ISSUE 4

ARIA Newsletter

April 2022

Inside This Issue

***ARIA** aims to form an international and intersectoral network of organizations working on a joint research program in numerical modelling, specifically in the fields of model reduction and convergence between data and models.*

EDITORIAL

Welcome to the fourth issue of the ARIA newsletter.

The first half of the ARIA journey is already behind us. In this first quarter of the third year , step by step, we continue to move forward, always with our goals in mind. We are also happy that the secondments have been resumed in the project after 2 years of interruption. Some results and contents of the secondments are described below in this issue. In the next periods to come, we will achieve crucial goals and reach important milestones of the project.

ARIA's members and partners have continued to cooperate strongly in publishing new articles that are available on our project website: https://project.inria.fr/aria/publications/

We organized the 3rd online free seminar open to public on 10 March 2022 on the topic of numerical modeling of Aortic Abdominal Aneurysms. The next seminar will be in September 2022 on the topic of renewable energy. We will keep you informed of the date and registration process.

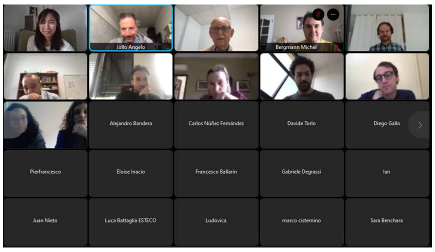
The next issue will be published in September 2022 in which we will give you updates on the projects workshops, continue to report results from our secondments, selecting highlights on the major research results.

The project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant No 872442

ARIA'S 3rd Online Seminar – 10 Mars 2022

ARIA is a Horizon 2020 project under the programme Marie Sklodowska-Curie Actions - Re-search and Innovation Staff Exchange (RISE) for boosting the carrier perspectives of researchers through staff exchange.

The third online seminar of ARIA project focused on the topic of numerical modeling of Aortic Abdominal Aneurysms with 42 participants.



Tutorials of this seminar: https://project.inria.fr/aria/seminar-march-2022/

The talks were given by scientists of ARIA project.

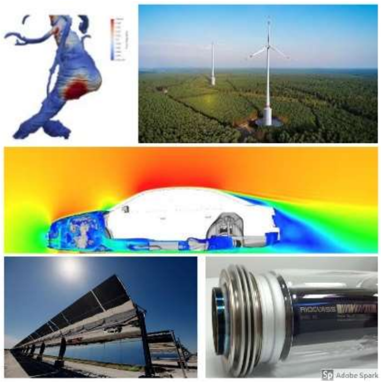
Florian Bernard from the start-up company Nurea started the seminar with the talk on "*Why biomechanics will help clinicians ?*" . In his talk, he went through daily clinicians challenges, to try to understand why biomechanics will help in the decision making process, and what are the last scientific barriers that we need to face.

Ludovica Saccaro from Inria Bordeaux presented on "*Parametrisation and Generation Abdominal Aortic Aneurysm in Reduced Dimensional Spaces*". She presented a new generative model of aneurysm shapes that allows to employ unsupervised learning approaches to generate statistically significant new aneurysms. And this new set of data, that can be arbitrarily large, can be used to conceive and assess the reliability of new premature rupture risk indicator.

Karol Calò and Valentina Mazzi from Politecnico di Torino continued to talk about "In silico characterization of near-wall and intravascular hemodynamics in Abdominal Aortic Aneurysms". They presented advanced tools of analysis for the hemodynamic characterization and visualization of near-wall and intravascular flow features in personalized CFD models of AAAs, with the aim of enriching the current understanding of the hemodynamic environment characterizing the AAA disease.

Francesco Ballarin from Catholic University of the Sacred Heart in Italy – a new member of ARIA consortium then presented on "Optimal control and reduced order models: enablers to assimilate boundary conditions from data for cardiovascular simulations". In his talk, he summarized how the formulation of the assimilation task as an optimal control problem, and its reduction by means of reduced order modelling techniques, can contribute to devising the automated procedures.

To end the seminar, Simona Perotto from Politecnico di Milano brought audience through the topic of "Hierarchical model reduction in haemodynamics: in terms of advances and challenges" in which she focused on the most recent advances of an approach, which include the generalization of HiMod to a parametric setting and the proposal of a specific procedure to manage bifurcation geometries. The talk also concluded a quick panorama on the issues currently under investigation.



