainty affects other potential sources of CFD errors like the numerical ones, caused by the discretization of the equations, the modelling ones, due to the description of fluid phenomena and, at lower lever, the user or software errors.

A complex model, that contains many important uncertainties, is presented in this work, which main purpose is a sensitivity analysis on key operating parameters of a gear pump studied with both numerical and experimental techniques. In particular, the study is focused on the calibration of the fixed displacement machine clearances.

Gear pumps represent the majority of the fixed displacement machines used for flow generation in fluid power systems. The internal conformation of this system contains many undetermined variables, due to both the manufacturing techniques and the breaking-in pressure, that strongly affect the pump performance. The 3D CFD model of this type of products is particularly difficult to develop [1], because of the deforming volumes in-between the gears, the structural deformation of the case during the functioning and the moving operating point. These transient modifications of the initial geometry of the pump highly influence the outer mass flow and it must be estimated through mathematical methods.

A classical methodology was used for the purpose by starting from the 3D geometry of the pump. Subsequently, the fluid domain was extracted, the mesh was created and the moving boundary conditions were set. The deformation of the fluid domain was managed by the skewness level of the mesh and deformed with a smoothing and remeshing approach by using a dynamic mesh. The model was solved with a commercial code, and then post processed.

The comparison between experimental and numerical results, united with the widely investigated Richardson Extrapolation (RE) method for the discretization error estimation [2], led to an accurate sensitivity analysis of the clearances.

The future aim of this work is to obtain, thanks to the sensitivity analysis, the pump volumetric efficiency as a function of the leakages between the machine gears and case, which highly affect the numerical results. A future purpose is to provide the characteristic curves of the gear pump depending on the breaking-in pressure.

The results obtained is a sensitivity analysis that is able to compare the gap between the gears, at different mesh level of accuracy, with the experimental data in order to evaluate the influence of the analyzed parameters on the numerical results.

[1] S. Mancò, N. Nervegna, "Simulation on an external gear pump and experimental verification" In *Proceedings of the JHPS International Symposium on Fluid Power*, 139-152, (Tokio, Japan,1989).

[2] Celik, I. B., Ghia, U., Roache, P.J. Freitas, C. J., Coleman, Raad, P. E., "*Procedure for Estimation and Reporting of Uncertainty Due to Discretization in CFD Applications*," ASME J. Fluids Eng., **130**(7), (2008).

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Geometric Uncertainty Quantification of a Film Cooled Gas Turbine Blade

Andrea Gamannossi,[1] ***and Alberto Amerini,***[2] ***and Lorenzo Mazzei,***[2] ***and Matteo Poggiali,***[2] ***and Antonio Andreini,***[2]

[1]DIA, University of Parma, Italy – andrea.gamannossi@studenti.unipr.it

[2]DIEF, University of Florence, Italy – alberto.amerini@stud.unifi.it

Key words: Uncertainty quantification, Computational Fluid Dynamics, Film Cooling, Gas Turbine, Blade

CFD is nowadays a must-have tool for the design phase of the gas turbine components. However, the results are often presented in a deterministic way, with a "single-line" plot and a certain solution. Experimentalists are required to insert a confidence interval with its relative error within the results, showing how the measurements can be affected by all the source of errors arising from the experiment itself. Instead, most of numerical studies do not include all the source of error arising from the simulation: starting from the boundary conditions, passing by the numerical model and the discretization error. Uncertainty quantification is the field studying these effects and how an input uncertain variable propagates through the simulations and affects the result. This work presents an uncertainty quantification approach applied to CFD: an industrial prismatic gas turbine blade with film cooling on the suction side only and standard shaped holes configuration. The blade is made by additive manufacturing (AM) process and the hole are then manufactured by electric discharge machining (EDM) process. Both manufacturing processes feature geometric uncertainty on the final shape: the AM is more related to the shape itself while EDM is related to the difference between the nominal and the final geometry. The blade was part of an initial experimental test campaign which revealed many output results in terms of adiabatic effectiveness and heat transfer. CFD analyses are conducted on this profile; a bi-fluid approach to measure the effectiveness is adopted: air for the main flow and CO2/SF6 for the coolant flow. Regarding uncertainty quantification an analysis is carried out varying the hole dimension and position with respect to the blade, including the fillet radius. Input variation are selected based on data available from an industrial partner. Polynomial-chaos approach is used in conjunction with the probabilistic collocation method for both analyses. With a 2nd order polynomial approximation the total number of simulation required is 8. This method is able to reproduce what the normal Montecarlo analysis does (with more than a thousand of simulations) with an optimum grade of accuracy. For the uncertainty quantification framework Dakota [1] is used. RANS approach with k—w SST turbulence model is adopted for the simulations. Results show the confidence interval for both analyses and prove how the position tolerance of the blade, as well as the hole dimension, is extremely important for the effectiveness. In particular, when dealing with additive manufacturing and EDM processes.

[1] Adams, B.M., Bauman, L.E., Bohnhoff, W.J., Dalbey, K.R., Ebeida, M.S., Eddy, J.P., Eldred, M.S., Hough, P.D., Hu, K.T., Jakeman, J.D., Stephens, J.A., Swiler, L.P., Vigil, D.M., and Wildey, T.M., "Dakota, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 6.9 User's Manual,," Sandia Technical Report SAND2014-4633, November 2018.

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Towards a Consistent Stochastic Modeling of Oceanic Dynamics

L. Li,[1,2] ***W. Bauer,***[2] ***and E. Mémin,***[2]

[1]Université Rennes I France

[2]Fluminance Group Inria Rennes France

Key words: Stochastic Modeling, Oceanic Dynamics, Ensemble Forecasting, Uncertainty Quantification

For several years, there is a growing interest in geophysical sciences such as oceanography or meteorology to incorporate random flows. These models aims at representing processes such as unknown physical forcing or uncertainty coming either from a large–scale approximate description or from the nature of discrete numerical schemes used. The modeling of these uncertainties along time is paramount in both uncertainty quantification and ensemble forecasting.

In this work, we propose to follow a recent derivation [1, 2] that comes from a decomposition of the Lagrangian fluid particle displacement into a smooth component and a time–uncorrelated uncertainty

$$\mathrm{d}\mathbf{X}_t = \mathbf{u}(\mathbf{X}_t)\mathrm{d}t + \boldsymbol{\sigma}(\mathbf{X}_t)\mathrm{d}\mathbf{B}_t. \tag{1}$$

A random passive tracer transported along such a stochastic flow (1) is then found through a generalized Itô formula,

$$\mathrm{D}_t\theta \triangleq \mathrm{d}_t\theta + \Big((\mathbf{u} - \frac{1}{2}\nabla\cdot\mathbf{a})\mathrm{d}t + \boldsymbol{\sigma}\mathrm{d}\mathbf{B}_t\Big)\cdot\nabla\theta - \frac{1}{2}\nabla\cdot(\mathbf{a}\nabla\theta)\mathrm{d}t = 0, \tag{2}$$

in which a variance operator $\mathbf{a}$ of the random field $\boldsymbol{\sigma}\mathrm{d}\mathbf{B}_t$ is involved. The energy of such a random tracer is shown to be well conserved along time for each realization, characterizing hence the essence of a transport. Such stochastic transport operator can then be used as a fundamental tool to derive stochastic representation of fluid flow dynamics [1, 2].

Such a stochastic principle, termed modeling under location uncertainty, has been tested for the numerical simulation of the wind-driven circulation in a shallow ocean basin, which is widely used to characterize the role of mesoscale eddies and their effect on mean circulation. This kind of model describes the incompressible barotropic flows by assuming the hydrostatic balance, the beta–plane approximation, geostrophic balance and horizontal eddy viscosity parametrization. The governing equations under our stochastic framework can be written as

$$\mathrm{D}_t q = S_1(\nabla\mathbf{u})\mathrm{d}t + S_2(\nabla\mathbf{u})\mathrm{d}\mathbf{B}_t + D + F, \tag{3}$$

in which the potential vorticity (PV) q is driven by a symmetric double-gyre forcing F, a viscous dissipation D and some source processes S_1, S_2 due to asymmetry of the stochastic advections in (2). In the absence of dissipation and forcing, this random system (3) have a consistent set of energetics for each realization.

The numerical assement shows that the proposed random model (LU), compared to a classical large eddy simulation (LES) approach, can capture better on a coarse mesh the correct four–gyre time–averaged circulation structure, as predicted by a direct numerical simulation (DNS) at a much finer resolution (cf. figure 1).

Then the performance of our random model has been evaluated and analyzed in terms of uncertainty quantification and ensemble forecasting. Some common criterions (e.g. Talagrand histogram) are used to quantify

the prediction accuracy, compared to observations provided by DNS (cf. figure 2). We will otherwise show that the proposed random model, under both homogeneous and heterogeneous uncertainty, is more efficient than a deterministic model with a pertubation of the initial condition. This ability is in particular essential for data assimilation applications.

In this study we show also the influence of a structure-preserving numerical scheme on the performances of both time–statistics and ensemble forecasting.

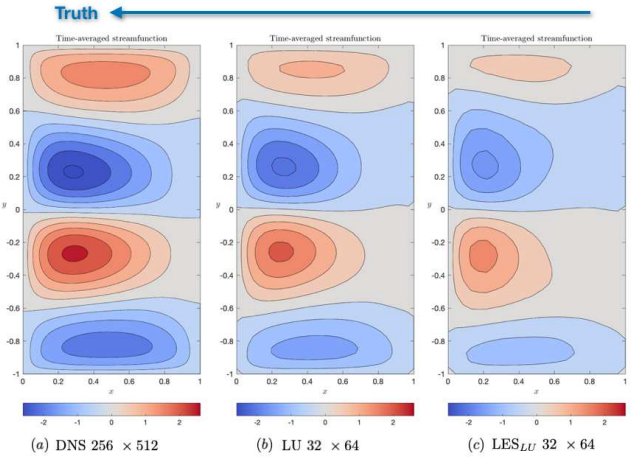


Figure 1: Illustration of time–averaged streamfunction contours : (a) DNS results at a fine resolution; (b) LU results at a coarse resolution; (c) LES results at the same resolution as in LU, but by removing the time-uncorrelated term in (2).

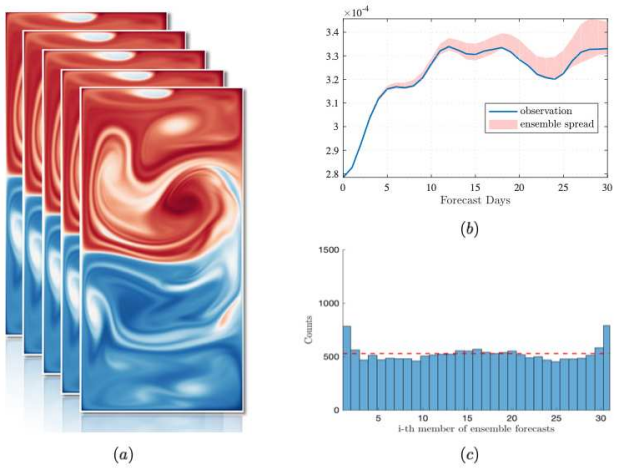


Figure 2: Illustration of a reliable ensemble forecasting prediction : (a) Ensemble of instantaneous PV field; (b) Time history of locally averaged PV field (observed v.s. ensemble spread); (c) Rank histrogram of instantaneous PV field.

[1] E. Mémin (2014), “Fluid flow dynamics under location uncertainty," Geophysical and Astrophysical Fluid Dynamics **108**, 119-146.

[2] V. Resseguier, E. Mémin and B. Chapron (2017), “Geophysical flows under location uncertainty, Part I: random transport and general models," Geophysical and Astrophysical Fluid Dynamics **111**, 149-176.

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Bayesian Inference and Markov Chain Monte Carlo Sampling for Lagrangian Particle Tracking in the Ocean

Samah El Mohtar, Omar Knio, and Ibrahim Hoteit,

King Abdullah University of Science and Technology, Thuwal 23955, Saudi Arabia –
samah.mohtar@kaust.edu.sa, omar.knio@kaust.edu.sa, ibrahim.hoteit@kaust.edu.sa

Key words: Uncertainty quantification, Bayesian inference, MCMC, Lagrangian particle tracking

Estimation of Lagrangian particle tracking (LPT) model parameters is challenging due to the irreversible nature of processes affecting the particles. In the ocean, several methods have been proposed to tackle this problem, but each has its limitations. In this work, we present a generic method that employs Bayesian inference and Markov chain Monte Carlo (MCMC) sampling to construct the probability distributions of parameters of interest. The forward model used within the MCMC machinery enables the use of existing application-specific modules built on top of LPT models. Furthermore, various types of observations can be considered depending on available data. This framework allows the method to serve different applications of LPT in the ocean. The method has been tested using a simple LPT advection-diffusion model in a double-gyre synthetic flow field. Different data types were tested, ranging from the simple location of particles, to measurements of concentration and contours of spills. Inference of the location of the source, time and duration of release is presented as a probability distribution that quantifies uncertainties and correlations between parameters.

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Forward and Backward Lagrangian Particle Tracking in Ensemble Flow Fields

Samah El Mohtar,[1] ***Ibrahim Hoteit,***[1] ***Omar Knio,***[1] ***Leila Issa,***[2] ***and Issam Lakkis,***[3]

[1]King Abdullah University of Science and Technology, Thuwal 23955, Saudi Arabia – samah.mohtar@kaust.edu.sa, ibrahim.hoteit@kaust.edu.sa, omar.knio@kaust.edu.sa

[2]Department of Computer Science and Mathematics, Lebanese American University, Beirut, Lebanon – leila.issa@lau.edu.lb

[3]Department of Mechanical Engineering, American University of Beirut, Beirut, Lebanon – il01@aub.edu.lb

Key words: Stochastic flow fields, Red sea, Lagrangian tracking

Ocean ensemble data assimilation systems generate ensembles of independent velocity field realizations after every assimilation cycle. Lagrangian tracking of passive tracers within such a framework is challenging due to the exponential growth in the number of particles that arises from describing the behavior of velocity over time as a set of possible combinations of the different realizations. This contribution addresses the problem of efficiently advecting particles, forward and backward in time, in ensemble flow fields, whose statistics are prescribed by an underlying assimilated ensemble. To this end, a parallel adaptive binning procedure that conserves the zeroth, first and second moments of probability is introduced to control the growth in the number of particles. The adaptive binning process offers a tradeoff between speed and accuracy by limiting the number of particles to a desired maximum. To validate the proposed method, we conducted various forward and backward particles tracking experiments within a realistic high-resolution ensemble assimilation setting of the Red Sea, focusing on the effect of the maximum number of particles, the time step, the variance of the ensemble, the travel time, the source location, and history of transport. We also demonstrate the efficiency of the method for possibly identifying (backward in time) a moving target from observed released materials.

