ISSUE 5

ARIA Newsletter

December 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 fifth issue of the ARIA newsletter.

In this last quarter of the third year, we continue to move forward with the implementation of more secondments involved in the project. Some results and contents of the secondments are described below in this issue.

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/

The dissemination activities of ARIA went on with the participation to several events engaged to the general public including the European Researchers' Night in September 2022 and other dissemination events.

We organized ARIA-VT workshop and the 4th online free seminar open to public. The next seminar will be on 27th January 2023 with the topic on the development of test suites to validate and assess model order reduction techniques for specific classes of applications in computational mechanics. Additionally, we will organize another face to face workshop on 8-10 March 2023 at Inria Bordeaux, France. The information and registration to these events will be updated on our project website – http://rise-aria.eu

Stay tuned and happy reading!

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 – VT Workshop – 06-08 July 2022

This workshop was organized at the Department of Biomedical Engineering and Mechanics & Department of Mathematics, Virginia Tech, U.S.A.

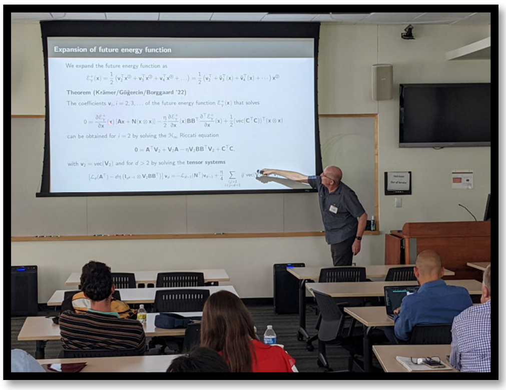
The main purpose of this conference was to serve as a forum for the ROM community to exchange their views on both the achievements and the open problems in reduced order modeling of industrial applications. The conference aimed at building a stronger community of reduced order modelers who are genuinely interested in developing the next generation of ROMs for industrial applications.

Tutorials of this seminar: shorturl.at/cN159

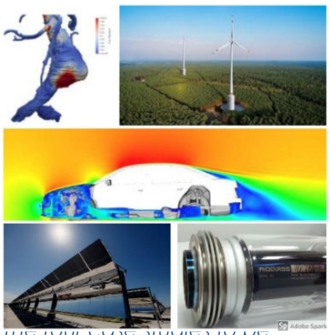
The organizing committee of the workshop are: Traian Iliescu (Chair- ARIA associated member), John Burns, Raffaella De Vita, Angelo Iollo (U. Bordeaux & Inria – ARIA Scientific Coordinator)) and Honghu Liu.

The speakers of the workshop are experts in ROM including ARIA members such as Francesco Ballarin (UCSC), Rozza Gianluigi (SISSA), Tommaso Taddei (Inria/U. Bordeaux).

The workshop involved fruitful discussions between ARIA representatives and other participants around the topic on reduced order modeling of industrial applications.



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 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*

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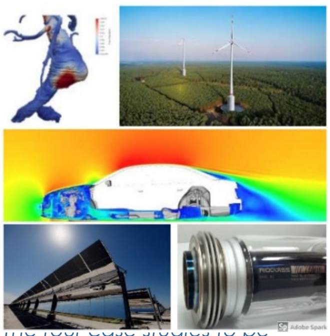

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ARIA engaged to the general public

ARIA is proud to attend wide public events that display the diversity of science and its impact on citizens' daily lives in fun, inspiring ways.

ARIA members participated European Researchers' Night in September 2022 in both Bordeaux (France)and Brescia (Italy). This participation helped raise the awareness on science careers and the enhance the public recognition of researchers in general.