The four case studies to be implemented in ARIA:

- *Nurea - a test case on vascular disease problem*
- *VW – a test case on Ahmed body problem*
- *Valorem – a test case on wind engineering problem*
- *Virtualmech – a test case on heat transfer problem*

In silico characterization of Abdominal Aortic Aneurysms hemodynamics

Karol Calò/Valentina Mazzi/Umberto Morbiducci (Politecnico di Torino)

Abdominal aortic aneurysm (AAA) is a pathological condition consisting of an unphysiological localized enlargement (greater than 3 cm) of the abdominal aortic lumen, a consequence of the structural and mechanical degradation of the vessel wall. The current clinical standards regulating AAA treatment are based on aneurysm size and growth rate. In particular, indications for surgical treatment depend on the estimated maximum aortic diameter, with a suggested critical threshold value of 5.5 cm, or on AAA growth rate, with a critical threshold of 1 cm/year. However, these diameter-based criteria for surgical intervention have been widely recognized as insufficient.

The onset and development of the aneurysmatic disease is still unclear, but it is widely accepted the hypothesis that AAA pathogenesis is highly influenced by different risk factors, such as systemic (hypertension, obesity, etc.) and biomechanical (pressure forces, wall stresses). Among the latter, hemodynamics plays a key role in modulating the pathogenesis of the AAA disease by regulating multiple aspects of vascular pathophysiology. It is well known, in fact, that various vascular pathologies, including aneurysms, tend to develop preferentially where blood flow patterns are more complex and intricate. Moreover, hemodynamic forces may contribute to intraluminal thrombus formation and growth, and to aneurysm rupture. All of this has led to the formulation of the so-called "hemodynamic hypothesis", according to which there is a localizing hemodynamic risk factor for vascular disease, characterized by a complex interplay between vessel geometry, wall shear stress (WSS) and intravascular flow. WSS is defined as the tangential force exerted by the flowing blood on the endothelial lining covering the intima surface of vascular wall. In the presence of aggravating flow events, WSS may trigger abnormal biological responses such as endothelial dysfunction/injury, increased wall permeability, and platelets activation/aggregation/deposition which are responsible for the thrombotic disease, thus making WSS a marker of thrombus formation. Besides the WSS, also the organization of intravascular blood flow patterns plays an important role in the aneurysmatic disease progression. In particular, flow recirculation is positively correlated with biomarkers of thrombotic risk. Moreover, the presence and organization of vortical structures affect platelets dynamics, and helical flow plays a beneficial role in suppressing flow reversal and recirculation, reducing platelet adhesion and thrombotic risk.

For all these reasons, the study of local arterial hemodynamics is essential for a better understanding of the risk associated with the onset and progression of AAA vascular disease. In this context, the personalized Computational Fluid Dynamics (CFD) represents the most powerful tool to model blood flow in silico. Recent advances in medical imaging and CFD have allowed to model local blood flow patterns in realistic, personalized cardiovascular models, fostering understanding of the relationship between hemodynamics and arterial homeostasis. In this scenario, our contribution to the ARIA project aims at providing advanced tools of analysis for the hemodynamic characterization of personalized CFD models of AAA. In a wider perspective, such tools could be useful to identify more accurate clinical markers for AAA risk prediction, integrating the current clinal standards in the decision-making process.

In this case, several reasons can be given for the change of trend. Phenomena involving domain movements are variations on themes of fairly similar solutions (in the sense of some well-defined norm) unless there are dramatic changes in the set of parameters strongly affecting the solution (e.g. large variety of displacements or extreme changes in obstacle geometries). This helps the research of a Reduced Basis (RB) which is more sensitive to the variation of the parameter and, thus, allows to reduce the degrees of freedom.

A numerical reason for reducing the problem in foreground instead that in the background consists in the recovery of the RB. Typically it is sought by exploiting data from different full simulations. Let us suppose to have different simulations of the same phenomenon for different velocities of displacement of the obstacle. This means that, for a given time instant, for some simulations some cells in the background do not exist because they are covered by the foreground and, consequently no data are directly available on those cells. This implies a loss of information and a loss of quality for the RB. On the contrary, this never happens for the foreground because the movement never affects the existence of the cell but only its shape. Thus it is always possible to collect information to store in a dataset and, in a training stage, to build a RB.

MEMPHIS team in INRIA Bordeaux Sud-Ouest and the OPTIMAD engineering s.r.l. company are exploiting the two approaches (the one here described and the one discussed in the previous article) by preserving the possibility to parallelise all the processes and to consider a wide range of possible movements for incompressible flows.