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Bayesian Convolutional Neural Networks as a Tool to Detect Discharges of Pollutants to Marine Waters through Time Series Classification

Kristian Gundersen[1]***, Guttorm Alendal***[2]***, Anna Oleynik***[3]

[1]Department of Mathematics, University of Bergen, Norway – Kristian.Gundersen@uib.no

[2]University of Bergen, Norway – Guttorm.Alendal@uib.no

[3]University of Bergen, Norway – Anna.Oleynik@uib.no

Key words: Deep Learning, Uncertainty quantification, Bayesian Convolutional Neural Network, Time Series Classification

The world's oceans are already under tremendous stress from climate change, acidification and other human activities [1]. In fact, UN has declared 2021-2030 as the decade for marine science[1]. Monitoring the marine environment is a part of ecosystem based Marine Spatial Planning [2] and Life under Water is one of UN's Sustainable Development Goals. Here we study the use of Bayesian Convolutional Neural Networks for classification of time series from marine monitoring programs in order to detect discharges of pollutants in the ocean. These discharges can in general be composed of a mixture of chemical, biological and radioactive matters, and a real challenge is to distinguish a signal of a discharge in noisy time series. The problem is even more complicated if the pollutants are naturally present in the environment and if a large area has to be monitored. Monitoring programs associated with offshore geological storage projects are in this category. Hence, there is a need for data analysis methods that can detect a weak signal in noisy time series in a probabilistic manner, as input to making decisions for mobilising more comprehensive and costly surveys.

The key concept of Bayesian Neural Network (BNN) is to introduce a prior distribution over the weights of the neural network and, thus, add stochasticity in the framework. In the time-series classification settings, the outcome of a traditional neural network is a probability (point-estimate) of the class that the time series belongs to. The outcome of a BNN is a probability distribution that gives information not only about the class, but also about the uncertainties in the predictive power of the model. Despite these uncertainties can be expressed analytically [3], the practical use of the BNNs may fail due to large computational costs. Gal and Ghahramani [4] have recently proposed an approach addressing this issue. The main idea is to use dropout as a variational inference approximation; a method to estimate posteriori densities for Bayesian models. The benefits of variational inference over more traditional methods, such as Markov Chain Monte Carlo (MCMC) method, are better scalability to large datasets and an easier implementation [5]. Instead of using sampling, an optimization problem can be formulated. It can be shown that the simple approach of using Bernoulli dropout during both training and testing stages can be viewed as an approximative variational inference technique [4]. During prediction, we simply do n forward passes for each time series in the test data set to generate empirical probability distributions of which class the time series belongs to.

Here we present a solution to a classification problem applied to the detection of CO_2 seeps to the marine environment from a subsurface reservoir at the Scottish Goldeneye area. We use Bayesian Convolutional Neural Network (BCNN) [6] for time series classification, motivated by their ability to automatically generate features. Some of the most promising advances in time series classification the last few year have been with different

[1]https://en.unesco.org/ocean-decade

variations of convolutional neural networks [7]. We use time series produced by a General Circulation Model (GCM) with additional tracers for training, validating, and testing the network. All data is standardized and labeled as "leak" or "no-leak".

We argue that the use of modeling data in this case is a necessity since the data corresponding to the leak scenarios is difficult and, in some cases, impossible to obtain. Moreover, and this is our main argument, the trained deep neural network can be used in a transfer learning setting [8]. That is, we can use a pre-trained neural network on the model data, fix the parameter weights in the first few layers, and then train the network with the limited real data as input. The conjecture is that the first few layers adequately represent the core feature characteristics of the time series, and thus significantly reducing the need of in-situ data.

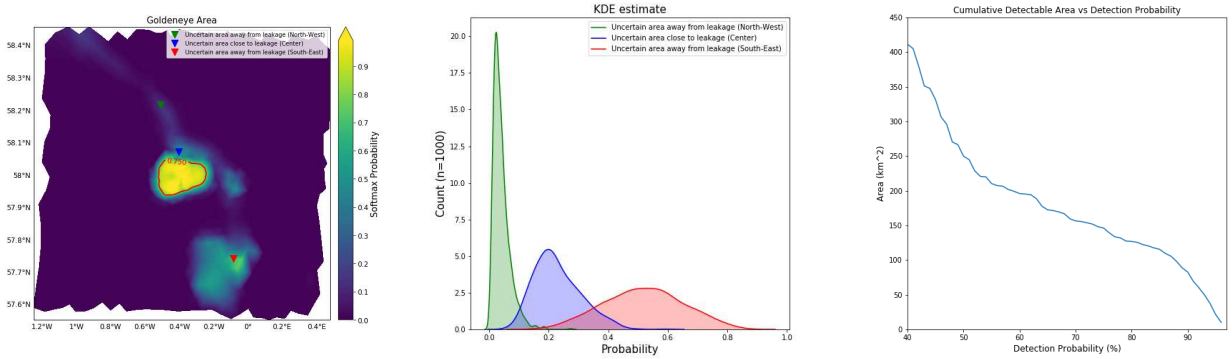


Figure 1: Left Panel: *Plot of the predictive mean of the leak class for the Goldeneye area for a CO_2 pollutant released at the center with a flux of 300T per/day CO_2. The red line enclosure indicates an area where the seepage is detected with a predictive mean above 75 %.* ***Middle Panel:*** *KDE-estimate for the three different locations visualized on the predictive mean plot.* ***Right Panel:*** *Shows the cumulative area vs the probability of detection.*

We trained the network based on four 3D simulations, three leak and one no-leak scenario. Each of four simulations contain 1736×23 time series of CO_2 concentrations over approximately 100km $\times$ 100km area with 23 vertical layers. In all leak scenarios the leakage was placed at the seafloor in the center of the two dimensional domain. All the data, except the bottom layer, was used for training and validation, while the time series at the bottom layer was used for testing. Figure 1(Left panel) shows the predictive mean of the ensemble of the 1000 forward realizations for each of the 1736 time series at the bottom layer. The empirical standard deviation is used as a measure of the uncertainty in the predictions, see Figure 1(Middle panel). Figure 1(Right panel) shows trade - off between the footprint size and the confidence in the prediction. The uncertainty estimate obtained from BCNN would allow for more informative decisions when designing monitoring program.

References

[1] Benjamin S Halpern, Catherine Longo, Darren Hardy, Karen L McLeod, Jameal F Samhouri, Steven K Katona, Kristin Kleisner, Sarah E Lester, Jennifer O'Leary, Marla Ranelletti, Andrew A Rosenberg, Courtney Scarborough, Elizabeth R Selig, Benjamin D Best, Daniel R Brumbaugh, F Stuart Chapin, Larry B Crowder, Kendra L Daly, Scott C Doney, Cristiane Elfes, Michael J Fogarty, Steven D Gaines, Kelsey I Jacobsen, Leah Bunce Karrer, Heather M Leslie, Elizabeth Neeley, Daniel Pauly, Stephen Polasky, Bud Ris, Kevin St Martin, Gregory S Stone, U Rashid Sumaila, and Dirk Zeller. An index to assess the health and benefits of the global ocean. *Nature*, 488(7413):615–620, August 2012.

[2] Elianny Domínguez-Tejo, Graciela Metternicht, Emma Johnston, and Luke Hedge. Marine Spatial Planning advancing the Ecosystem-Based Approach to coastal zone management: A review. *Marine Policy*, 72:115–130, October 2016.

[3] David JC MacKay. A practical Bayesian framework for backpropagation networks. *Neural computation*, 4(3):448–472, 1992.

[4] Yarin Gal and Zoubin Ghahramani. Dropout as a Bayesian approximation: Representing model uncertainty in deep learning. In *international conference on machine learning*, pages 1050–1059, 2016.

[5] David M Blei, Alp Kucukelbir, and Jon D McAuliffe. Variational inference: A review for statisticians. *Journal of the American Statistical Association*, 112(518):859–877, 2017.

[6] Yarin Gal and Zoubin Ghahramani. Bayesian convolutional neural networks with Bernoulli approximate variational inference. *arXiv preprint arXiv:1506.02158*, 2015.

[7] Hassan Ismail Fawaz, Germain Forestier, Jonathan Weber, Lhassane Idoumghar, and Pierre-Alain Muller. Deep learning for time series classification: a review. *Data Mining and Knowledge Discovery*, pages 1–47, 2019.

[8] Sinno Jialin Pan and Qiang Yang. A survey on transfer learning. *IEEE Transactions on knowledge and data engineering*, 22(10):1345–1359, 2009.

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Emulating environmental modeling systems in presence of uncertainties: overview and challenges

***Mélanie C. Rochoux*[1], *Aurélien Costes*[1,2], *Ronan Paugam*[1], *Géraldine Rea*[1], *Laëtitia Thouron*[1], *Andrea Trucchia*[3], *Cong Zhang*[4], *Thomas Jaravel*[1], *Christine Lac*[2], *Valéry Masson*[2], *Arnaud Trouvé*[4], *Olivier Vermorel*[5], *Didier Lucor*[6]**

[1]CECI, Université de Toulouse, CNRS, CERFACS, Toulouse, France – melanie.rochoux@cerfacs.fr, geraldine.rea@polytechnique.edu, laetitia.thouron@cerfacs.fr, ronan.paugam@cerfacs.fr, thomas.jaravel@cerfacs.fr

[2]CNRM, Université de Toulouse, CNRS, Météo-France, Toulouse, France – aurelien.costes@meteo.fr, christine.lac@meteo.fr, valery.masson@meteo.fr

[3]BCAM, Basque Center for Applied Mathematics, Bilbao, Spain – atrucchia@bcamath.org

[4]University of Maryland, Department of Fire Protection Engineering, Maryland, USA – cong0129@umd.edu, atrouve@umd.edu

[5]CERFACS, Toulouse, France – olivier.vermorel@cerfacs.fr

[6]LIMSI, CNRS, Université Paris-Saclay, Orsay, France – didier.lucor@limsi.fr

Key words: Emulators, air quality, wildfire, front dynamics, plume dynamics, uncertainty quantification, sensitivity analysis, data assimilation

Accurately predicting the evolution of environmental systems remains a challenge for risk assessment. Large eddy simulation has been identified as a promising tool to tackle this challenge. At the scale of micro-meteorology, simulating the land surface processes and the flow dynamics is a multi-physics multi-scale problem due to the complex flow dynamics induced by land surface heterogeneity, time-transient meteorological conditions and surface/atmosphere interactions. We thus need to analyze the impact of both modeling uncertainties and aleatory uncertainties on the simulated quantities of interest due to modeling choices and the internal variability of the target environmental systems. Since large eddy simulations are computationally expensive, we have access to a limited number of simulations. To overcome this issue, we investigate the use of emulators to quantify model output uncertainties and analyze model output sensitivity with respect to inlet flow conditions and physical model parameters. Fast emulators based on generalized polynomial chaos expansion and gaussian process [1, 2] are trained to approximate probability distributions and corresponding statistical moments as well as Sobol' sensitivity indices. The use of sparse basis is investigated [3]. Specific measures can be used to track flow structures in terms of shape and topology [2]. These emulators can be integrated in ensemble-based data assimilation system to accelerate the inverse modeling procedure [4]. Our emulation strategy will be illustrated for two environmental applications using field-scale experimental data sets: wildland fire behavior modeling [5, 6] on the one hand, urban outdoor air quality modeling [7] on the other hand.

[1] P.T. Roy, N. El Moçayd, S. Ricci, J-C. Jouhaud, N. Goutal, M. De Lozzo and M.C. Rochoux: Comparison of polynomial chaos and Gaussian process surrogates for uncertainty quantification and correlation estimation of spatially distributed open-channel steady flows Stochastic Environmental Research and Risk Assessment **32**, 1723-1741 (2018).

[2] M.C. Rochoux, A. Collin, C. Zhang, A. Trouvé, D. Lucor and P. Moireau: Front shape similarity measure for shape-oriented sensitivity analysis and data assimilation for Eikonal equation, ESAIM Proceedings and Surveys **63**, 215-236 (2018).

[3] A. Trucchia, V. Egorova, G. Pagnini and M.C. Rochoux: On the merits of sparse surrogates for global sensitivity analysis of multi-scale nonlinear problems: Application to turbulence and fire-spotting model in wildland fire simulators Communications in Nonlinear Science and Numerical Simulation **73**, 120-145 (2019).

[4] M.C. Rochoux, S. Ricci, D. Lucor, B. Cuenot and A. Trouvé: Towards predictive data-driven simulations of wildfire spread - Part I: Reduced-cost Ensemble Kalman Filter based on a Polynomial Chaos surrogate model for parameter estimation, Natural Hazards and Earth System Science **14**, 2951-2973 (2014).

[5] A. Costes, C. Lac, V. Masson and M.C. Rochoux: "Bi-directional fire-atmosphere coupling for on-demand simulations in case of forest fires," In *Proceedings of the VIII International Conference on Forest Fire Research*, Advances in Forest Fire Research, Imprensa da Universidade de Coimbra, Viegas, Domingo Xavier (ed.), Coimbra, Portugal (2018).

[6] R. Paugam, M.C. Rochoux, N. Cazard, C. Lapeyre, W. Mell and M. Wooster: "Computing high resolution fire behavior metrics from prescribed burn using handheld airborne thermal camera observations," In *Proceedings of the EGU General Assembly*, EGU2019-13804, Vienna, Austria (2019).

[7] G. Rea, M.C. Rochoux, L. Thouron, F. Auguste, T. Jaravel and O. Vermorel: Large eddy simulations of micro-scale meteorology and pollutant dispersion: model intercomparison for the MUST experiment In preparation for submission to Atmospheric and Environment.

Keynote Lecture - V. Heuveline - Uncertainty quantification with application to medical engineering: towards a more reliable medicine?
Session Chair: O. Ernst
Auditorium

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Uncertainty quantification with application to medical engineering: towards a more reliable medicine?