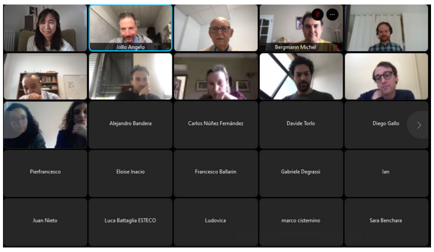
Photo: Ludovica Saccaro – ARIA's secondee at European Researchers' Night in Bordeaux

Another dissemination event attended by UCSC on October 21, 2022 was in the context of the Celebration of Mind initiative, a world-wide series of dissemination events held in honor of Martin Gardner's birthday. This was the occasion for additional groups of high school students (around 550) to attend some of the 50 presentations offered by UCSC researchers. Dr. F.Ballarin (UCSC), ARIA member, presented a topic of "Fluid dynamics in the aorta based on CT scan data". After a brief summary of the role of the aorta in the human circulatory system, attendees were introduced to a specific disease, the "coarctation of the aorta", in which a part of the blood vessel has an abnormal narrowing, called "coarctation" or "stenosis". It is of interest to introduce a parametrization on the stenosis to be able to compare e.g. a healthy case to a diseased case with mild, moderate or severe stenosis. Volunteers were then sought among the attendees so that they could carry out themselves at least one out of three tasks that are often needed to go from the clinical data to the computational model.

Figure 1: heart (top left), healthy aorta (top right, rotated upside down), diseased aorta with mild stenosis (bottom right, rotated counterclockwise), and diseased aorta with moderate stenosis (bottom left, rotated clockwise) printed with a 3D printer.

ARIA'S 4th Online Seminar – 03 October 2022

The fourth online seminar of ARIA project focused on the topic of renewable energy.



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

The talks were given by scientists of ARIA project.

Juan Valverde from Virtualmech started the seminar with the talk on "*Non-intrusive ROMs for heat transfer and fluid flow problems in Concentrated Solar Power (CSP) applications?*" . In his talk, he tackled a class of problems that arise in CSP receivers of central tower technology in a design and optimization environment and are computationally very intensive.

Michel Bergmann from Inria/Bordeaux University talked about "*POD-assisted computations of incompressible fluid flows: applications to wind and marine energy*" with the interests in numerical modeling of complex flows. He proposed a sampling strategy of the input parameter space based on the distance between POD subspaces, with the introduction of a new Energy-weighted PABS (principal angle between subspace) metric. He also showed that this metric performs better than classical ones like PABS or Grassmann geodesics.

Federico Roman from IEFLUIDS company continued to share insights on "Large Eddy Simulation on a marine turbine with stable stratification". He focused on the evaluation of the impact of marine stable stratification on turbine performance and wake characteristics.

To end the seminar, Mejdi Azaiez from Inria/Bordeaux University shared interest on physical problems that can be modeled by partial differential equations having the form of gradient flows. He then gave a talk on" Certified Reduced Order Method for Parametrized Allen-Cahn Equation". He proposed to consider a parametrized Allen-Cahn equation and suggested a certified model reduction strategy to approximate it.

All the talks of this seminar were recorded and can be accessed on our project website - http://rise-aria.eu

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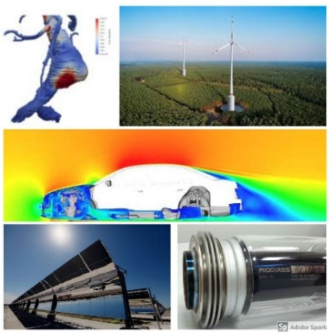

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Ludovica's insight on a secondment with OPTIMAD

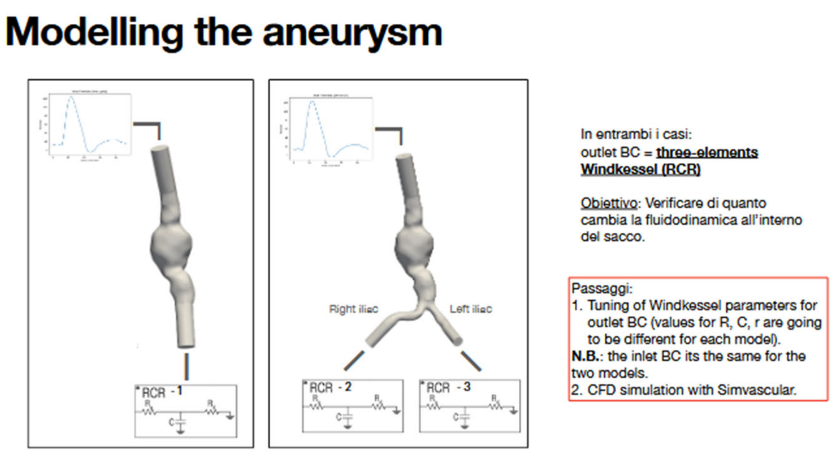
Ludovica Saccaro (Inria)

Simulation in numeric is crucial and absolutely necessary. The researcher has to master the simulation tools to assure the correct setting of the simulation and the best choices for the fastest and better result. The work is completed by interpreting the results, as mistakes and misinterpretation may lead to erroneous conclusions.

