ISSUE 6

ARIA Newsletter

July 2023

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 sixth issue of the ARIA newsletter.

In this period, secondments are still on-going from academy to industrial and vice versa and we have achieved progresses in the project research.

We organized ARIA's face to face workshop on 8-10 March 2023 at Inria Bordeaux, France where the major experts in the different fields have been invited, including the US partners belonging to the project. Thanks to this workshop, ARIA participants can progress towards key advances in modeling multi-scale nonlinear physical phenomena.

The fifth online seminar of the project was organized early this year presented the initiative on the development of test suites to validate and assess model order reduction techniques for specific classes of applications in computational mechanics.

During this period, we have two new partners joining the consortium including University of Trieste and CNAM. And to ensure the widest possible dissemination, all journal papers are open access through self-archiving and all suitable data is available on the open access section of the public web site.

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 Workshop, 08-10 March 2023

This workshop was organized at Centre Inria de l'université de Bordeaux. This was an open international conference on Reduced Order Models aimed to progress towards key advances in modeling multi-scale nonlinear physical phenomena.

Tutorials of this workshop: https://project.inria.fr/aria/dissemination/training-materials/aria-workshop-08-10-march-2023/

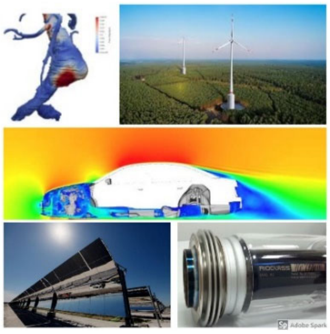
The organizing committee of the workshop were: Angelo Iollo (U. Bordeaux & Inria – ARIA Scientific Coordinator), Tommaso Taddei and Michel Bergmann (U. Bordeaux & Inria)

The speakers of the workshop were experts of the domain coming from both academic and industrial parties coming all over Europe and America such as:

- Charbel Farhat (Stanford University)
- Denis Sipp (ONERA)
- Laurent Cordier (CNRS)
- Virginie Ehlarcher (Ecole des Ponts ParisTech)
- Simone Camarri (University of Pisa)
- Traian Iliescu (Virginia Tech)
- William Wolf (University of Campinas)
- Matteo Diez (CNR -INM)
- Irina Tezaur (Sandia)
- Giovanni Stabile (University of Urbino)
- Luc Pastur (Institut Polytechnique de Paris)

The workshop involved fruitful talks on interesting topics around ROMs with active participation and discussion among the 60 participants. The talks included the following topics:

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*

- Data-driven flow modeling using Machine Learning and Data Assimilation
- Wasserstein-type interpolation for generic mixture models:,application to model-order reduction in quantum chemistry
- Control design by stability analysis: an overview and a,possible integration in reduced-order models
- Regularized Reduced Order Models (Reg-ROMs),for Turbulent Flows
- Neural Network Surrogate Models for Flow Control and Image Feature Extraction
- Design-Space Dimensionality Reduction in Global Optimization of Functional Surfaces: Recent Developments and Way Forward
- Component–based coupling of first–principles and data–driven models
- Nonlinear manifold ROM with Convolutional Autoencoders and Reduced Over-Collocation method
- Non-generic coincidence of local bifurcations in the fluidic pinball

There was also a poster session under the scope of the workshop. This was the chance for 16 Phds coming around Europe to present their research topics and results integrated with fruitful and active discussion with all the attendants.

This first face to face workshop was a success with the participation of 60 attendants coming from around Europe and America including professors, engineers, researchers, early stage researchers. The workshop was a chance to disseminate ARIA project to public and allowed ARIA members to progress towards key advances in modeling multi-scale nonlinear physical phenomena.

There was a video captured some events at the workshop: https://youtu.be/h7yCQrnoQrw

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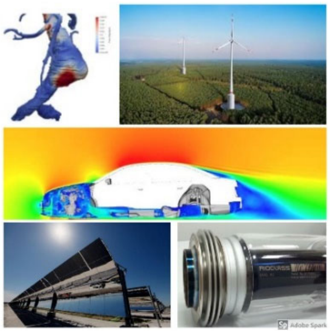

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ARIA’S 5th Online Seminar – 27 January 2023

SAVE THE DATE

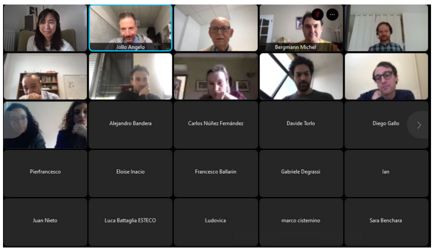
ARIA ONLINE SEMINAR
on
MOR Test case Initiatives
27.01.2022 at 14:00 (CET)

Register: http://rise-aria.eu

INVITED SPEAKERS

Bernd Noack (Harbin Institute of Technology, China)
Nan Deng (Harbin Institute of Technology, China)
Patrick Blonigan (Sandia National Labs, US)
Masayuki Yano (University of Toronto, Canada)
Matthew Zahr (University of Notre Dame, US)
Cheng Huang (University of Kansas, US)

The fifth online seminar of ARIA presented the initiative on the development of test suites to validate and assess model order reduction techniques for specific classes of applications in computational mechanics. The seminar consisted of three talks that described three test suites; talks were followed by a panel discussion.