Vincent Heuveline

Universität Heidelberg, Germany – vincent.heuveline@uni-heidelberg.de

Key words: Uncertainty Quantification, Medical Engineering

In the last decades, the understanding of medical processes has been improved, which deals as a foundation of applying mathematical modeling techniques in this application field. Numerical models provide the means of predicting biomechanical behavior and processes, which is fundamental for improving current medical treatment approaches. Medical applications benefit from numerical modeling including medical device design, heart function simulation, disease diagnosis, tumor prediction, amongst others. However, many modeling approaches so far are deterministic. Especially in the life sciences, the occurring parameters can not always be assumed to be known accurately due to complex geometry, unknown boundary conditions, measurement as well as modeling errors. Taking such uncertainties into account by stochastic models results in a parametrization by a set of independent random variables. This leads to a blown up system size requiring even more scalable numerical schemes in order to take advantage of the capabilities of high performance computers (HPCs). As the available compute power on HPCs is still increasing exponentially, the underlying biological mechanisms can be simulated with increasing accuracy. This talk discusses the impact of emerging uncertainty quantification (UQ) modeling for medical applications. The link between contemporary deterministic approaches and intrusive schemes based on stochastic Galerkin methods using Polynomial Chaos will be established. A simplified performance model based on the computational intensity is presented and allows to evaluate the quality and the efficiency of UQ approaches in the context of medicine. Numerical experiments assuming complex flow problems arising in medical processes are presented.

ST5– Biological flows

Session Chair: V. Heuveline

Auditorium

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Semi-intrusive uncertainty quantification analysis with a surrogate model for in-stent restenosis 2D model

***Dongwei Ye*[1], *Anna Nikishova*[1], *Lourens Veen*[2], *Pavel Zun*[1,3] *and Alfons G. Hoekstra*[1,3]**

[1]Computational Science Lab, Institute for Informatics, University of Amsterdam, The Netherlands – {D.Ye, A.Nikishova, A.G.Hoekstra}@uva.nl

[2]Netherlands eScience Center, Amsterdam, The Netherlands – L.Veen@esciencecenter.nl

[3]ITMO University, Saint Petersburg, Russia – Pavel.Zun@gmail.com

Key words: Uncertainty Quantification, Surrogate modelling, Gaussian process regression, Multiscale simulation, Semi-intrusive method

The two-dimensional in-stent restenosis model (ISR2D) is a multi-scale simulation of the post-stenting healing response of a coronary artery [1, 2]. The model is composed of three submodels: a model to calculate the initial geometry of vessel wall after stenting, an agent-based model to compute the proliferation of smooth muscle cells and endothelium recovery, and a Lattice-Boltzmann model to simulate the blood flow through the artery in changing geometries, reflecting the developing restenosis. An uncertainty quantification analysis for the ISR2D model is performed based on the semi-intrusive multi-scale algorithm proposed by [3, 4]. The algorithm allows the replacement of the most expensive part of the multiscale ISR2D simulation which is the blood flow model, with a surrogate model. In this work, the surrogate model is based on a Gaussian process. The vessel wall geometry features and blood flow velocity at the inlet are used as the input for the Gaussian process. Results of uncertainty estimation of the neointimal area are well approximated compared to the estimation from the quasi Monte-Carlo algorithm [5]. Result of sensitivity analysis shows that the overall variance and partial variances are overestimated however the correct order of the partial variances is preserved. Additionally, both accuracy and computational efficiency of the result outperformed previous results using nearest-neighborhood interpolation [4]. The result shows that the semi-intrusive method with the surrogate is a valid method to perform uncertainty quantification in an efficient way for the ISR2D model. The implication for the more realistic 3D verison of the ISR model [6] will be discussed.

[1] H. Tahir, A. G. Hoekstra, E. Lorenz, P. V. Lawford, D. R. Hose, J. Gunn, D. J. W. Evans, "Multi-scale simulations of the dynamics of in-stent resteno- sis: impact of stent deployment and design", Interface Focus **1** (3) (2011)

[2] H. Tahir, C. Bona-Casas, A. G. Hoekstra, "Modelling the effect of a functional endothelium on the development of in-stent restenosis", PLoS One **8** (6) (2013)

[3] A. Nikishova, A. G. Hoekstra, "Semi-intrusive uncertainty quantification for multiscale models", arXiv:1806.09341

[4] A. Nikishova, L. Veen, P. Zun, A. G. Hoekstra, "Semi-intrusive multiscale metamodelling uncertainty quantification with application to a model of in-stent restenosis", Phil. Trans R. Soc. A **377** (2142) (2019

[5] A. Nikishova, L. Veen, P. Zun, A. G. Hoekstra, " Uncertainty quantification of a multiscale model for in-stent restenosis", Cardiovascular Engineering and Technology **9** (4) (2018)

[6] P. S. Zun, T. Anikina, A. Svitenkov, A. G. Hoekstra, "A Comparison of Fully-Coupled 3D In-Stent Restenosis Simulations to In-vivo Data", Frontiers in Physiology **8** (2017) 284

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Sensitivity analysis of an electrophysiology model for the left heart

Giulio Del Corso,[1]***, Francesco Viola,***[2] ***and Roberto Verzicco,***[1,2,3]

[1]GSSI - Gran Sasso Science Institute, Italy – giulio.delcorso@gssi.it

[2]PoF group, University of Twente, The Netherlands – f.viola@utwente.nl

[3]Department of Industrial Engineering, University of Roma Tor Vergata, Italy – verzicco@uniroma2.it

Key words: Uncertainty quantification, Sensitivity Analysis, Fluid Dynamics, Electrophysiology, Heart Model

Modeling the human heart functioning is a very challenging task since it needs to account for the deforming geometries, such as the opening and closing of the heart valves and the periodic expansion and contraction of the ventricles and atria. This synchronized motion of the heart tissues generates a pulsatile and turbulent hemodynamics within the heart chambers and a strong fluid-structure interaction (FSI). Furthermore, ventricles and atria can not be modeled as passive tissues (as done for blood vessels) due to the active contraction of the heart muscle fibers that provides the cardiac rhythmicity. Thus, an electrophysiology model solving for the active potential propagation in the heart and the consequent muscle contraction has to be included in the FSI [1]. This involved multi-physics model also requires many input parameters (elastic properties of the tissue, electrical conductivities, anatomincal details), which can vary among different individuals and that can be hardly measured *in-vivo*, thus calling for an uncertainty quantification approach.

Due to the complexity of the full fluid-structure-electrophysiology problem we focus here on the electrophysiology model with the aim of studying the model sensitivity with respect to the input parameters and the propagation of their uncertainties. The electrophysiology solver is based on the so-called *bidomain* model that consists of a diffusion-reaction equation for the muscular transmembrane potential (the *action potential*), which is coupled with a cell-model representing the ion fluxes through the ion channels placed at the myocytes membrane [2, 3]. Here, we consider two different cellular models, the FitzHugh-Nagumo model [5] for the atrium and the Ten Tusscher-Panfilov [4] for the ventricle. The solution of the system provides the action potential propagation over the myocardium and the subsequent muscle contraction, as shown in Figure 1 for the case of a left heart with an electrical stimulus propagating in the ventricle (a-c) and atrium (d,e). The model, however, is strictly dependent on the input parameters such as the anisotropic conductivity tensors of the media and the specific membrane capacitance [1], which depend on the tissue microstructure and fibers orientation as well as age, sex and genetic of each person. Therefore we study here the the propagation of uncertainties on the electrical parameters of the electrophysiology equations.

Firstly, we study the sensitivity of the electrophysiology on the input parameters including the conductivity tensors using a Sobol' method based on ANOVA-HDMR decomposition [6, 7, 8] and the FAST (Fourier amplitude sensitivity test) method [6, 9]. The resulting total sensitivity indices characterize to what parameters the muscular activation of the ventricular myocardium is most sensitive. Henceforth, the forward propagation of uncertainty on these parameters is investigated using an adaptive polynomial chaos expansion [10, 11]. This work is a starting point to study how these uncertainties propagate, not only in the electrophysiology model, but also through the multi-physics heart model [1] including hemodynamics and structure deformation. Indeed, a modification on the muscular activation of the ventricle, due to an uncertainty on the input electrical parameter, can potentially alter the hemodynamics and modify the heart pumping efficiency as well as the hydrodynamics loads experienced by the cardiac tissues.

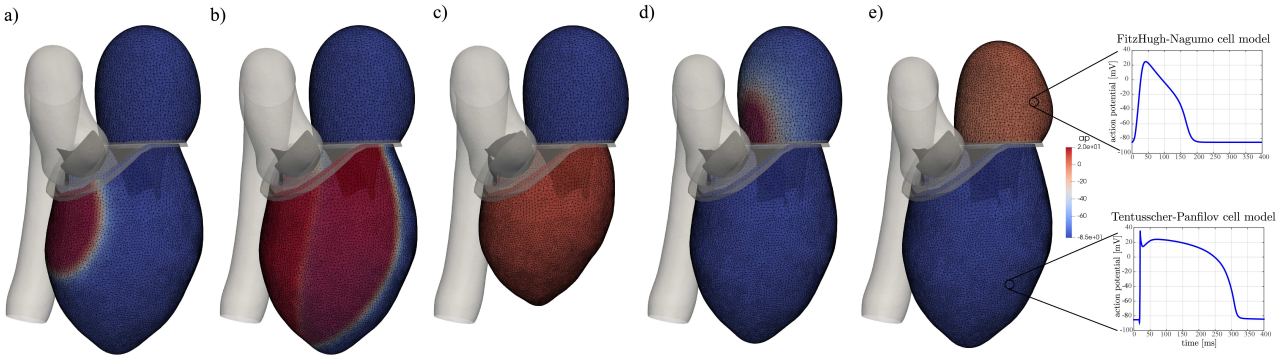


Figure 1: Snapshots of the action potential for the left heart during a heart beat. The different cellular models for atrium and ventricle are shown in the lateral insets.

[1] F. Viola, V. Meschini, R. Verzicco, "A multi-way coupled model for the left-heart: Fluid-Structure-Electrophysiology interaction (FSEI), Under revision (2019).

[2] L. Tung, "A bi-domain model for describing ischemic myocardial dc potential", Ph.D. thesis, Massachusetts Institute of Technology (1978)

[3] R. H. Clayton, A. V. Panfilov, "A guide to modelling cardiac electrical activity in anatomically detailed ventricles", Progress in biophysics and molecular biology 96 (1) (2008) 19-43

[4] K. Ten Tusscher, A. Panfilov, "Cell model for efficient simulation of wave propagation in human ventricular tissue under normal and pathological conditions", Physics in Medicine & Biology 51 (23) (2006)

[5] R. Fitzhugh, "Thresholds and plateaus in the Hodgkin-Huxley nerve equations", The Journal of general physiology 43 (5) (1960) 867-896

[6] K. Chanm S. Tarantola, A. Saltelli and I. Sobol'. "Variance-based methods". In: Sensitivity Analysis. Ed. by A. Saltelli, K. Chand and E. M. Scott. Chinchester: John Wiley and Sons, Ltd., 2000.

[7] I. Sobol'. "Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates". In: Mathematics and Computers in Simulation 55.1-3 (Feb. 2001), pp. 271-280.

[8] I. Sobol'. "Sensitivity analysis for non linear mathematical models". In: Math. Model. Comput. Exp. 1 (1993) pp. 407-414.

[9] A. Saltelli, S. Tarantola, and K. P.-S- Chan, "A quantitative model independent method for global sensitivity analysys of model output". In. Technometrics 41.1 (Feb. 1999), pp. 39-56.

[10] G. Blatman, B. Sudret. "Adaptive sparse polynomial chaos expansions based on least angle regression". Journal of Computational Physics, (2011), pp. 2345-2367.

[11] B. Sudret. "Polynomial chaos expansions and stochastic finite element methods". In: Risk and Reliability in Geotechnical Engineering (2014)

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Stochastic analysis of the effect of inlet conditions in the hemodynamics simulation of a thoracic aortic aneurysm

Alessandro Mariotti,[1] ***Simona Celi,***[2] ***Katia Capellini,***[2,3] ***and Maria Vittoria Salvetti,***[1]

[1]DICI, University of Pisa, Pisa, Italy – alessandro.mariotti@unipi.it, mv.salvetti@ing.unipi.it
[2]BioCardioLab - Heart Hospital, Fondazione Toscana G. Monasterio, Massa, Italy – s.celi@ftgm.it, katia.capellini@ftgm.it
[3]DII, University of Pisa, Pisa, Italy

Key words: Ascending thoracic aortic aneurysm, hemodynamics simulations, polynomial chaos

An Ascending Thoracic Aortic Aneurysm (ATAA) is a permanent dilatation occurring in the ascending part of the thoracic aorta. This disease represents a clinical challenge due to the significant mortality risk carried by both complications and surgical repair. Currently, decisions about clinical management are based on the maximum aneurysm diameter: surgery is recommended whether the aneurysm diameter reaches $5.5cm$. However, ascending aortic dissections may occur also with smaller diameters. In the initiation and progression of cardiovascular diseases, such as in case of ascending thoracic aortic aneurysm, an important role is played by hemodynamic forces ([1]). Among the hemodynamic descriptors, the wall shear stresses can have an important effect on vessel wall mechanical properties, and, therefore, on the aneurysm rupture risk.

In this context, Computational Fluid Dynamics (CFD) permits the investigation of pressure and flow field at a temporal and spatial resolution unachievable by any clinical methodology. A variety of variables and indicators difficult to be obtained from *in-vivo* measurements can be easily quantify through CFD and, even better, the combination of medical imaging with CFD permits to investigate hemodynamics on a patient-specific basis (see e.g. [4]). Nonetheless, the accuracy of CFD predictions strongly depends on modeling assumptions and computational set-up. An important critical aspect is represented by boundary conditions, which must be correctly prescribed to reproduce the effect of organs and vessels outside the portion of aorta that is actually simulated. Both inflow and outflow boundary conditions should be patient specific and can only seldom be obtained from *in-vivo* measurements (and, when available, experimental data are often characterized by a space and time resolution not adequate for numerical simulation).

In an our previous work we investigated on the impact of outflow boundary conditions based on the three-element Windkessel model, by performing a stochastic analysis of the effect of the uncertainties in the Windkessel parameters ([2]). The results highlighted that a fine tuning of RCR parameters is not needed and that the values of the RCR parameters can be set in order to obtain a desired physiological behavior of the pressure profile in the simplified fully lumped model in which the contribution of the computational domain is neglected. Moreover, we deterministic investigated on the effect of the wall compliance ([3]), observing some discrepancies between numerical results, obtained with a homogeneous linear elastic model, and in-vivo data.