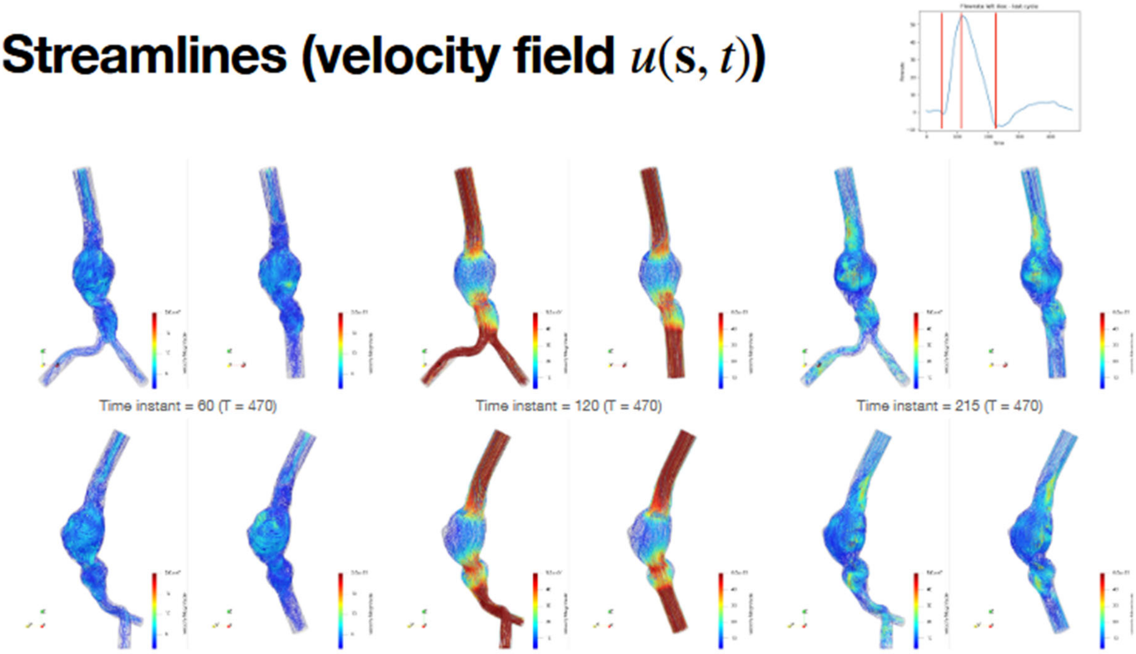
Simvascular (https://simvascular.github.io/) is an opensource software package providing a complete pipeline from medical image data segmentation to patient specific blood flow simulation and analysis. Its high efficiency allows to carry fluid dynamical simulation in blood vessels with high accuracy.

In this setting, my secondment in OPTMAD in May 2022 has been devoted to both improve my knowledge of Simvascular software, to independently set and run realistic simulation of the blood flowing in the aorta, and to learn how to read the simulations results. While OPTIMAD provided me with the technical and informatics support and help, I was also sided by Karol Calò and Valentina Mazzi from Politecnico di Torino. Their help was also focused on the interpretation of the results from a biomedical point of view, namely to compute the hemodynamic indicators used in biomechanics form the fluid dynamics resulting from Simvascular. In particular the boundary conditions to be set at the entrance of the aorta and the exit have been considered: pressure and inflow coming from measures in literature, and the use of Windkessel model as and outflow boundary condition. At the outlet, the influence of the iliac bifurcation on the hemodynamics in the aneurysm sac has also been investigated, proving how the geometry and of the domain considered in biomedical simulations might change the results.