More specifically, near-wall flow was characterized analyzing those WSS features (e.g., WSS magnitude/direction, WSS fixed points and manifolds) known to be involved in the pathophysiological mechanisms leading to AAA development and progression, whereas intravascular blood flow was investigated through the identification/characterization of internal vortical and helical structures, flow separation and stagnation.

The application of this framework combining patient-specific CFD and advanced fluid mechanics tools of analysis in prospective and/or longitudinal studies could contribute to increase the chance of finding mechanistic explanations to clinical observations, and to provide potential clinical markers for rupture risk prediction.

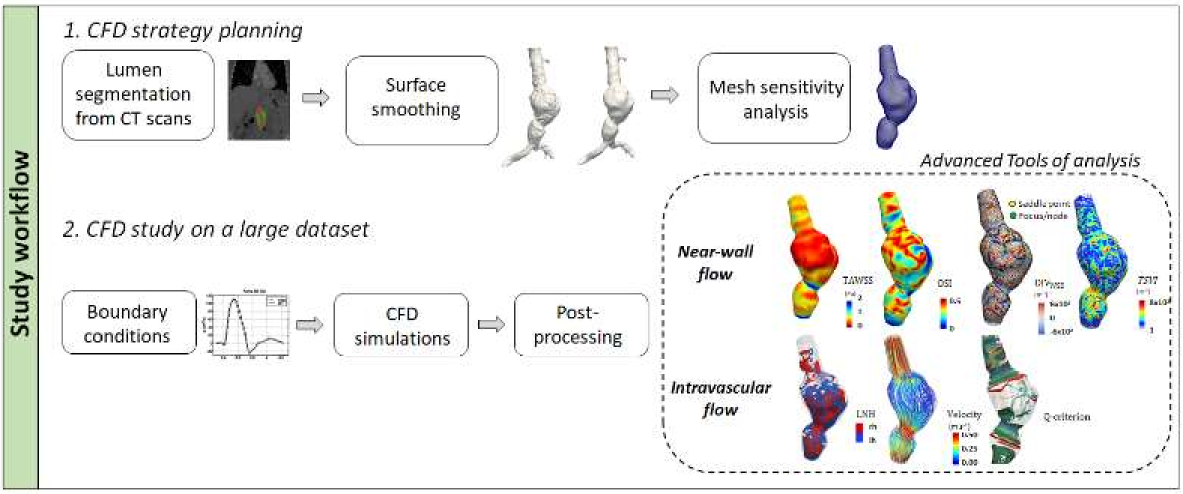


Fig 1. Study workflow of patient-specific AAA local hemodynamics.

Adaptive sampling and Active Subspaces

Gabriele Degrassi (ESTECO), Mauro Munerato (ESTECO), Angela Scardigli (OPTIMAD), Laura Balasso (OPTIMAD)

During the secondments carried out by Gabriele Degrassi and Mauro Munerato from ESTECO, and Angela Scardigli and Laura Balasso from OPTIMAD, two main topics were discussed as part of the ARIA project: adaptive sampling for ROMs and Active Subspaces for dimensionality reduction.

Adaptive sampling for Reduced Order Models

This analysis was carried out with the purpose of finding a proper way of adding new samples efficiently to the dataset to improve the ROM accuracy over the whole parameter space. The index used to estimate the ROM performance is the leave-one-out cross-validation error and its trend was employed to drive different sampling strategies.

Two models were used as test cases: the viscous analysis of a 5-parameters airfoil, simulated through XFOIL, and the incompressible turbulent flow past the Ahmed body, parameterized as a function of the slant angle varying from 15° to 35°.

The whole study was conducted thanks to OPTIMAD technology for ROMs training, error estimation and usage, and ESTECO products modeFRONTIER, for process automation and design optimization, and VOLTA, for Simulation Process and Data Management.

The first step was to automate the sampling process and modeFRONTIER proved to be very effective, resulting in the structure described in figure 1.1.