We focus herein on inlet boundary conditions. A common practice is the imposition of a flow rate waveform. We consider a real aneurysm geometry acquired by Magnetic Resonance Imaging (MRI), shown in Figure 1a, and perform the simulations with the open-source software *SimVascular*. We carried out a systematic sensitivity analysis to the shape of the inlet flow rate waveform, and, in particular, to the flow stroke volume and to the period of the cardiac cycle. For this analysis we decide to consider plug flow (uniform spatial distribution of the inlet velocity). Both rigid and deformable walls are considered. A deterministic analysis of the influence of these parameters is difficult because of the significant cost of each simulation. An efficient alternative is to use a stochastic approach, in which the selected parameters are considered as random variables with a given probability distribution. The uncertainty can, thus, be propagated through the CFD model and a continuous response surface of the output quantities of interest in the parameter space can be recovered through

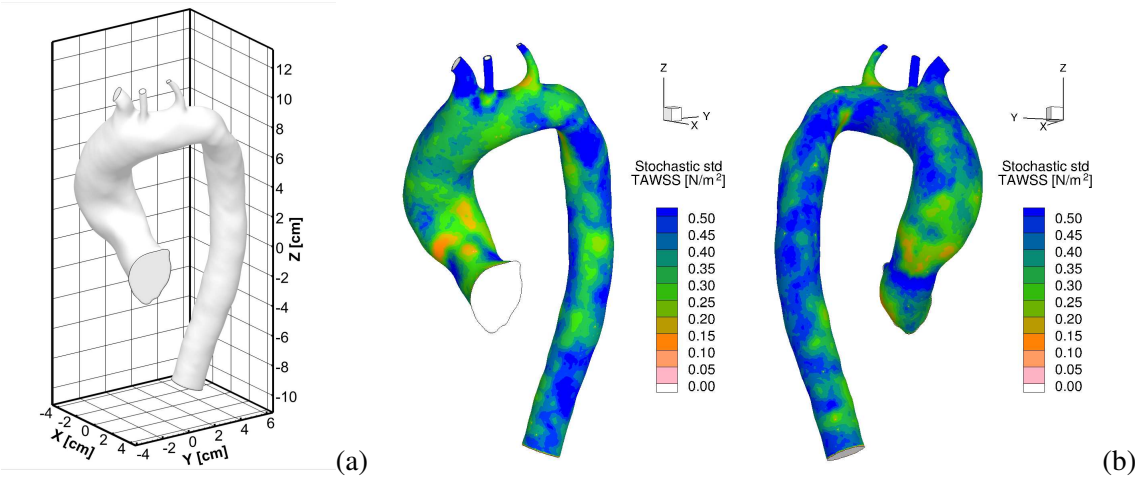


Figure 1: Sketch of the considered geometry (a). Stochastic standard deviation of TAWSS (b): effect of uncertainties in the values of the cardiac cycle period T and of the stroke volume SV, beta PDF distributions for the case of rigid walls.

a "surrogate" model, which requires a limited number of deterministic simulations. In the present work, we use the generalized Polynomial Chaos (gPC) approach is used in its not intrusive form. For both selected uncertain parameters, viz. the flow stroke volume and to the period of the cardiac cycle, we used clinical data to construct more accurate beta PDFs. The polynomial expansion being truncated to the third order in each of the input parameter, 16 simulations were needed to compute the coefficients of the expansion. An example of the obtained results is given in Figure 1b, in which the stochastic standard deviation of the cycle-averaged wall shear stresses (TAWSS) is shown. As will be presented at the conference, the two input parameters showed a deep influence on wall shear stresses, confirming the need of using patient-specific inlet conditions.

Currently, we are investigating on the effects of the spatial distribution of the inlet velocity. Again a stochastic approach is chosen and patient specific data are considered. The results will be shown in the final presentation.

[1] K. Capellini, E. Vignali, E. Costa, et al., "Computational fluid dynamic study for aTAA hemodynamics: an integrated image-based and radial basis functions mesh morphing approach," J Biomech Eng, **140(11)**, 111007 (2018).

[2] A. Boccadifuoco, A. Mariotti, S. Celi, N. Martini, and M. V. Salvetti, "Impact of uncertainties in outflow boundary conditions on the predictions of hemodynamic simulations of ascending thoracic aortic aneurysms," Comput Fluids, **165**, 96-115, (2018).

[3] A. Boccadifuoco, A. Mariotti, K. Capellini, S. Celi, and M. V. Salvetti, "Validation of numerical simulations of thoracic aorta hemodynamics: comparison with in-vivo measurements and stochastic sensitivity analysis," Cardiovasc Eng Technol, **9(4)**, 688-706, (2018).

[4] Morbiducci, U., Ponzini, R., Rizzo, G., Cadioli, M., Esposito, A., Montevecchi, F.M. and Redaelli, A. "Mechanistic insight into the physiological relevance of helical blood flow in the human aorta: An in vivo study," Biomechanics and Modeling in Mechanobiology, **10(3)**, 339-355, (2011).

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

An integrated approach of uncertainty quantification and 3D MRI techniques in guiding CFD analysis for a non-invasive study of aortic coarctation

***Maria Nicole Antonuccio*[1,2], *Benigno Marco Fanni*[1,2], *Katia Capellini*[1,2], *Emilie Sauvage*[3], *Alessandro Mariotti*[4], *Claudio Capelli*[3] and *Simona Celi*,[1]**

[1]BioCardioLab - Heart Hospital, Fondazione Toscana G. Monasterio, Massa, Italy – bmfanni@ftgm.it, kcapellini@ftgm.it, s.celi@ftgm.it
[2]DII, University of Pisa, Italy – m.antonuccio@studenti.unipi.it
[3]DICI, University of Pisa, Italy – e.sauvage@ucl.ac.uk, c.capelli@ucl.ac.uk
[4]DICI, University of Pisa, Italy – alessandro.mariotti@for.unipi.it

Key words: Uncertainty quantification, Computation Fluid Dynamics, Aortic coartation

Coarctation of aorta (CoA) is a congenital cardiovascular disease characterized by an abnormal narrowing of the proximal descending aorta, leading to a pressure gradient (ΔP) across the coarctation, increased afterload and reduced peripheral perfusion pressures [1]. Currently, the correction of CoA is based on invasive treatments and the main indication relies on the value of the maximal trans-coarctation pressure ($\Delta P \geq 20$ mmHg) [2]. Investigations of the hemodynamics and biomechanical basis of morbidity in CoA plays a fundamental role considering recent advancements in computational modeling. In this context, the computational fluid dynamics (CFD) approach represents a powerful tool to investigate hemodynamic quantities in a non-invasive way.
In this work, a patient-specific CFD framework was developed for the non invasive assessment of the hemodynamics of the CoA, starting from the patient-specific imaging to the related computational model and the appropriate boundary conditions. In particular, the aim was to assess the capability of the presented framework to capture the correct patient-specific ΔP across the CoA. In this context, the definition of the correct boundary conditions within the computational models still represents a challenge since the overall patient-specific flow dynamics strongly depends on the outflow conditions [3]. The work-flow of the process is reported in Figure 1. The 3D model was obtained from magnetic resonance imaging (MRI). The inflow boundary condition was imposed at the valve level of the ascending aorta, considering patient-specific phase contrast MRI data.

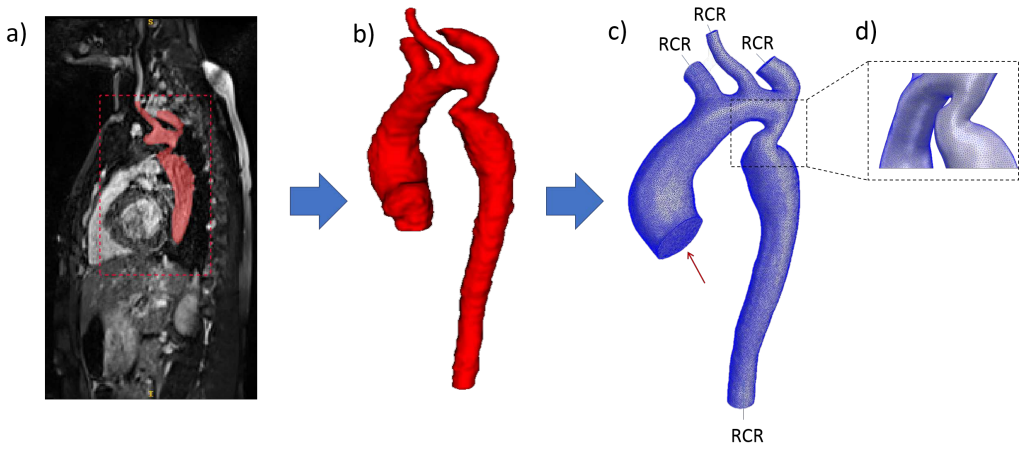


Figure 1: Patient-specific CFD framework: MRI dataset segmentation (a); segmented model (b); 3D CFD mesh with 0-D RCR coupling (c) and zoom on CoA (d).

The effects of the downstream organs and vessels were implemented with a three-element RCR Windkessel model for each outlet, i.e. the three supra-aortic vessels and the descending aorta[4]. The initial RCR parameters were firstly determined with a custom code based on the patient-specific flow, as retrieved from imaging, and *in vivo* pressure measurements. After reconstructing the geometry and setting up the inlet and the outlet boundary conditions, patient-specific CFD simulations were performed. The open-source software *SimVascular* was used. The ΔP evaluated *in silico* at the coarctation level was compared against the invasive intravascular trans-CoA pressure measurements. Hemodynamic quantities and indices of interest, including pressure loss, time-averaged wall shear stress, and oscillatory shear index, were also quantified. A stochastic approach is still under investigation for the assessment of the correct RCR parameters to be applied on each aortic branch in order to obtain the best fit between *in vivo* and *in silico* data in terms of outflows and pressure drops. Figure 2 depicts, as example, the results of a deterministic simulation.

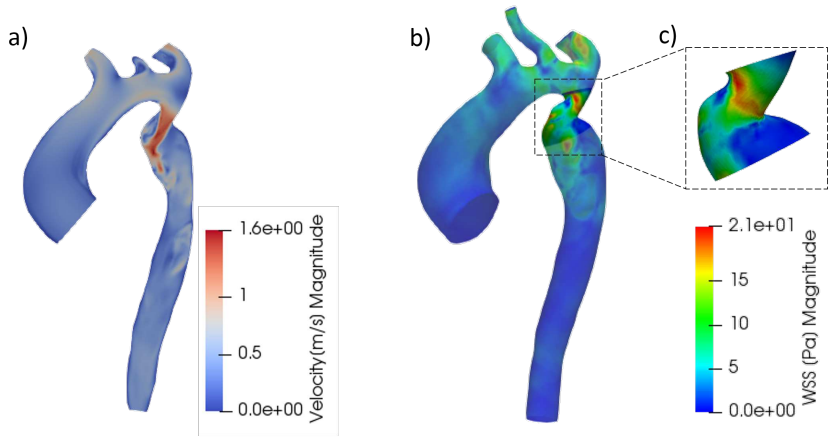


Figure 2: Velocity field at systolic peak in a long axis plane (a); WSS at systolic peak (b) and zoom in CoA (c).

In particular, we are investigating how the uncertainties in the Windkessel model parameters may affect the results of the numerical simulation. We are adopting a stochastic approach in which the parameters are considered as random variables with a given probability distribution. We are analyzing different strategies to obtain a continuous surface in the parameters space starting from a few deterministic numerical simulation. The generalized polynomial chaos (gPC) seems to be the best choice in terms of feasibility and properties of convergence. In particular, we are adopting the not intrusive form of the gPC with the big advantage that it is possible to use deterministic finite element tools, such as the solver *SimVascular*, as a black box to sample the model solutions.

[1] L.S. Teo, T. Cannel, A. Babu-Narayan, et al., "Prevalence of Associated Cardiovascular Abnormalities in 500 Patients with Aortic Coarctation Referred for Cardiovascular Magnetic Resonance Imaging to a Tertiary Center," Pediatr Cardiol, **32(8)**, 1120-1127, (2011)

[2] C. A. Warnes, R. Williams, et al., "ACC/AHA 2008 guidelines for the management of adults with congenital heart disease: a report of the American College of Cardiology/American Heart Association Task Force on Practice Guidelines (writing committee to develop guidelines on the management of adults with congenital heart disease)," Circulation **118(23)**, 714-833, (2008)

[3] A. Boccadifuoco, A. Mariotti, S. Celi, N. Martini, M.V. Salvetti, "Impact of uncertainties in outflow boundary conditions on the predictions of hemodynamic simulations of ascending thoracic aortic aneurysms" Comput Fluids, **165**, 96-115, (2018)

[4] I.E. Vignon-Clementel, C.A. Figueroa, K.E. Jansen, C.A. Taylor, "Outflow boundary conditions for three-dimensional finite element modeling of blood flow and pressure in arteries" Comput. Methods Appl. Mech. Engrg., **195**, 3776-3796, (2006)

ST6– Environmental II

Session Chair: Gorodetsky A.A.

Auditorium

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Refining the input space of plausible future debris flows using noisy data and multiple models of the physics

Andrea Bevilacqua,[1] ***Abani Patra,***[2] ***Marcus Bursik,***[3] ***E. Bruce Pitman,***[4]
José Luis Macías,[5] ***Ricardo Saucedo,***[6] ***David Hyman***[7]

[1]INGV, Sezione di Pisa, Italy – andrea.bevilacqua@ingv.it
[2]Dpt. of Mechanical and Aerospace Engineering, UB, NY, USA – abani.patra@buffalo.edu
[3]Dpt. of Earth Sciences, [4]Dpt. of Material Design and Innovation, UB, NY, USA
[5]Departamento de Vulcanología, Instituto de Geofísica, UNAM, Mexico City, DF, Mexico
[6]Instituto de Geología, Facultad de Ingeniería, UASLP, San Luis, SLP, Mexico
[7]Cooperative Institute for Meteorological Satellite Studies, UW, Madison, WI, USA

Key words: Uncertainty quantification, Geophysical Flows, Inverse Problems, Model Inadequacy

Forecasts of future geophysical mass flows, fundamental in hazard assessment, usually rely on the reconstruction of past flows that occurred in the region of interest using models of physics that have been successful in hindcasting. The available pieces of data $D_i \in \mathcal{D}$, are commonly related to the properties of the deposit left by the flows and to historical documentation. Nevertheless, this information can be fragmentary and affected by relevant sources of uncertainty (e.g., erosion and remobilization, superposition of subsequent events, unknown duration, and source). Moreover, different past flows may have had significantly different physical properties, and even a single flow may change its physics with respect to time and location, making the application of a single model inappropriate.