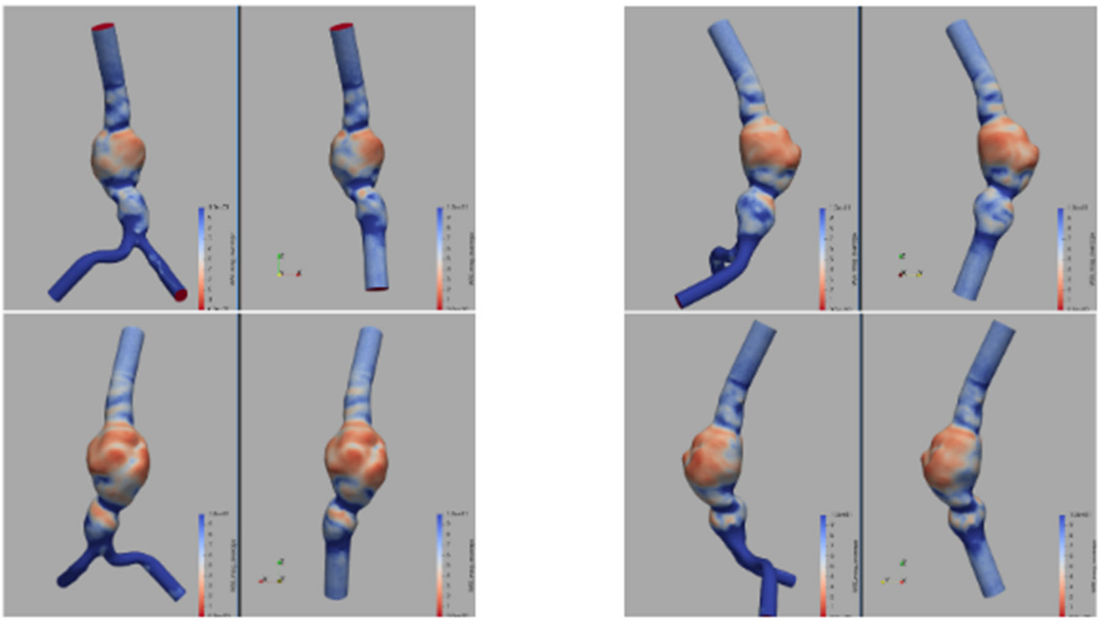
Both Karol and Valentina have also come to Bordeaux in the framework of the ARIA project at the beginning of the year (academic year, October 2022), and the discussion and confrontation about the hemodynamic indicators have thus advanced during my staying in Torino.



Streamlines (velocity field $u(s, t)$)



TAWSS - time averaged wall shear stress



Data assimilation and model order reduction for cardiovascular simulations

Francesco Ballarin, Università Cattolica del Sacro Cuore, Brescia, Italy

Recent decades have seen an increasing demand for computational models capable of predicting blood flow in patients affected by cardiovascular diseases. Data to create patient-specific computational models is nowadays increasingly available from non-invasive medical imaging techniques, including the geometry of the blood vessel itself (e.g., by means of CT or MRI scans) and the state of the system (e.g., velocity measurements by means of 4D flow MRI). A possible mathematical model of the blood flow relies on numerical solutions of Navier-Stokes equations in the 3D patient-specific computational domain reconstructed from CT/MRI geometrical data. Obtaining accurate simulations however still poses several challenges, some of which we are addressing thanks to collaborations between institutions involved in the ARIA project.

The first challenge is that it is unfeasible to image, reconstruct and discretize the entire cardiovascular system, and thus the vasculature not included in the 3D model must be replaced by boundary conditions. Still, the choice of such boundary conditions critically affects quantities of clinical interest computed by the simulation, such as pressure and flow rates. In [1], we propose a technique for the automated estimation of outlet boundary conditions based on an optimization formulation ("optimal control") constrained to the Navier-Stokes model. The values of resistive boundary conditions are set as the variables to be optimized ("controls"), with the goal of matching available patient-specific data. A graphical summary of the proposed workflow is shown in Figure 1. We further show that the proposed framework can indeed assimilate 4D flow MRI data more accurately than very common techniques based on Murray's law and Ohm's law.