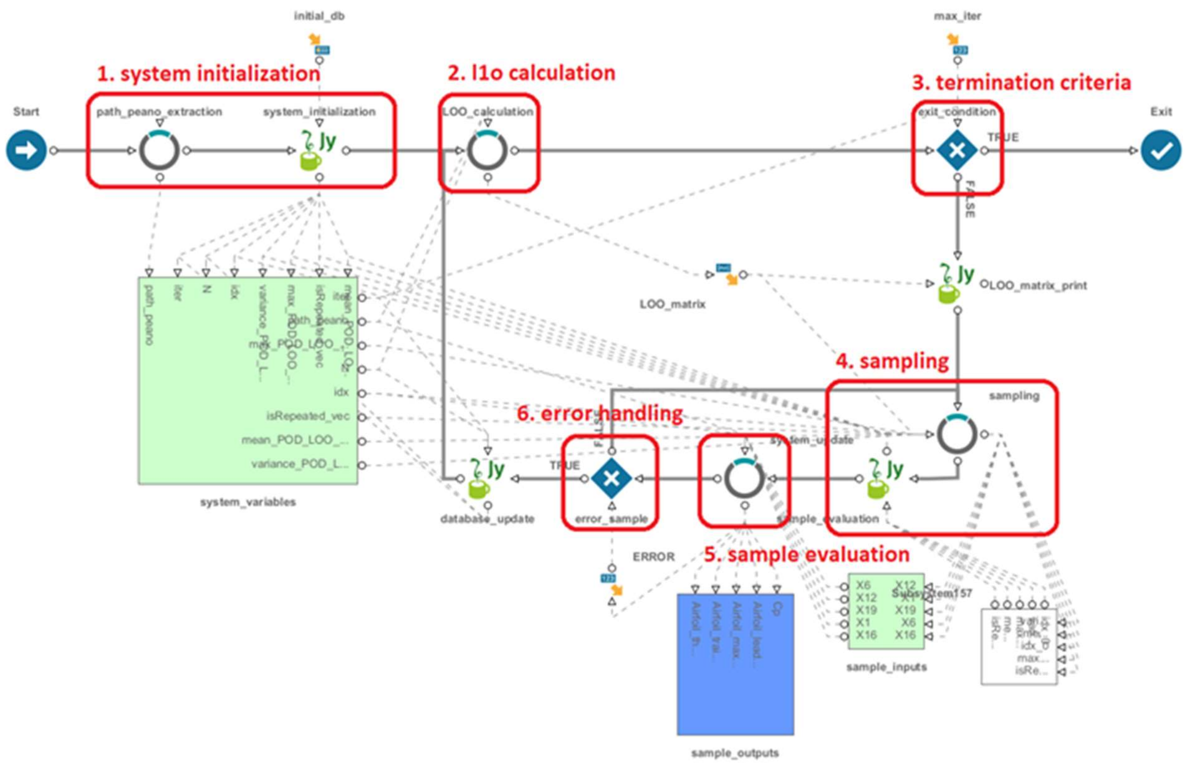


Figure 1.1: Process automation workflow for adaptive sampling

In particular, the study focused on the sampling phase, testing different strategies:

- MACK/Lipschitz sampling (modeFRONTIER algorithms);
- Error maximization using an error predictor response surface;
- Gaussian Mixture Distribution (with Incremental Space Filler)

For the airfoil problem, the analysis was carried out starting from 21 samples as initial database and 50 more were added using the different strategies. Furthermore, different starting datasets were tested. Instead, for the Ahmed body simulation, the starting dataset was the simulation of the two extreme configurations: 15° and 35°, and 18 designs were added.

To avoid biases due to different initial datasets, the leave-one-out error used to compare the different strategies was computed over a fixed dataset.

The results were quite promising for some of the strategies, when compared to a random sampling, especially for small sizes of the training set. The charts in figure 1.2 show mean and standard deviation values for l1o error at different phases of the sampling for all the analyzed strategies.