In a probabilistic framework, for each model $M \in \mathcal{M}$ we define (M, P_M), where P_M is a probability measure over the parameter space of M. While the support of P_M can be restricted to a single value by solving an inverse problem for the optimal reconstruction of a particular flow, the inverse problem is not always well posed. That is, no input values are able to produce outputs consistent with all observed information [5]. Choices based on limited data using classical calibration techniques (i.e. optimized data inversion) are often misleading since they do not reflect all potential event characteristics and can be error prone due to incorrectly limited event space. Sometimes the strict replication of a past flow may lead to overconstraining the model, especially if we are interested in the general predictive capabilities of a model over a whole range of possible future events.

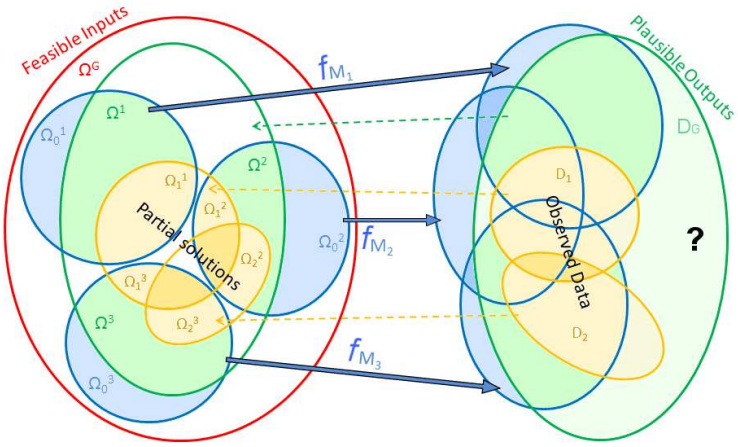


Figure 1: Diagram of input spaces, model functions, and output space (blue), with feasible inputs domain (red), plausible output codomain and specialized inputs (green), and observed data and partial solutions subsets (orange). The question mark emphasizes that the covering of other plausible outputs could be enabled by adding more models if necessary.

In this study, we use a multi-model ensemble and a plausible region approach to provide a more prediction-oriented probabilistic framework for input space characterization in hazard analysis. In other words, we gener-

alize a poorly constrained inverse problem, decomposing it into a hierarchy of simpler problems.

We apply our procedure to the case study of the Atenquique volcaniclastic debris flow, which occurred on the flanks of Nevado de Colima volcano (Mexico) in 1955. We adopt and compare three depth-averaged models. Input spaces are explored by Monte Carlo simulation based on Latin hypercube sampling. The three models are incorporated in our large-scale mass flow simulation framework TITAN2D [3, 4]. Our meta-modeling framework is fully described in Fig.1 with a Venn diagram of input and output sets, and in Fig. 2 with a flowchart of the algorithm. See also [1] for more details on the study.

Our approach is characterized by three steps: **(STEP 1)** Let us assume that each model $M_j \in \mathcal{M}$ is represented by an operator: $f_{M_j} : \Omega_0^j \longrightarrow \mathbb{R}^d$, where $d \in \mathbb{N}$ is a dimensional parameter which is independent of the model chosen and characterizes a common output space. This operator simply links the input values in Ω_0^j to the related output values in $\mathbb{R}^d$. Thus we define the global set of feasible inputs: $\Omega_G := \bigsqcup_j \Omega_0^j$. This puts all the models in a natural meta-modeling framework, only requiring essential properties of feasibility in the models, namely the existence of the numerical output and the realism of the underlying physics. **(STEP 2)** After a preliminary screening, we characterize the codomain $D_G \subset \mathbb{R}^d$ of plausible outputs: that is, the target of our simulations – it includes all the outputs consistent with the observed data, plus additional outputs which differ in arbitrary but plausible ways[1]. For instance, having a robust numerical simulation without spurious effects, and with meaningful flow dynamics, and/or the capability to inundate a designated region. Thus $\forall j$, the specialized input space is defined as[2]: $\Omega^j = f_{M_j}^{-1}(D)$. **(STEP 3)** Furthermore, through more detailed testing, $\forall i \in I$, we can thus define the subspace $\Omega_i^j \subseteq \Omega^j$ of the inputs that are consistent with a piece of empirical data D_i. Formally, $\forall i$, $\Omega_i^j = f_{M_j}^{-1}(D_i)$, and for this reason those sets are called partial solutions to the inverse problem. In our case study, model selection appears to be inherently linked to the inversion problem. That is, the partial inverse problems enable us to find models depending on the example characteristics and spatial location.

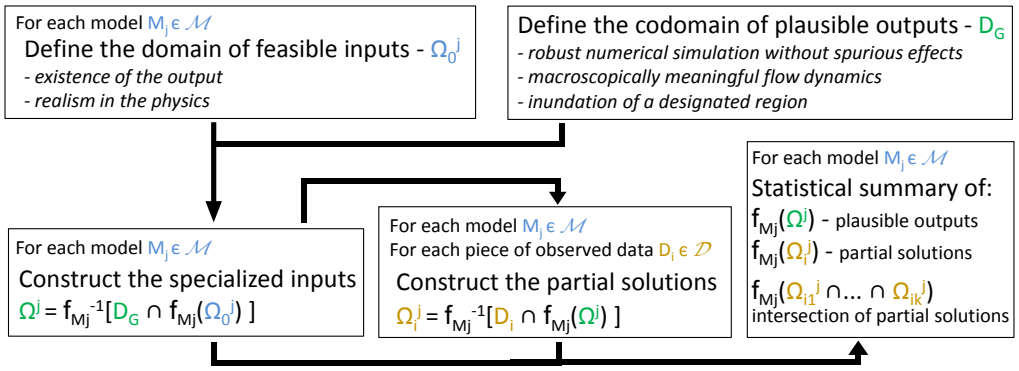


Figure 2: Diagram of the steps of our meta-modeling approach.

[1] A. Bevilacqua, A.K. Patra, M.I. Bursik, E.B. Pitman, J.L. Macías, R. Saucedo, D. Hyman, "Probabilistic forecasting of plausible debris flows from Nevado de Colima (Mexico) using data from the Atenquique debris flow, 1955", Natural Hazards Earth System Science **19**, 791-820 (2019).

[2] K. Farrell, J. Tinsley Oden, D. Faghihi, "A Bayesian framework for adaptive selection, calibration, and validation of coarse-grained models of atomistic systems", Journal of Computational Physics **295**, 189-208 (2015).

[3] A.K. Patra, A.C. Bauer, C.C. Nichita, E.B. Pitman, M.F. Sheridan, M.I. Bursik, B. Rupp, A. Webber, A.J. Stinton, L.M. Namikawa, C.S. Renschler, "Parallel adaptive numerical simulation of dry avalanches over natural terrain", Journal of Volcanology and Geothermal Research **139**, 1–21 (2005).

[4] A.K. Patra, C.C. Nichita, A.C. Bauer, E.B. Pitman, M.I. Bursik, M.F. Sheridan, "Parallel adaptive discontinuous Galerkin approximation for thin layer avalanche modeling", Computers & Geosciences **32**, 912–926 (2006).

[5] A. Tarantola and B. Valette, "Inverse Problems = Quest for Information", Journal of Geophysics **50**, 159-170 (1982).

[1] Our notion of output plausibility is not related to the model plausibility defined in [2].

[2] For the sake of simplicity, we use the same notation for each piece of data D_i and the set of outputs consistent with it.

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Surrogate-based parameter inference in a debris flow model

Maria Navarro,[1] ***Olivier Le Maître,***[2] ***Ibrahim Hoteit***[3]***, David George,***[4] ***Kyle Mandli,***[5] ***and Omar M. Knio***[6]

[1]King Abdullah University of Science and Technology, Saudi Arabia – mariaisabel.navarrojimenez@kaust.edu.sa

[2]LIMSI-CNRS, France – olm@limsi.fr

[3]King Abdullah University of Science and Technology, Saudi Arabia – ibrahim.hoteit@kaust.edu.sa

[4]U.S. Geological Survey, Vancouver, WA 98683 – dgeorge@usgs.gov

[5]Columbia University, New York, NY 10027 – kyle.mandli@columbia.edu

[6]King Abdullah University of Science and Technology, Saudi Arabia – omar.knio@kaust.edu.sa

Key words: Bayesian inference, Polynomial Chaos Expansion, Debris Flow, Uncertainty Quantification

This work tackles the problem of calibrating the unknown parameters of a debris flow model with the drawback that the information regarding the experimental data treatment and processing is not available. In particular, we focus on the the evolution over time of the flow thickness of the debris with dam-break initial conditions. The proposed methodology consists of establishing an approximation of the numerical model using a polynomial chaos expansion that is used in place of the original model, saving computational burden. The values of the parameters are then inferred through a Bayesian approach with a particular focus on inference discrepancies that some of the important features predicted by the model exhibit. We build the model approximation using a preconditioned non-intrusive method and show that a suitable prior parameter distribution is critical to the construction of an accurate surrogate model. The results of the Bayesian inference suggest that utilizing directly the available experimental data could lead to incorrect conclusions, including the over-determination of parameters. To avoid such drawbacks, we propose to base the inference on few significant features extracted from the original data. Our experiments confirm the validity of this approach, and shown that it does not lead to significant loss of information. It is further computationally more efficient than the direct approach, and can avoid the construction of an elaborate error model.

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Propagation of Uncertainties in Density-Driven Flow

Alexander Litvinenko[1]***, Dmitry Logashenko***[2]***, Raul Tempone***[1,2]***, Gabriel Wittum***[2] ***and David Keyes***[2]

[1]RWTH Aachen, Germany, – {litvinenko, tempone}@uq.rwth-aachen.de

[2]KAUST, Thuwal, Saudi Arabia – {dmitry.logashenko, raul.tempone, gabriel.wittum, david.keyes}@kaust.edu.sa

Key words: Uncertainty quantification, density driven flow, subsurface flow, uncertain porosity

Accurate modeling of contamination in subsurface flow and water aquifers is crucial for agriculture and environmental protection. Here, we demonstrate an efficient parallel algorithm to quantify the propagation of the uncertainty in the dispersal of pollution in subsurface flow. Specifically, we consider the density-driven flow and estimate how uncertainty from permeability and porosity propagates to the solution. We take an Elder-like problem as a numerical benchmark and we use random fields to model the limited knowledge on the porosity and permeability. We construct a low-cost generalized polynomial chaos expansion (gPCE) surrogate model, where the gPCE coefficients are computed by projection on sparse and full tensor grids. We parallelize both the numerical solver for the deterministic problem based on the multigrid method, and the quadrature over the parametric space.

[1] A. Litvinenko, D. Logashenko, R. Tempone, G. Wittum, and D. Keyes "Propagation of Uncertainties in Density-Driven Flow", arXiv preprint, April 2019.

[2] S. Reiter, A. Vogel, I. Heppner, M. Rupp, and G. Wittum, "A massively parallel geometric multigrid solver on hierarchically distributed grids", Computing and visualization in science 16, 4 (2013), pp 151-164, DOI: 10.1007/s00791-014-0231-x

[3] A. Vogel, S. Reiter, M. Rupp, A.Nagel, and G. Wittum, "UG4 — a novel flexible software system for simulating PDE based models on high performance computers". Computing and visualization in science 16, 4 (2013), pp 165-179, DOI: 10.1007/s00791-014-0232-9

[4] A. Schneider, H. Zhao, J. Wolf, D. Logashenko, S. Reiter, M. Howahr, M. Eley, M. Gelleszun, H. Wiederhold, "Modeling saltwater intrusion scenarios for a coastal aquifer at the German North Sea", E3S Web of Conferences 54, 00031 (2018), DOI:10.1051/e3sconf/20185400031

[5] M. Espig, W. Hackbusch, A. Litvinenko, H.G. Matthies, E. Zander, "Efficient analysis of high dimensional data in tensor formats", Sparse Grids and Applications, LNCSE, volume 88, pp 31-56, 2012

[6] S. Dolgov, B.N. Khoromskij, A. Litvinenko, and H.G. Matthies, "Polynomial Chaos Expansion of Random Coefficients and the Solution of Stochastic Partial Differential Equations in the Tensor Train Format", IAM/ASA J. Uncertainty Quantification 3 (1), pp 1109-1135, 2015

[7] A. Litvinenko, H.G. Matthies, T.A. El-Moselhy, "Sampling and low-rank tensor approximation of the response surface", Monte Carlo and Quasi-Monte Carlo Methods 2012, PROMS, volume 65, pp 535-551, 2013

[8] A. Litvinenko, H.G. Matthies, "Numerical Methods for Uncertainty Quantification and Bayesian Update in Aerodynamics", In: Eisfeld B., Barnewitz H., Fritz W., Thiele F. (eds) Management and Minimisation of Uncertainties and Errors in Numerical Aerodynamics. Notes on Numerical Fluid Mechanics and Multidisciplinary Design, vol 122. Springer, Berlin, Heidelberg, 2013

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

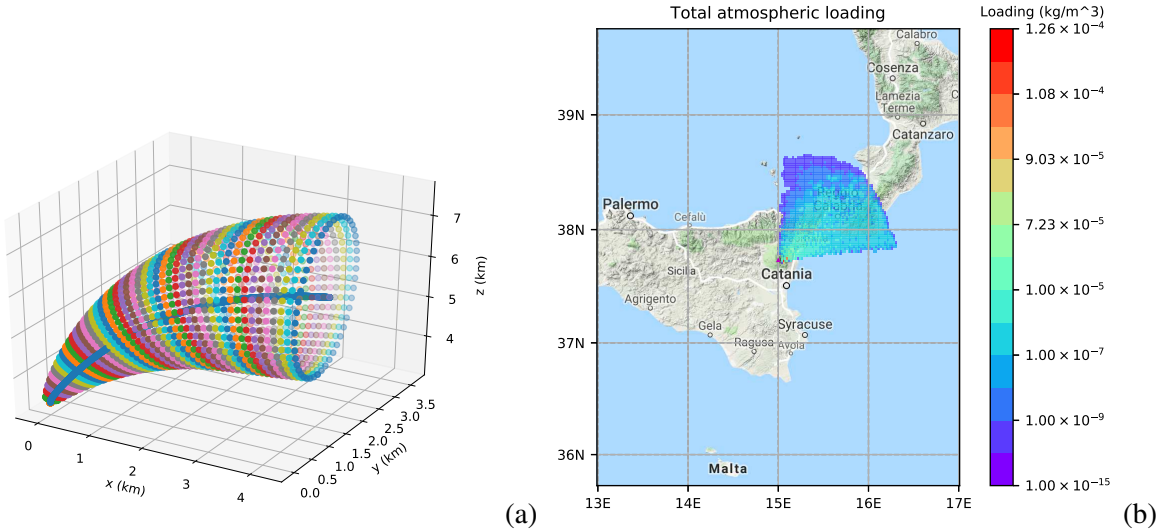
Uncertainty quantification in explosive volcanic eruptions: from volcanic column generation to ash dispersion and deposition