The second challenge is that even a single 3D numerical simulation is computationally expensive. Since the assimilation procedures discussed above may require multiple evaluations of the numerical model, it is essential to employ reduced order modelling techniques to obtain cheaper model evaluations. Several techniques are suitable to reach such a goal. In particular, in [2] we employ data-driven models which combine proper orthogonal decomposition and feedforward neural networks, and apply them to cases of coronary artery disease with parameters accounting for boundary conditions and severity of the disease. Furthermore, in [3] we apply a Hierarchical Model (HiMod) reduction when modelling the transport of a passive scalar in a microchannel. Such a geometric configuration, as many other configurations in hemodynamics, provides an ideal setting to test a HiMod approximation, which exploits the presence of a leading dynamics to commute the original 3D model into a system of 1D coupled problems.

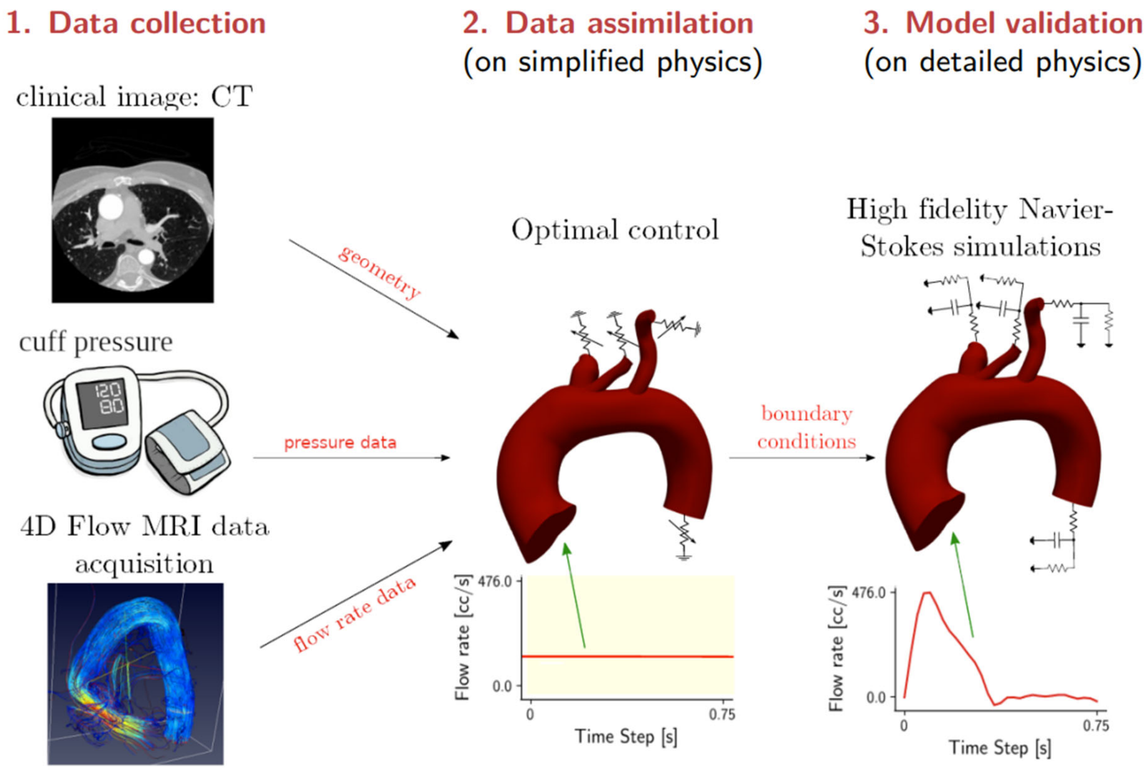


Figure 1: Data assimilation workflow proposed in [1].

References:

[1] E. Fevola, F. Ballarin, L. Jiménez-Juan, S. Fremes, S. Grivet-Talocia, G. Rozza, and P. Triverio, An optimal control approach to determine resistance-type boundary conditions from in-vivo data for cardiovascular simulations, International Journal for Numerical Methods in Biomedical Engineering, 37(10), e3516, 2021, arXiv: 2104.13284.