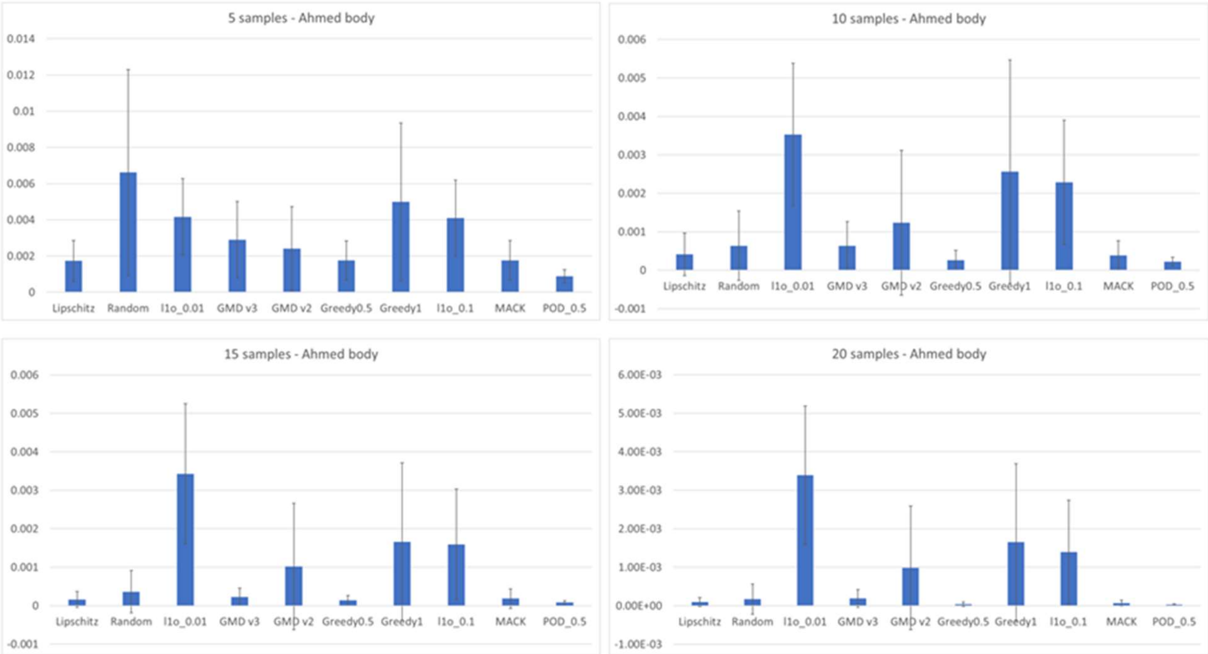


Figure 1.2: Mean and Standard deviation l1o errors at different phases of the adaptive sampling strategies for Ahmed body simulation.

In the end, the study clearly showed that Lipschitz and MACK implementations present in modeFRONTIER seem to be quite efficient. GMD (Gaussian Mixture Distribution) strategy also worked fine but with some parameter tuning requirements. The error maximization strategy, instead, still requires further investigation to find the proper setup, as in the tests it proved to be worse than random sampling.

To give an idea, for the Ahmed body test case we expected to have more points added in the area around 25° and 29°, when flow separation occurs on the slanted surface, but for some strategies this wasn't the case, as pictured in figure 1.3.

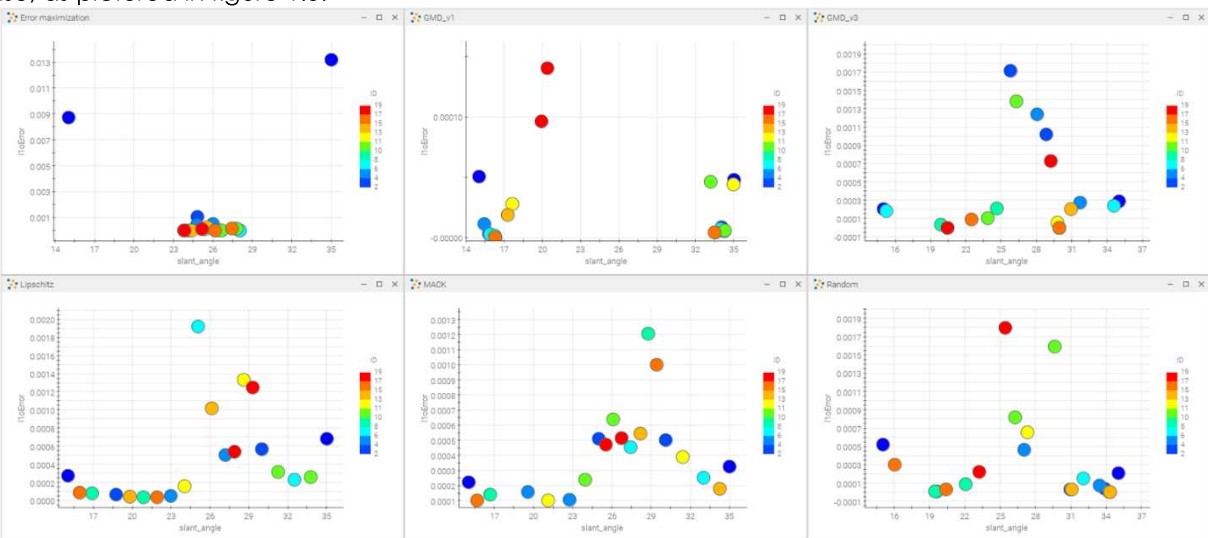


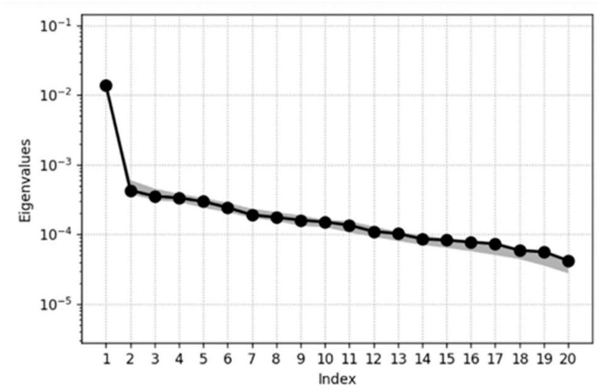
Figure 1.3: Bubble charts showing the slant angle on x-axis, the l1o error on the y-axis and the iteration as the color.