***Federica Pardini*[1], *Mattia de' Michieli Vitturi*[1], *Samantha Louise Engwell*[2], *Sara Barsotti*[3], *and Augusto Neri*[1]**

[1]Istituto Nazionale di Geofisica e Vulcanologia, Sezione di Pisa, Pisa, Italy
[2]British Geological Survey, Edinburgh, United Kingdom
[3]Vedurstofa Íslands, Icelandic Met Office, Reykjavík, Iceland

Key words: Uncertainty quantification, Eruptive column models, Ash dispersion, Volcanic hazard

Explosive volcanic eruptions produce hot plumes of gas and particles whose behaviour is complex and dependent on both eruptive source parameters (e.g. exit velocity, gas fraction, temperature and grain-size distribution) and atmospheric environment. Assessing the way in which these elements influence plume height and subsequent ash dispersal patterns (both in the atmosphere and on the ground) is of fundamental importance for volcanic hazard mitigation. Here, we present the results of uncertainty quantification and sensitivity analysis performed through latin hypercube sampling and polynomial chaos expansion, aimed at identifying and quantifying the source parameters exerting a major role on plume height and trajectory. The analysis is applied to the integral column model PLUME-MoM 2.0. The model describes the rise of a pyroclastic mixture by solving the equations for the conservation of mass, momentum and energy for the gas-ash mixture, accounting for important processes such as particles settling, particle aggregation, phase changes of water and effects of moisture. The continuous polydispersity of pyroclastic particles is described using a quadrature-based moment method, an innovative approach in volcanology well-suited for the description of the multiphase nature of magmatic mixtures. The study is further extended beyond the dynamics of the rising plume to investigate the effects that uncertain eruptive source parameters have on ash dispersion in the atmosphere and deposition on the ground. Indeed, the column model has been integrated with the dispersal model HYSPLIT, which simulates the transport and dispersion of particles into the atmosphere. Particles lost from the column enter into the atmospheric environment and are transported and dispersed until they deposit on the ground. The uncertainty quantification analysis allows us to construct statistical particle size distributions, both in the air and on the ground, at various distances from the volcanic vent. The cases study for the present analysis are two eruptive scenario, weak and strong plume, at Mt.Etna, Italy.



(a) (b)

Figure 1: Image of the volcanic column from PLUME-MoM 2.0 (a) and atmospheric ash loading as simulated by HYSPLIT (b)

[1] M. de' Michieli Vitturi, A. Neri, and S. Barsotti, "PLUME-MoM 1.0: A new integral model of volcanic plumes based on the method of moments," Geoscientific Model Development **8**, 2447-2463 (2015).

[2] M. de' Michieli Vitturi, S.L. Engwell, A. Neri, and S. Barsotti, "Uncertainty quantification and sensitivity analysis of volcanic columns models: Results from the integral model PLUME-MoM," Journal of Volcanology and Geothermal Research **326**, 77-91 (2016).

[3] A.F. Stein, R.R. Draxler, G.D. Rolph, B.J.B. Stunder, M.D. Cohen, and F. Ngan, "NOAA's HYSPLIT atmospheric transport and dispersion modeling system," Bulletin of the American Meteorological Societyt **96**, 2059-2077 (2015).

Keynote Lecture - E.F. Campana - Sailing in a storm: UQ for ship optimization in a stochastic environment with operational uncertainty
Session Chair: P. Cinnella
Auditorium

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Sailing in a Storm: UQ for Ship Optimization in a Stochastic Environment with Operational Uncertainty

Emilio F. Campana[1] ***and Matteo Diez***[2]

[1]CNR-DIITET, Italy – emiliofortunato.campana@cnr.it

[2]CNR-INM, Italy – matteo.diez@cnr.it

Key words: Ship Design, Uncertainty Quantification, Design Optimization, Stochastic Optimization

The ocean is an intrinsic stochastic environment and ships operations are permeated by uncertainty stemming from environmental conditions (wave energy spectra, significant wave height, modal period, and direction, wind, etc.) and operational parameters (speed, heading, payload, etc.). Therefore, a robust and reliable assessment of ship performance (resistance, seakeeping, maneuverability, stability and control) must consider the uncertainty associated to all relevant input parameters and evaluate its propagation to the relevant outputs through the analysis process. Furthermore, high-fidelity simulations (e.g., large-grid CFD and/or FEA computations) are often required to ensure accuracy and reliability of the analysis outcomes and the subsequent decision making. This is particularly true for stormy conditions, high sea states, high and steep waves, and violent impacts, where low-fidelity tools usually fail to provide reliable predictions. It is worthwhile to recall that international vessel registers expect, as an effect of climate changes, an increase in the near future of both the average sea state in the oceans and the frequency of extreme wave events. Consequently, modern ship design must incorporate uncertainty quantification (UQ) methods with high fidelity analyses. The affordability of combining these tools with (global) optimization algorithms into a fully digital and automated design processes depends on the availability of efficient methods for operational and design space exploration, i.e. UQ and optimization.

The talk will focus on the integration of UQ methods into a simulation-based design global optimization framework to increase ships operational efficiency and effectiveness in real ocean environments. The use of collocation methods and adaptive metamodels with Monte Carlo simulation will be discussed as well as the efficient application of design space dimensionality reduction techniques based on the Karhunen-Loève expansion of hull shape- and physics-related variables. Examples will be provided based on recent international collaborative research within NATO Science and Technology Organization Applied Vehicle Technology task group AVT-252 on ”Stochastic Design Optimization for Naval and Aero Military Vehicles,” where a naval-destroyer hull form was optimized to increase its operational efficiency and effectiveness in realistic ocean environment and operations.

[1] Serani, A., Diez, M., Wackers, J., Visonneau, M. and Stern, F., 2019. Stochastic Shape Optimization via Design-Space Augmented Dimensionality Reduction and RANS Computations. In AIAA Scitech 2019 Forum (p. 2218).

[2] Diez, M., Campana, E.F. and Stern, F., 2018. Stochastic optimization methods for ship resistance and operational efficiency via CFD. Structural and Multidisciplinary Optimization, 57(2), pp.735-758.

[3] Volpi, S., Diez, M., Gaul, N.J., Song, H., Iemma, U., Choi, K.K., Campana, E.F. and Stern, F., 2015. Development and validation of a dynamic metamodel based on stochastic radial basis functions and uncertainty quantification. Structural and Multidisciplinary Optimization, 51(2), pp.347-368.

[4] Diez, M., Campana, E.F. and Stern, F., 2015. Design-space dimensionality reduction in shape optimization by Karhunen-Loève expansion. Computer Methods in Applied Mechanics and Engineering, 283, pp.1525-1544.

SF1 – Applications III

Session Chair: E.F. Campana

Auditorium

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Uncertainty Quantification by Adaptive Multifidelity Surrogates of Noisy CFD Data

***Jeroen Wackers*[†]*, Michel Visonneau*[†]*, Andrea Serani*[*]*, Riccardo Pellegrini*[*]*, Riccardo Broglia, and Matteo Diez*[*]

[†] LHEEA Lab, Ecole Centrale de Nantes, CNRS-UMR 6598, Nantes, France
– jeroen.wackers@ec-nantes.fr, michel.visonneau@ec-nantes.fr

[*] CNR-INM, National Research Council-Institute of Marine Engineering, Rome, Italy
– andrea.serani@inm.cnr.it, riccardo.pellegrini@inm.cnr.it, riccardo.broglia@cnr.it, matteo.diez@cnr.it

Key words: Uncertainty quantification, Multifidelity analysis, Surrogate models, Computational Fluid Dynamics, Adaptive grid refinement, Multi-grid method

Ship performance depends on design and operational/environmental parameters. The accurate prediction of performance metrics (such as the hydrodynamic resistance) requires high-fidelity computational tools, especially for innovative configurations and extreme/off-design conditions. These tools are generally computationally expensive, making the design/operational-space exploration and associated uncertainty quantification (UQ) a technological challenge.

To reduce the computational cost, supervised machine learning/surrogate (or metamodeling) methods are applied. Dynamic/adaptive surrogates update dynamically their training sets, exploiting the information that becomes available during the analysis process: training points are added where it is most useful, reducing the number of function evaluations required to represent the desired function [1, 2]. Unfortunately, the adaptive sampling process is affected by the computational-output noise. Adaptive sampling methods may react to noise by adding many training points in noisy regions, rather than selecting new points in unseen regions. This deteriorates the model quality/efficiency and has to be considered carefully [3].

In addition to dynamic/adaptive surrogates and with the aim of reducing further the computational cost, multi-fidelity (MF) methods combine the accuracy of high-fidelity solvers with the computational cost of low-fidelity solvers. MF metamodels use mainly low-fidelity simulations and only few high-fidelity simulations are used to preserve the model accuracy. Several metamodels are used with MF data. An example of application of radial basis functions (RBF) is shown in [1, 2]. In CFD-based UQ, different fidelity levels may be obtained by varying the physical model, the grid size, and/or combining experimental data with simulations.

The objective of the present work is to present an adaptive RBF-based N-fidelity (NF) surrogate for UQ of complex industrial problems, fully exploiting the potential of simulation methods that naturally produce results spanning a range of fidelity levels: RANS (Reynolds-Averaged Navier-Stokes) simulations with adaptive grid refinement [4], and/or multi-grid resolution [5]. The NF method is further advanced to reduce the effects of the noise in the CFD outputs through regression and in-the-loop optimization of the model.

The NF method is developed based on authors' previous work [1, 2, 6, 3, 7] and demonstrated for the UQ of (i) a NACA hydrofoil and (ii) a roll-on/roll-off passengers (RoPax) ferry subject to uncertain shape/operating parameters. CFD is based on two RANS solvers: (1) ISIS-CFD [4], developed at ECN/CNRS and integrated in the FINE/Marine suite (NUMECA Int), and (2) Xnavis [5], developed at CNR-INM. In ISIS-CFD, different fidelity levels are defined by the grid refinement ratio in adaptive grid refinement. In Xnavis, different fidelities are obtained exploiting the multi-grid approach.

[1] S. Volpi, M. Diez, N. J. Gaul, H. Song, U. Iemma, K. K. Choi, E. F. Campana, and F. Stern, "Development and validation of a dynamic metamodel based on stochastic radial basis functions and uncertainty quantification," *Structural and Multidisciplinary Optimization*, vol. 51, no. 2, pp. 347–368, 2015.

[2] R. Pellegrini, A. Serani, M. Diez, J. Wackers, P. Queutey, and M. Visonneau, "Adaptive sampling criteria for multi-fidelity metamodels in CFD-based shape optimization," in *7th European Conference on Computational Fluid Dynamics (ECFD 7), Glasgow, UK, June*, 2018.

[3] J. Wackers, A. Serani, R. Pellegrini, R. Broglia, M. Diez, and M. Visonneau, "Adaptive multifidelity shape optimization based on noisy CFD data," in *International Conference on Adaptive Modeling and Simulation, ADMOS 2019, El Campello (Alicante), May*, 2019.

[4] P. Queutey and M. Visonneau, "An interface capturing method for free-surface hydrodynamic flows," *Computers & fluids*, vol. 36, no. 9, pp. 1481–1510, 2007.

[5] R. Broglia and D. Durante, "Accurate prediction of complex free surface flow around a high speed craft using a single-phase level set method," *Computational Mechanics*, vol. 62, no. 3, pp. 421–437, 2018.

[6] A. Serani, R. Pellegrini, R. Broglia, J. Wackers, M. Visonneau, and M. Diez, "An adaptive n-fidelity metamodel for design and operational-uncertainty space exploration of complex industrial problems," in *VIII International Conference on Computational Methods in Marine Engineering, MARINE 2019, Gothenburg, Sweden, May*, 2019.

[7] J. Wackers, M. Visonneau, A. Serani, R. Pellegrini, R. Broglia, and M. Diez, "Multi-fidelity machine learning from adaptive- and multi-grid RANS simulations," in *submitted to 33rd Symposium on Naval Hydrodynamics, Osaka, Japan, May*, 2020.

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Gradient Based Empirical Cumulative Distribution Function Approximation for Robust Aerodynamic Design

Andrea Bornaccioni,[1] ***Elisa Morales Tirado,***[2] ***Domenico Quagliarella***[2] ***and Umberto Iemma***[1]

[1]Roma Tre University, Italy – andrea.bornaccioni@uniroma3.it, umberto.iemma@uniroma3.it

[2]CIRA, Italy – e.moralestirado@cira.it, d.quagliarella@cira.it

Key words: Robust Design, RANS Solver, Adjoint Solver, Uncertainty Quantification, Risk Functions, Empirical Cumulative Distribution Function

A robust optimization approach based on the use of risk functions, namely VaR and CVaR [1], is presented together with an application to a robust aerodynamic design problem of the central airfoil of a tailless flying-wing aircraft at transonic cruise conditions. The characteristic feature of this design exercise is that for such a configuration the central section must provide not only a specified amount of lift but a definite nose-up pitching moment too. Thus, an additional aerodynamic constraint is required. The robust approach to this optimization problem helps to obtain solutions that do not deteriorate excessively in the presence of uncertainties on the airfoil contour or the operating conditions. The uncertainties on the airfoil section are due, for example, to machining tolerances, to deformations of the shape under load or the accumulation of debris on the wing surface. Furthermore, the aircraft may operate in speed and load conditions quite different from the design ones, and, hence they have to be considered as uncertain parameters too. Risk functions are here estimated using an approach based on the empirical cumulative probability distribution (ECDF). The quantities of interest (QoI) of the risk functions are the aerodynamic characteristics of the airfoil, namely lift, drag and pitching moment coefficients, which are computed solving the compressible Reynolds-averaged Navier-Stokes equations with the open source fluid-dynamic solver SU2 [3]. In the present work, we consider the effect of uncertainties in the operational conditions, such as Mach number and angle of attack. Furthermore, we take into account uncertainties on the pitching moment coefficient in order to account for changes in the aircraft center of gravity. The use of a RANS solver makes VaR and CVaR calculation costly from the computational point of view, and the characterizing aspect of the work is the use of techniques and methods for the reduction of the cost mentioned above. In particular, the estimate of the empirical CDF is obtained by exploiting the QoI gradients with respect to the uncertain variables computed through the discrete adjoint module of SU2 [4]. The ECDF is thus approximated with a first-order series expansion using efficiently calculated gradients from SU2 which, thanks to the adjoint method, are available at the computational cost of one CFD solution whatever the number of uncertainties is. The robust approach based on risk functions is, without doubt, more powerful and flexible than the deterministic multi-point methodology that is generally used in this type of problem, given that the high number of uncertain operational parameters makes the definition of the multi-point design problem quite tricky and cumbersome. On the other hand, however, the method of risk functions is computationally expensive due to the relatively high number of samples required to define the ECDF estimation. The adjoint-based approach presented here allows a substantial reduction of the computational cost needed to estimate the ECDF.