[2] P. Siena, M. Girfoglio, F. Ballarin, and G. Rozza, Data-driven reduced order modelling for patient-specific hemodynamics of coronary artery bypass grafts with physical and geometrical parameters, submitted, 2022, arXiv:2203.13682.

[3] S. Perotto, G. Bellini, F. Ballarin, K. Calò, V. Mazzi, U. Morbiducci, Isogeometric Hierarchical Model Reduction for advection-diffusion process simulation in microchannels, accepted, 2022, arXiv:2205.08127.

Regularized reduced Navier-Stokes equations under linear feedback control laws

Maria Strazzullo, Politecnico di Torino, Mathematics Department "G.L. Lagrange"

Over the last few decades, many efforts have been made to study the controllability of nonlinear systems, such as Navier-Stokes equations. This line of research focuses on the need of achieving a more stable desired state by means of suitable external variables, the controls. Is it possible to steer the solution toward the desired configuration and how can we act on the system to reach this goal? This problem is of utmost importance in many engineering and industrial applications, where one wants to govern the flow dynamics aiming at more convenient and possibly safer behaviors. The control of the Navier-Stokes equations has been widely studied for decades, from both a theoretical and an experimental viewpoint. However, due to its complexity, the topic is still relatively unexplored in the setting of large Reynolds numbers (and turbulent regimes) combined with reduced order modelling: these were the topics we focused on as ARIA project partners, in collaboration with Virginia Tech and Università Cattolica del Sacro Cuore [1].

In our research, we first address the following question: is linear feedback control enough as a stabilization strategy when dealing with large Reynolds numbers? Numerical evidence showed that, even under a strong control action (and even if we propose a new control action suited to large Reynolds numbers), other regularizing techniques should be used to stabilize the problem at hand. Indeed, in marginally-resolved regimes, i.e., when the computational mesh is not fine enough to capture all the dynamics and vortexcs of the flow, spurious numerical oscillations may arise. When this happens, the control action is affected, and, reaching the desired configuration becomes harder and harder. To tackle this issue, we propose an adaptive evolve filter and relax algorithm (aEFR) as a regularized strategy. The new approach:

1. alleviates the numerical and non-physical oscillations of the system, and
2. allows a better convergence of the system towards the desired configuration.

A second task is represented by the reduced formulation of the regularized control problem. Reduced order models (ROM) are an asset when the simulation is required in a short time and for several parametric configurations, for example. A parameter may represent physical, geometrical, or particular control features. ROMs aim at building a low-dimensional framework that represents the control system with a certain degree of accuracy, accelerating the time needed for a complete simulation. We want to investigate how the novel aEFR linear feedback control problem performs in a reduced framework and whether the aEFR strategy is beneficial also in the reduced context, as already assessed in [2] for the Navier-Stokes equations under no control action for the standard evolve filter and relax approach.

Some preliminary results showed that in the under-resolved ROM regime, i.e., when a small number of basis functions are used to describe the controlled system, employing aEFR at the reduced level can be beneficial in terms of accuracy with respect to the expected solution, without increasing the computational costs.

These investigations are the first steps towards more complicated applications of interest in the ARIA project context, such as data-driven modeling and boundary and active controls.