Active Subspaces

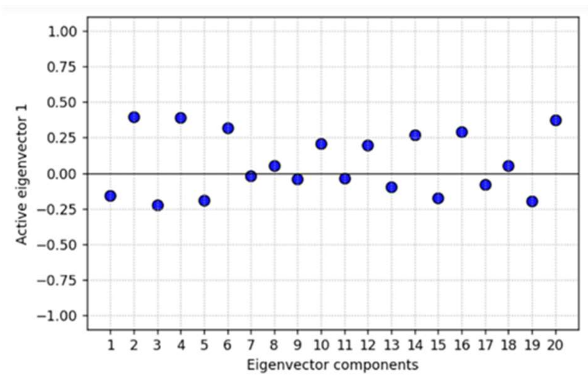
Modeling high dimensional problems can be challenging and the reduction of the input space is often needed to perform optimization or approximation. In order to properly reduce the dimensionality of the input space, one can consider that sometimes models defined on high dimensional domains vary primarily along a few directions. Classic sensitivity analysis can only be applied when these directions correspond to coordinates directions, while methods like PCA (Principal Component Analysis) do not consider the function's shape. Active Subspaces (AS) method instead, allows to detect the directions of strongest variability of a function using evaluations of the gradient and to approximate the function on a low-dimensional subspace of the domain, i.e., the active subspace.

The test case used to assess this method is the flow past 2D airfoils with varying shape, the same used for the sampling, but parametrized with 20 deformation coefficients instead of 5. The pressure distribution on each airfoil is obtained via XFOIL simulations, and the resulting lift coefficient (CL) is considered as a function defined on the 20-dimensional input space. The aim is to exploit AS to approximate the CL function on a low dimensional domain by detecting few directions along which it varies the most.
Since AS requires evaluations of the gradient on sample points, three different methods of approximation were employed: (i) finite differences computed by running additional simulations; gradient extracted from a surrogate (ii) local and (iii) global model (Gaussian Process Regression) interpolating data. Results are presented for method (iii).

The gradient is used to compute a rotation W of the input space such that the eigenvalues associated to each direction quantify how strongly the function varies along that direction. In Figure 2.1 are represented the eigenvalues in decreasing order and the components of the first direction of the rotated space. There is a large difference between the first and the second eigenvalue, suggesting that the CL function varies primarily along the first direction of the rotated space.



(a)



(b)

Figure 2.1: (a) eigenvalues associated to each direction of the rotated input space and (b) the components of the first eigenvector.

In fact, if we project the sample points on the subspace defined by the first direction only, we obtain a point cloud that is not so dispersed with respect to an approximating univariate response surface (Figure 2.2).

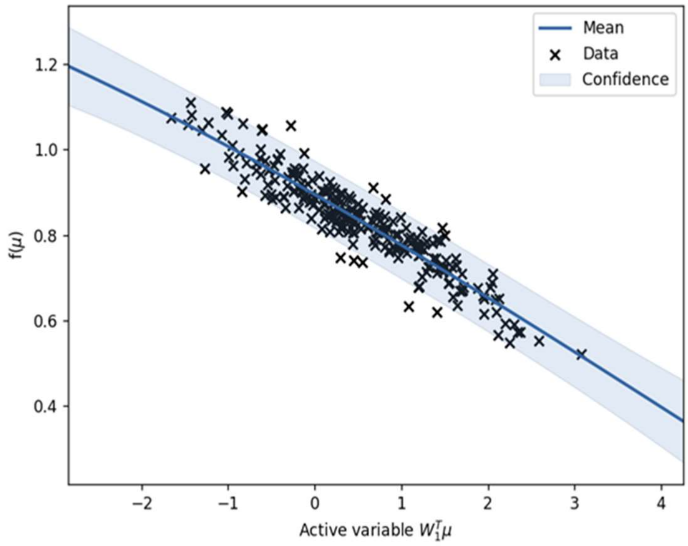


Figure 2.2: sample points projected on the first direction of strongest variability.