[1] D. Quagliarella, "Value-at-Risk and Conditional Value-at-Risk in Optimization Under Uncertainty," In *Uncertainty Management for Robust Industrial Design in Aeronautics*, 541-565 (Springer, Cham, 2019).

[2] M. A. Sargeant, T. P. Hynes, W. R. Graham, J. I. Hileman and M. Drela, "Stability of hybrid-wing-body-type aircraft with centerbody leading-edge carving. Journal of Aircraft," Journal of Aircraft **47**, 3 (2010).

[3] T. D. Economon, F. Palacios, S. R. Copeland, T. W. Lukaczyk and J. J. Alonso, "SU2: An open-source suite for multiphysics simulation and design," Aiaa Journal **54**, 3 (2015).

[4] T. A. Albring, M. Sagebaum and N. R. Gauger, “Efficient aerodynamic design using the discrete adjoint method in SU2," In *17th AIAA/ISSMO multidisciplinary analysis and optimization conference*, 3518 (2016).

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Assessment of Gradient-Based Surrogate Models for Robust Optimization in Computational Fluid Dynamics

Aldo Serafino,[1,2] ***Benoit Obert,***[1] ***and Paola Cinnella,***[2]

[1] Enertime, Courbevoie, France – aldo.serafino@enertime.com

[2] Lab. Dynfluid, École Nationale Supérieure d'Arts et Métiers, Paris, France – aldo.serafino@ensam.eu

Key words: Robust optimization, CFD for industrial applications, continuous adjoint method, discrete adjoint, gradient enhanced Kriging

Robust Design (RD) represents an important tool for the design of industrial products under uncertainty [1]. Because of the strong link between the concepts of design and optimization, RD is usually referred to as robust design optimization (RDO) or robust optimization (RO), as well. Several RO strategies are nowadays available: among them, some techniques can be considered rather prominent like Taguchi's [2] or the Low-Quantile one [3] or the "Horsetail Matching" [4].

The RO approaches studied in the literature often combine evolutionary optimization algorithms, like genetic algorithms (GA) and techniques for the quantification of the uncertainty (UQ). Unfortunately, the UQ for complex systems requiring to be simulated with Computational Fluid Dynamics (CFD) comes up against the high computational cost of CFD models for configurations of practical interest. As a consequence of this, the propagation of the uncertainty is not feasible with methods like Montecarlo (MC), even with improved sampling techniques (i.e., Latin Hypercube Sampling).

In the present work we investigate RDO techniques well-suited for industrial applications. The main requirements are: 1) greatest possible parsimony in terms of costly CFD simulations (for a given accuracy level) and 2) non intrusiveness (as in industry the use of black-box CFD codes can be usual). In this respect, a promising non-intrusive RDO technique has been introduced in [5], based on the coupling of two nested Kriging surrogates: the first one is used to compute the required statistics of the objective functions in the uncertain parameter space, while the second one is used to model the response of these statistics to the design variables. An expected improvement criterion is used to update the second Kriging surrogate during convergence towards the optimum. Such an approach has been successfully applied to the design of turbine blades for Organic Rankine Cycles [6] and to the RDO of the thermodynamic cycle [7]. The approach was shown to require $O(10 \times n \times d)$ function evaluations (with n the number of uncertain parameters and d the number of design variables) at the first generation of the GA, in order to generate the Kriging surrogates, which can be efficiently parallelized on a high-performance computer, while additional $O(10 \times n)$ evaluations are required for each update of the external Kriging surrogate. Typically, only a few updates during the GA iterations are sufficient to obtain an accurate approximation of the Pareto front. Despite considerable efficiency gains with respect to other surrogate models like Polynomial Chaos Expansion (see for instance [8]) or Probabilistic Collocation Method [9], the nested Kriging approach remains too expensive for industrial problems, especially if a large number of uncertain parameters has to be taken into account and if massively parallel computers are not available. Thus, RDO is typically limited to uncertain spaces of low to moderate dimensionality (up to about 8 uncertain parameters).

With the aim of enabling the application of RDO to higher dimensional parameter spaces and/or to more realistic and complex fluid flow problems, a further reduction of the computational cost is mandatory. In order to achieve this goal, in the present work we investigate a RDO methodology based on the coupling of a Gradient Enhanced Kriging (GEK) [10] for the UQ step with a Kriging surrogate for the optimization step. The gradients required for GEK are efficiently computed by means of the Continuous [11] or Discrete Adjoint method [12], allowing to strongly reduce the dependency of the computational cost of the UQ step on the number of uncertain

parameters. Specifically, the continous adjoint is suitable for a non-intrusive coupling with industrial CFD solvers, although the discretization of the adjoint equations and the implementation of the boundary conditions may be a delicate task and introduce errors in the calculated gradients. The continuous-adjoint GEK RDO is assessed against the discrete-adjoint one and a GEK using finite-difference approximations of the function derivatives in terms of accuracy and computational cost. For that purpose, we restrict our attention to an inexpensive test problem, namely, the supersonic flow in a quasi-1D nozzle, already studied in [13]. For this toy problem, the solutions of the Gradient-Enhanced RDO strategies can be compared to a reference RDO using Monte Carlo sampling for the UQ step and no surrogate modeling for the optimization step.

[1] H.G. Beyer and B. Sendhoff. "Robust optimization: A comprehensive survey." Computer Methods in Applied Mechanics and Engineering, 196(33), July 2007, pp. 3190-3218.

[2] G.Taguchi. *System of experimental design: engineering methods to optimize quality and minimize costs.* UNIPUB/Kraus International Publications, 1987.

[3] M. Moustapha, B. Sudret, J.M. Bourinet and B. Guillaume. "Quantile-based optimization under uncertainties usingadaptive Kriging surrogate models." Struct Multidisc Optim (2016) 54:1403-1421.

[4] L.W. Cook and J.P. Jarrett. "Horsetail matching: a flexible approach to optimization under uncertainty." Engineering Optimization(2018), 50:4, 549-567.

[5] P. Cinnella and E. Bufi. "Robust Optimization Using Nested Kriging Surrogates: Application to Supersonic ORC Nozzle Guide Vanes." ERCOFTAC Bulletin 110, mar 2017.

[6] E.A. Bufi and P. Cinnella. "Robust optimization of supersonic ORC nozzle guide vanes." J. Phys.(2017): Conf. Ser.821 012014.

[7] A. Serafino, B. Obert, H. Hagi and P. Cinnella. "Assessment of an Innovative Technique for the Robust Optimization of Organic Rankine Cycles." In *ASME TurboExpo2019, 17-21 June 2019, Phoenix, AZ (USA).*

[8] P. Cinnella and S.J. Hercus. "Robust Optimization of Dense Gas Flows Under Uncertain Operating Conditions." Computers Fluids, 39(10):1893 - 1908, 2010.

[9] G.J.A. Loeven. *Efficient Uncertainty Quantification in Computational Fluid Dynamics.* PhD thesis, TU Delft, 2010.

[10] J.H.S. de Baar, R.P. Dwight, and H. Bijl. "Improvements to Gradient-Enhanced Kriging Using a Bayesian Interpretation." International Journal for Uncertainty Quantification, 4(3), 2014.

[11] A. Jameson, L. Martinelli and N.A. Pierce. "Optimum Aerodynamic Design Using the Navier-Stokes Equations." Theoret. Comput. Fluid Dynamics, 10(1):213-237, January 1998.

[12] M.B. Giles, M.C. Duta, J.D. Muller and N.A. Pierce. "Algorithm Developments for Discrete Adjoint Methods." AIAA Journal, 41(2): 198-205, February 2003.

[13] P. Cinnella and M. Pini. "Hybrid Adjoint-based Robust Optimization Approach for Fluid-Dynamics Problems." In *54th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference.*

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Quantification of Parametric Uncertainty in Wind Farm Wake Modeling

Jincheng Zhang,[1] ***and Xiaowei Zhao,***[1]

[1]School of Engineering, The University of Warwick, Coventry, UK

Key words: Uncertainty Quantification, Wake Modeling, Bayesian Inference, Wind Farm Simulations

Accurate prediction of wind turbine wakes is essential for the optimal operation of wind farms. In order to achieve this, the parametric uncertainty of analytical wake model is investigated for the first time in this work. Specifically, Bayesian inference is employed for calibrating the wake model. A series of Large Eddy Simulations (LES) of wind farms is carried out with different turbine settings and the generated high-fidelity flow field data is used to infer the model parameters. After model calibration, the posterior model check shows that the predicted mean velocity profile with the quantified uncertainty matches well with the high-fidelity LES data. The prediction of other quantities, such as turbine power output, is also carried out. Further analysis demonstrates that the data-driven wake model with the model parameters specified by their posterior distributions can be seen as the stochastic extension of the original wake model. As most of the existing wake models are static, the resulting stochastic model shows a great advantage over the original model, as it can give not only the steady wind farm properties but also some estimations about the unsteadiness of the wind farm.

[1] P. Gebraad, F. Teeuwisse, J. Wingerden, P. A. Fleming, S. Ruben, J. Marden and L. Pao, "Wind plant power optimization through yaw control using a parametric model for wake effects - a CFD simulation study," Wind Energy, 19, 95-114, 2016.

[2] P. A. Fleming, P. Gebraad, S. Lee, J. Wingerden, K. Johnson, M. Churchfield, J. Michalakes, P. Spalart and P. Moriarty, "Evaluating techniques for redirecting turbine wakes using SOWFA," Renewable Energy, 70, 211-218, 2014.

[3] M.C. Kennedy and A. O'Hagan, "Bayesian calibration of computer models," Journal of the Royal Statistical Society: Series B (Statistical Methodology), 63 (3): 425-464, 2001.

[4] S. H. Cheung, T. A. Oliver, E. E. Prudencio, S. Prudhomme and R. D. Moser, "Bayesian uncertainty analysis with applications to turbulence modeling," Reliability Engineering & System Safety, 96(9), 1137-1149, 2011.

[5] J. Zhang and S. Fu, "An efficient Bayesian uncertainty quantification approach with application to k-ω-γ transition modeling," Computers & Fluids, 161: 211-224, 2018.

[6] J. Zhang and S. Fu, "An efficient approach for quantifying parameter uncertainty in the SST turbulence model," Computers & Fluids, 181: 173-187, 2019.

SF2 – Methodology IV

Session Chair: D. Lucor

Auditorium

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Multifidelity Uncertainty Quantification for Fluid Dynamics applications

Alex A. Gorodetsky,[1] ***Gianluca Geraci,***[2] ***Michael S. Eldred,***[2] ***and John D. Jakeman,***[2]

[1]Aerospace Engineering, University of Michigan, MI, USA – goroda@umich.edu

[2]Optimization and Uncertainty Quantification, Sandia National Laboratories, NM, USA – {ggeraci,mseldre,jdjakem}@sandia.gov

Key words: Uncertainty quantification, Multifidelity, Fluid Dynamics

Creating predictive numerical simulations requires characterizing and quantifying the impact of uncertainty. In computational fluid dynamics (CFD) applications, computationally expensive models (Direct Numerical Simulation, Large Eddy Simulation, *etc.*) are often required to resolve all the important spatial and temporal scales of the solution. Moreover, practical engineering systems which involve fluid dynamics phenomena very often also comprise additional physics (as for instance radiation transport [1], combustion [2], *etc.*) whose accurate solution further increases the computational burden. In such situations the extreme computational cost of the numerical simulation coupled with a very large number of uncertainty sources heavily limits our ability to create large enough datasets for accurate Uncertainty Quantification (UQ).

Indeed, despite huge advances in UQ algorithms in the last two decades, UQ for realistic systems remains prohibitive in these extreme computational regimes where even a few simulations can be prohibitively expensive. To overcome this issue, the concept of multifidelity UQ has been introduced. This concept closely follows ideas that matured in the field of optimization [3, 4]. Several flavors of multifidelity UQ have been introduced, and they are all based on the aggregation of large numbers of lower accuracy realizations with a limited number of high-fidelity data. Historically the most natural way of deriving lower accuracy models has been to directly leverage coarsening along the spatial and temporal dimensions [9, 10, 11].

Recently, it has become increasingly important to also consider different modeling choices that share similar physics during multifidelity analysis. In CFD applications for turbulence simulations one might rely on either Large Eddy Simulations or Reynolds Averaged Navier-Stokes equations to produce very rough approximations of some global trends in Direct Numerical Simulations. In these circumstances, existing algorithms must be adapted to efficiently exploit relationship among models (see for instance [8, 7]).

In this work we consider algorithms for propagating uncertainty through computational simulation models of varying fidelities. Our goal is to estimate, or predict, quantities of interest from a specified high-fidelity model when only a limited number of these simulations is available. To aid in this task, lower fidelity models can be used to reduce the uncertainty of the high-fidelity predictions. We discuss existing sampling-based and surrogate-based algorithms from an information transfer perspective, and we first demonstrate the way in which these algorithms leverage information (e.g., correlations and discrepancies) between models. We show that algorithms based on recursion, e.g., multi-fidelity Monte Carlo [8] or recursive co-kriging [12], can inefficiently make full use of available information. We then propose new approaches based on approximate control variates (for sampling-based variance reduction) [6] and Bayesian networks (for surrogate-based approaches) [5] that mitigate these problems and achieve significant, sometimes reaching an order of magnitude, gains in efficiency. Numerical results for the proposed approach will be reported for several test cases and possibly for more realistic applications.

[1] L. Jofre, G. Geraci, H. Fairbanks, A. Doostan and G. Iaccarino, "Multi-fidelity uncertainty quantification of irradiated particle-laden turbulence," arXiv preprint arXiv:1801.06062 (2018).

[2] X. Huan, C. Safta, K. Sargsyan, G. Geraci, M.S. Eldred, Z.P. Vane, G. Lacaze, J.C. Oefelein and H.N. Najm "Global Sensitivity Analysis and Estimation of Model Error, Toward Uncertainty Quantification in Scramjet Computations," AIAA Journal **56:**3, pp. 1170–1184 (2018).

[3] M. Alexandrov, J. E. Dennis, Jr., R. M. Lewis, and V. Torczon "A trust-region framework for managing the use of approximation models in optimization." Structural Optimization, **15**, pp. 16–23 (1998).