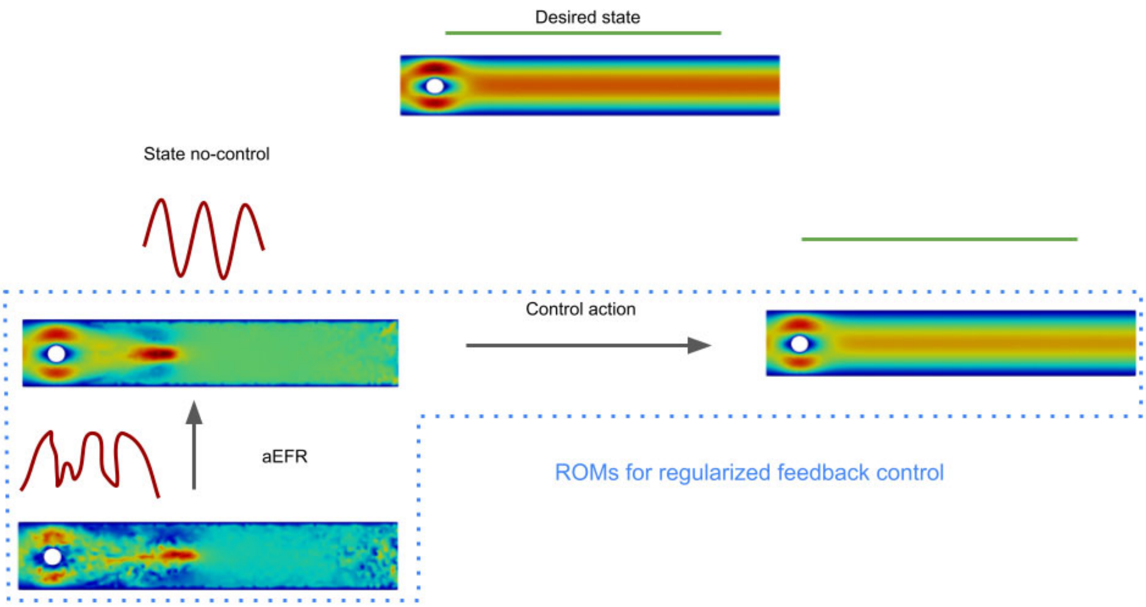


Figure 1: Workflow of aEFR feedback control for Navier-Stokes equations.

[1] Strazzullo, Ballarin, Canuto, and Iliescu "A reduced evolve-filter-relax regularization for feedback control of Navier-Stokes equations", in preparation (2022).
[2] Strazzullo, Girfoglio, Ballarin, Iliescu, and Rozza, "Consistency of the full and reduced order models for evolve-filter-relax regularization of convection-dominated, marginally-resolved flows." International Journal for Numerical Methods in Engineering 123.14 (2022): 3148-3178.

Secondment of Alejandro Bandera Moreno (University of Seville) at Valorem

1 Introduction

The aim of this secondment was to develop a posteriori error estimation based upon Kolmogórov turbulence theory.

This theory states that under the hypothesis of similarity (invariance under change of scale) and isotropy there exist an inertial range $[k_1, k_2]$ where the energy spectrum $E(k)$ can be expressed as a function of the wavenumber k and the turbulent dissipation ϵ, this is, $E(k) \sim \epsilon^\alpha k^\beta$ for some α, β to be determined, this can be done by simple dimensional analysis and yields $\alpha = 2/3$ and $\beta = -5/3$, that is the reason why this theory is also called the Kolmogórov -5/3 law.

The inertial range is determined by two wavenumbers, k_1 associated to the largest scales of the problem and k_2 associated to the smaller scale under which the viscosity takes an active part.

2 Advances in a posteriori error estimator

Now, if we let $E_N(k;\mu)$ be the energy spectrum associated to the reduced solution of dimension N $u_N(\mu)$, we can define the a posteriori error estimator as follows

$$\Delta_N(\mu) = \min_a \left(\int_{k_1}^{k_2} |E_N(k;\mu) - a(\mu)k^{-5/3}|^2 dk \right)^{1/2}.$$

This measures how close is a given solution to the theoretical Kolmogórov spectrum in the inertial range.

In practice, we need to substitute k_2 by $k_c < k_2$ as k_c is related to the smallest scale we can solve numerically (for instance, via the Smagorinsky model).

This estimator has been already been tested in [1] for a 2D academic example. Our main aim in this secondment was to develop a 3D numerical version of the a posteriori estimator, what we did successfully for functions defined in a cuboid domain.

A further problem was to compute the spectrum of a non periodic velocity. It was tackled by computing with enough precision, via quadrature formulas, the scalar products of the fourier transform.

The next step is to test the estimator for an academic example, as the final use of this estimator is to develop a reduced system of the flow after an aerogenerator so the simulations are less expensive computationally and so they can be performed in a shorter time.

References

[1] Caravaca García, C. (2022). Reduced Basis Method applied to the Smagorinsky Turbulence Model. (Tesis Doctoral Inédita). Universidad de Sevilla, Sevilla.

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