In order to assess how well the function can be approximated on a subspace of dimension N, the following steps were followed for each N (from 1 to 20): (i) the sample points are projected on the subspace defined by the first N direction of strongest variability detected by AS; (ii) an approximating Gaussian Process Regression (GPR) is fitted on the projected points; (iii) mean relative approximation error is computed.

The steps are repeated for each of the three methods for computing the gradient, as shown in Figure 2.3. This analysis allows us to compare the different methods for computing gradients and, most importantly, to choose a subspace dimension that leads to an acceptable approximation error.

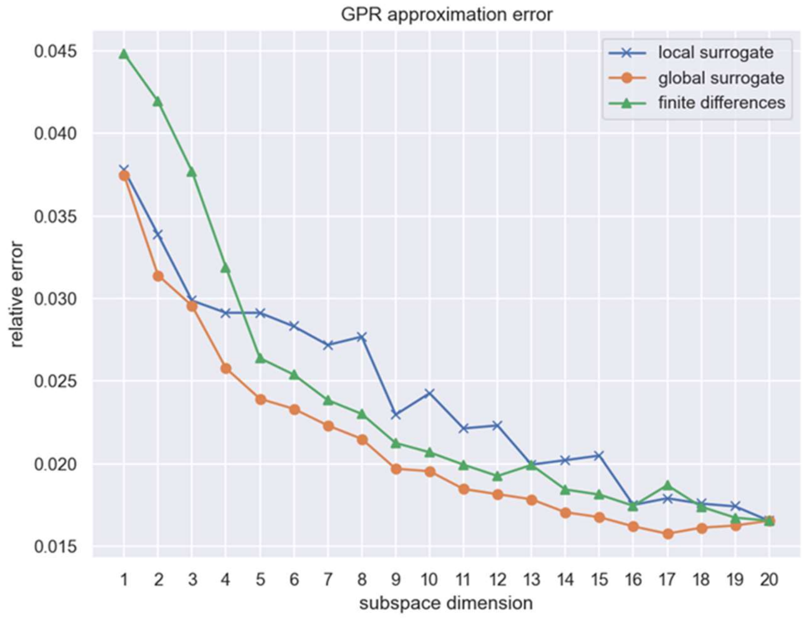


Figure 2.3: Response surface approximation error as a function of the input subspace defined by the first N directions detected by AS method.

References:

Active subspace methods in theory and practice: applications to Kriging surfaces, P.G. Costantine, E. Dow, Q. Wang https://arxiv.org/pdf/1304.2070.pdf

Secondment at Stanford University

M. Bergmann, A. Iollo and T. Taddei, Inria Bordeaux Sud-Ouest

M. Bergmann (MB), A. Iollo (AI) and T. Taddei (TT) (Inria Bordeaux) had a secondment at Stanford University in the research team of Prof. Farhat from February 9th to February 19th. The aim of the secondment was to discuss new developments in projection-based model order reduction (MOR) for a broad range of problems in nonlinear mechanics.

In more detail, MB, AI and TT were introduced to the recent contributions of Farhat's team: quadratic approximations; localized-in-parameter MOR; adaptive mesh refinement for MOR, and mechanics-informed neural networks for data-driven constitutive modeling. They also presented in the group meeting the recent works of the Inria team on registration methods for nonlinear MOR and on mapping of coherent structures via optimal transportation of Gaussian models.

Several lines of research were identified for further collaborations between the Inria team and Prof. Farhat's team: the aim is to combine the recent independent advances of the two teams on MOR to tackle the modeling of unsteady turbulent flows via low-dimensional models, and also the treatment of problems with moving discontinuities and/or with parametric geometries.

During this stay, they also discussed with researchers from Sandia Livermore National Lab (I. Tezaur, P. Kuberry, C. Sockwell, Y. Shimizu, P. Bochev) about hybrid high-fidelity / low-fidelity domain decomposition techniques for multi-scale, multi-fidelity and multi-physics problems. The same line of research was analyzed with Yougsoo Choi from Lawrence Livermore National Lab, including component-based ROM.