[4] M.S. Eldred and D.M. Dunlavy. "Formulations for surrogate-based optimization with data fit, multifidelity, and reduced-order models." In *AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference. American Institute of Aeronautics and Astronautics (AIAA)*, (AIAA 2006).

[5] A. Gorodetsky, G. Geraci, M.S. Eldred, J.D. Jakeman "Latent Variable Networks for Multifidelity Uncertainty Quantification and Data Fusion." In *7th European Conference on Computational Fluid Dynamics (ECFD 7)*, (International Center for Numerical Methods in Engineering CIMNE, 2018).

[6] A. Gorodetsky, G. Geraci, M.S. Eldred, J.D. Jakeman "A Generalized Framework for Approximate Control Variates'.' arXiv preprint arXiv:1811.04988 (2018).

[7] G. Geraci, M.S. Eldred, G. Iaccarino. "A multifidelity multilevel Monte Carlo method for uncertainty propagation in aerospace applications." In *19th AIAA Non-Deterministic Approaches Conference (AIAA)*, (AIAA 2017).

[8] B. Peherstorfer, K. Willcox and M. Gunzburger "Optimal model management for multifidelity Monte Carlo estimation." SIAM Journal on Scientific Computing, **38**:5, pp. A3163–A3194 (2016).

[9] M.B. Giles "Multilevel Monte Carlo path simulation." Oper. Res., **56**, pp. 607–617 (2008).

[10] M.B. Giles "Multilevel Monte Carlo methods." Acta Numerica, **24**, pp. 259–328 (2015).

[11] A. Haji-Ali, F. Nobile, R. Tempone "Multi-index Monte Carlo: when sparsity meets sampling" Numerische Mathematik, **132**(4), pp. 767-806 (2016)

[12] L. Le Gratiet, J. Garnier "Recursive co-kriging model for design of experiments with multiple levels of fidelity" International Journal for Uncertainty Quantification, **4**(5), pp. 365-386 (2014)

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Accurate statistical estimators by continuation MLMC for engineering design problems

Fabio Nobile, Quentin Ayoul-Guilmard and Sundar Ganesh

CSQI, École Polytechnique Fédérale de Lausanne, Switzerland
{fabio.nobile,quentin.ayoul-guilmard,sundar.ganesh}@epfl.ch

Key words: uncertainty quantification; optimisation under uncertainty; multi-level Monte Carlo; parallel computing; fluid dynamics.

An important challenge in civil engineering is to study the effects of wind uncertainties on structural loading for use in risk-averse design. Optimising the design of a structure for safety without factoring in these uncertainties can result in an unsafe or non-cost-optimal design. To control the effects of the uncertainties on structural loading, one has to leverage a multitude of concurrent design parameters, one of which is the shape of the structure. The optimal design problem can be written in abstract terms as

$$\begin{aligned} d^* &= \operatorname{argmin}\{J(d) : d \in D\} \\ \text{with} \quad J(d) &= \mathbb{E}\left(\phi\left(\hat{Q}(d,\cdot)\right)\right) + C(d-d_0). \end{aligned} \tag{1}$$

Here, $C(d-d_0)$ is a function that penalises the distance of a design d from a preferred design d_0; D is the design space; $\hat{Q}(d,\omega) := Q(u(\cdot,\omega,d))$ is the output quantity, whose statistics $\mathbb{E}(\phi(\hat{Q}))$ we aim to optimise, and which depends on the solution u of a Partial Differential Equation (PDE) with uncertain parameters ω that describes the underlying physics:

$$\begin{cases} \mathcal{L}u = 0 & \text{in } X_d, \\ f(u) = 0 & \text{on } \Gamma_d, \\ u = u_\omega & \text{on } \Gamma_\omega. \end{cases} \tag{2}$$

The domain boundary is partitioned as $\partial X_d = \Gamma_d \cup \Gamma_\omega$ where Γ_d is the shape-dependent part of the boundary on which the boundary condition defined by f is prescribed and Γ_ω is the portion on which the uncertain value u_ω is applied (e.g. inflow wind condition). Through different choices of ϕ and C, the objective function being minimised can depend on different types of statistics, ranging from the mean-variance risk measure to Conditional Value at Risk (CVaR), as well as on design-dependent costs. The solution of the optimisation problem can be solved in a number of ways, one of which is through gradient-based methods. These methods require the computation of the sensitivities $\nabla_d J$, which involve the solution of the adjoint problem corresponding to (2). In order to solve this optimisation problem, a number of challenges exist that we attempt to address in this work.

Of utmost importance is the accurate and efficient estimation of the target statistics and its sensitivity with respect to design parameters to enable the use of gradient-based optimisation techniques. We propose novel Multi-Level Monte Carlo (MLMC) estimators for these statistics [2, 3], and present a systematic procedure to adaptively tune these estimations, based on error indicators [4]. We also discuss possible ways of estimating the sensitivities $\nabla_d J$ by combining MLMC estimators with the adjoint equations corresponding to problem (2).

MLMC algorithms are well-suited to parallelisation aimed towards high-performance exascale computing, for which we use the PyCOMPSs [5] and Hyperloom [1] schedulers; this implementation is a joint work with the Centre Internacional de Mètodes Numèrics en Enginyeria, the Barcelona Supercomputing Centre and the Technische Universität München.

We illustrate these accurate and cost-efficient statistical estimations on numerical examples of engineering interest inspired by civil engineering and aerodynamics applications, featuring fluid-flow problems in combination with various uncertain inlet boundary conditions.

[1] Vojtěch Cima, Stanislav Böhm, Jan Martinovič, Jiří Dvorskỳ, Kateřina Janurová, Tom Vander Aa, Thomas J. Ashby, and Vladimir Chupakhin. Hyperloom: a platform for defining and executing scientific pipelines in distributed environments. In *Proceedings of the 9th Workshop and 7th Workshop on Parallel Programming and RunTime Management Techniques for Manycore Architectures and Design Tools and Architectures for Multicore Embedded Computing Platforms*, pages 1–6. ACM, 2018.

[2] Sebastian Krumscheid and Fabio Nobile. Multilevel Monte Carlo approximation of functions. *SIAM/ASA Journal on Uncertainty Quantification*, 6(3):1256–1293, 2018.

[3] Michele Pisaroni, Sebastian Krumscheid, and Fabio Nobile. Quantifying uncertain system outputs via the multilevel Monte Carlo method — Part I: central moment estimation. Technical Report 23.2017, MATHICSE, EPFL, 2017.

[4] Michele Pisaroni, Fabio Nobile, and Penelope Leyland. Continuation Multilevel Monte Carlo evolutionary algorithm for robust aerodynamic shape design. *Journal of Aircraft*, 56(2):771–786, 2019.

[5] Enric Tejedor, Yolanda Becerra, Guillem Alomar, Anna Queralt, Rosa M. Badia, Jordi Torres, Toni Cortes, and Jesús Labarta. PyCOMPSs: Parallel computational workflows in Python. *The International Journal of High Performance Computing Applications*, 31(1):66–82, 2017.

This research is being carried out within the ExaQUte project, funded by the European Union's Horizon 2020 research and innovation program under grant agreement No. 800898.

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Scalable distributed asynchronous Monte Carlo algorithms workflow design

Riccardo Tosi,[1] ***Ramon Amela,***[2] ***Jordi Pons,***[3] ***Rosa M. Badia*** [4] ***and Riccardo Rossi*** [5]

[1]CIMNE, Barcelona, Spain – rtosi@cimne.upc.edu

[2]BSC, Barcelona, Spain – ramon.amela@bsc.es

[3]CIMNE, Barcelona, Spain – jpons@cimne.upc.edu

[4]BSC, Barcelona, Spain – rosa.m.badia@bsc.es

[5]CIMNE, UPC, Barcelona, Spain – rrossi@cimne.upc.edu

Key words: Uncertainty quantification, HPC, Monte Carlo, Multi Level Monte Carlo, Fluid Dynamics

The aim of this work is to build a highly efficient framework in order to run Monte Carlo algorithms, such as standard Monte Carlo (MC), Multi Level Monte Carlo (MLMC) or Continuation Multi Level Monte Carlo (CMLMC) [3], in distributed environment. In the proposed models we work with adaptive mesh refinement, and we propose two different approaches:

- mesh generation and simulation running one after the other for each simulation,
- storage of the mesh for each accuracy level.

The latter optimizes the execution times, but losing mesh accuracy.

The whole work is developed inside KratosMultiphysics [1] (Kratos)[1], "a framework for building parallel, multi-disciplinary simulation software". The design is fully no file-based, meaning that the mesh has been read only once, and then it has been retrieved through a serializer for all the independent simulations, gaining remarkable computational time. The workflow is integrated with PyCOMPSs [2][2], a library which eases the running of applications in distributed environments. The critical point is to set up the optimal scheduling of the simulation onto the available hardware, due to the presence of a lot of tasks with really different granularity. The aim is to have a dynamic scheduling process, able to distribute the parallel Kratos simulations.

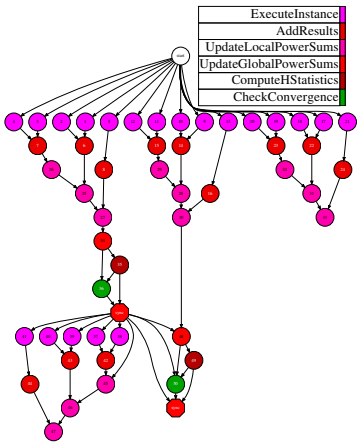


Figure 1: Graph connections of asynchronous MC algorithm dependencies.

A key element in distributed environments is to run asynchronous algorithms. Currently, asynchronous MC and synchronous MLMC are currently working, while asynchronous MLMC will be running soon. These algorithms present the great advantage of avoiding synchronization points that leave the machine empty when computing the statistics. Our idea is to run many MC/MLMC batches and to synchronize only one batch per time, that update the global statistics, while the others run and fill the machine. Therefore, we have four levels of parallelism:

- between batches,
- between levels,

[1]https://github.com/KratosMultiphysics/Kratos
[2]https://github.com/bsc-wdc/compss

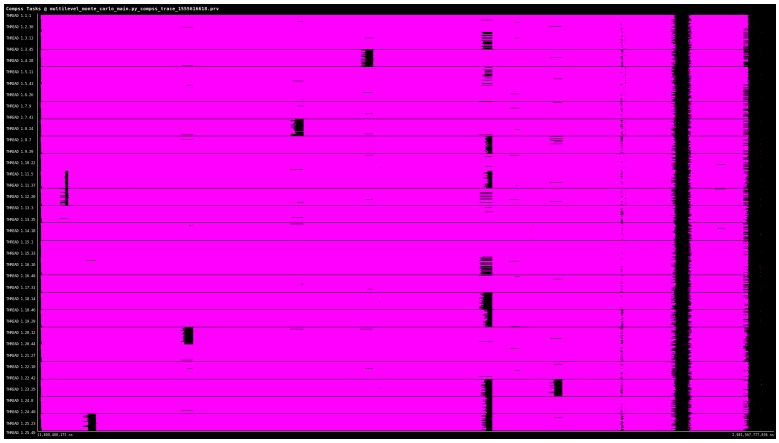


Figure 2: Trace of asynchronous MC execution with 25 nodes, 11 convergence checks and 110000 samples.

- between samples on each level,
- on the simulation of each sample.

The computation of the local statistics of each batch is computed in mini-batches, improving the performance of the algorithm.

The use of this framework is of interest for all complex engineering problems. In particular, our first application was dedicated to the statistical analysis of a 2d airfoil with random angle of attack and Mach number.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 800898.

[1] Dadvand, Pooyan and Rossi, Riccardo and Oñate, Eugenio, "An object-oriented environment for developing finite element codes for multi-disciplinary applications," Archives of computational methods in engineering **17**, pp. 253-297 (2010).

[2] Amela, Ramon and Ramon-Cortes, Cristian and Ejarque, Jorge and Conejero, Javier and Badia, Rosa M "Executing linear algebra kernels in heterogeneous distributed infrastructures with PyCOMPSs," Oil & Gas Science and Technology–Revue d'IFP Energies nouvelles **73**, 47 (2018).

[3] Pisaroni, Michele and Nobile, Fabio and Leyland, Pénélope "A continuation multi level Monte Carlo (C-MLMC) method for uncertainty quantification in compressible aerodynamics," Computer Methods in Applied Mechanics and Engineering **326**, pp. 20-50 (2017).

Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics
11–13 September 2019, Pisa, Italy

Towards risk averse structural design optimization with uncertain wind loading: Two-dimensional benchmarks

B. Keith,[1] ***A. Kodakkal,***[1] ***M. Nuñez,***[2] ***R. Rossi,***[2] ***R. Tosi,***[2] ***B. Wohlmuth,***[1] ***and R. Wüchner***[1]

[1]Technische Universität München, Germany —
{keith,wohlmuth}@ma.tum.de, {anoop.kodakkal,wuechner}@tum.de

[2]CIMNE, Barcelona, Spain — {rrossi,rtosi}@cimne.upc.edu

Key words: Wind loading, stochastic computational wind engineering, turbulent flow, shape optimization, risk-averse design

This talk will explore a longstanding question in civil engineering from a contemporary viewpoint: How best to design a structure under uncertain environmental conditions? Modern buildings must satisfy a number of well-defined, but computationally challenging, serviceability and failure criteria. For instance, tall or irregular structures are subjected to enormous stresses imparted by uncertain wind loading from turbulent atmospheric boundary layer flows and yet they must remain stable and reliable. Moreover, architects and other planners generally have specific design objectives and fixed expenditures for the final project. Each of these interests must be fully addressed long before construction begins. Informed by modern principles in risk-averse engineering design [1, 2], we will balance both sets of criteria and objectives in order to arrive at a new class of shape-optimization problems with uncertainty. We will then present and analyze a number of two-dimensional benchmark problems in this class which pave the way to the full three-dimensional setting and an answer to the question posed above.

This work was supported by ExaQUte, a European project funded by the European Unions Horizon 2020 research and innovation programme, that aims at constructing a framework to enable Uncertainty Quantification (UQ) and Optimization Under Uncertainties (OUU) in complex engineering problems using computational simulations on Exascale systems.

[1] R Tyrrell Rockafellar and Johannes O Royset, *On buffered failure probability in design and optimization of structures*, Reliability Engineering & System Safety **95** (2010), no. 5, 499–510.

[2] R Tyrrell Rockafellar and Johannes O Royset, *Engineering decisions under risk averseness*, ASCE-ASME Journal of Risk and Uncertainty in Engineering Systems, Part A: Civil Engineering **1** (2015), no. 2, 04015003.