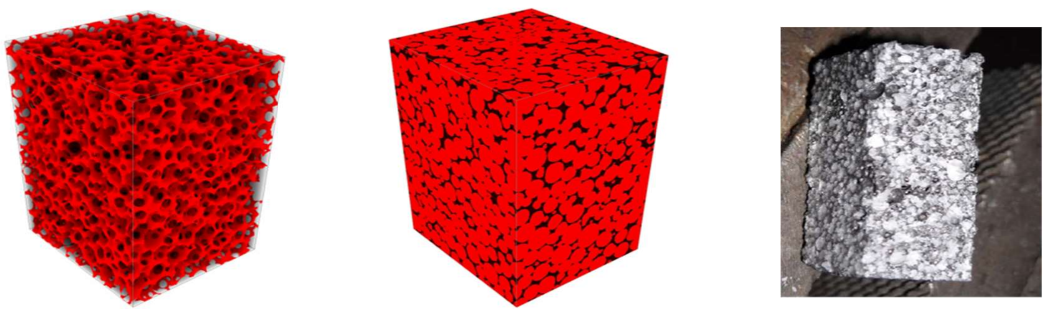
California folklore note: in the middle of February, the weather was perfect for surfing....

Model Reduction Oriented for Phase Change Material

M. AZAIEZ, Inria Bordeaux Sud-Ouest

Thermal energy storage (TES) is a key element for effective and efficient generation, and for utilization of heat when heat supply and heat demand do not match spatially and in time. This covers effective thermal management in the sectors of heating and cooling, process heat and power generation as well as increased utilization of renewable energy systems. A specific feature of thermal storage systems is that they are diversified with respect to temperature, power level and use of heat transfer fluids and that each application is characterized by its specific operation parameters. Thus, the availability of a broad portfolio of storage materials and design concepts is needed. Applications of TES systems are expected in several areas such as: 1) solar heating and cooling of buildings; 2) power generation using thermal conversion processes; 3) seasonal storage in combination with district heating systems; etc.

Heat can be stored essentially in three ways: 1) sensible heat storage, which results in an increase or decrease of the storage material temperature; 2) latent heat storage, which is connected with a phase transformation of the storage materials (phase change materials - PCMs), typically from solid to liquid and vice versa; and 3) thermochemical heat storage, which is based on reversible endo/exothermic chemical reactions. Currently commercially available TES systems are solely sensible heat storage systems to be used in connection with single phase heat transfer fluids. The technology of latent heat storage is today still a subject of R&D, with few specialists on the market that are familiar with designing and producing complete latent storage systems. Thermochemical storage is still in a fundamental, laboratory stage of development and research needs in the field have been identified and prioritized by the European Association for Storage Energy (EASE) and the European Energy Research Alliance (EERA)[1]. Improving relevant thermo-physical properties of PCMs and thermo-chemical storage materials by use of special additives or by developing composites has been recognized as one of the scientific challenges to close the gap between the TES targets and present performances. Additives and more specially carrier materials can efficiently contribute to enhance heat and/or mass transfer, to improve thermo-mechanical stability, to prevent undesirable effects like segregation or undercooling in PCMs, and to improve cyclability.



Example of PCM

1 Joint EASE/EERA recommendations for a European Energy Storage Technology Development, Roadmap toward 2030, March 2013.

One of the main difficulties in simulating phase change problems is due to the presence of moving boundary. Phase field model are known to be an efficient approach the evolution of the interface.

These models are to be coupled with conservation equations such as the heat equation and of Navier-Stokes. The numerical simulation of the coupled model is very time consuming and requires a large data storage. It is within this framework that we aim with VirtualMech and the group of Prof T. Chacon to propose a model reduction strategy to simulate the phase change process and to apply it for thermal energy process.

We started by considering models described by partial differential equations having the form of gradient flows. Such models come from energy gradient flows describe dynamics driven by a free energy, long used in many fields of science and engineering, particularly in materials science and fluid dynamics.

Typical examples include the Cahn-Hilliard and Allen-Cahn equations for multi-phase flows, for which the evolution PDE system is resulted from the energetic variation of the action functional of the total free energy in different Sobolev spaces.

Models of the gradient flow take the general form:

$$\frac{\partial \phi}{\partial t} = -\mathrm{grad}_H E(\phi),$$

where E is the free energy functional associated to the physical problem.

As can be seen from the literature, AC and CH models are now widely studied and analyzed. Stable schemes with high order accuracy in space and time are available. One can also appreciate several impressive simulations using these models to solve a complex physical phenomenon. However, in the area of model reduction and to our knowledge there are few papers dealing with the subject and even less when it comes to the parametrized problem.

To start we have considered a parameterized Allen-Cahn equation and we have proposed a certified model reduction strategy. We also established a stability analysis and error estimates for two fully discretized schemes with finite element approximation and reduced order element approximation in space respectively. The next step consists in extending our method by coupling the AC equation with the heat equation

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