Tutorials of this seminar: https://project.inria.fr/aria/aria-seminar-27-january-2023/

Nan Deng from Harbin Institute of Technology, China started the seminar with the talk on “Test suite for reduced-order modelling of bifurcation phenomena in fluid mechanics”. In his talk, he proposed the fluidic pinball [as a benchmark configuration for reduced-order modelling of successive bifurcations and complex dynamics of wake flow. In this talk, the numerical setup was introduced, then an overview of flow instabilities and bifurcation was given. He also presented results of the mean-field Galerkin model and hierarchical network model [6] for the transient and post-transient dynamics between multiple invariant sets are presented as examples.

Masayuki Yano (University of Toronto, Canada) was talking about Approximation of problems with parameter-dependent discontinuities in steady aerodynamics. In his talk, he proposed a family of test cases to validate and assess model reduction techniques for problems with parameter-dependent discontinuities, which arise in steady aerodynamics. He also proposed metrics that can be used to systematically assess various nonlinear model reduction techniques in terms of accuracy, online evaluation cost, and offline training cost.

Cheng Huang (University of Kansas, US) gave a talk on “Representation of long-term temporal dynamics and prediction of the solution to dynamical systems outside the training time window in combustion” in which he introduced the test suites to assess the model order reduction (MOR) techniques for combustion applications.

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

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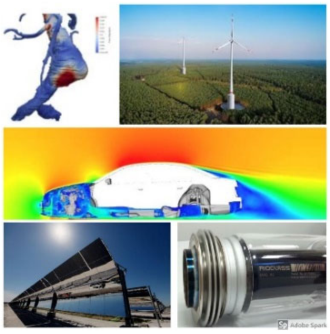

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IEFLUIDS and ARIA project

Federico Roman (IEFLUIDS)

Within the ARIA project, IEFLUIDS contributed mainly to the work-package 2, related to ROMS for incompressible turbulent and unsteady flows. The company collaborated with USE, INRIA and VALOREM to the industrial test case of the reproduction of a Wind Turbine (WT) wake.

A single wind turbine has been analyzed numerically taking advantage of Wall modeled Large Eddy Simulation (WLES), in this method only the large energy carrying scales of motion are directly solved, while the smaller ones, below the grid resolution, are modeled with an eddy viscosity approach; moreover, the viscous sub layer is not directly resolved but modeled through wall function, in order to reduce the computational cost. The test case considers a typical wind turbine used by VALOREM, with a rotor diameter of D=82m and with the hub located at approximatively 1D from the ground. The WT is considered on a flat field with a wall roughness associated to grass and bushes.

To investigate the WT wake 20 simulations have been run, spanning from the minimum to the maximum cutoff wind velocity measured at the hub height. To facilitate the reduced order model generation, instead of the velocity, the cases have been developed by using equal distributed magnitude for the streamwise pressure gradient. The wind turbine is not directly considered inside the domain, but its effect is modelled using a Blade Element Momentum theory (BEM), see for example Manwell et al. 2010, so adding a momentum sink term in the Navier Stokes equations. Several approach can be used in the BEM framework, at the present time it has been decided to adopt the simplest one, so a non-rotating actuator disk, see Wu and Porté-Agel 2013. The momentum sink has been calibrated using real data provided by VALOREM. For the turbulence model, a simple Smagorinsky model has been used with a fixed constant (no dynamic procedure), also in this case with the idea to maintain the numerical procedure as simple as possible.

The adopted domain is 4D in the vertical direction, 6D in the spanwise direction and 25D in the streamwise, the WT is located at 5D from the inlet, the employed dimensions are similar to that used by Stevens et al. 2018. For each case a precursor simulation has been run, without the wind turbine and considering a periodic condition in the streamwise direction. Turbulent flow planes have been stored in time to be provided as a boundary condition to the wind turbine simulation. This procedure has been adopted because the LES requires at the inlet the presence of coherent turbulent structures in order to sustain the turbulent kinetic energy production mechanism. All the simulations have been run till a steady state condition, then the time statistics have been collected over a proper period, to perform first order and second order analysis. All these data have been transferred to the project's partner to build the reduced order model. Figure 1 shows for the flow field, averaged in time, three iso-surface for the streamwise velocity component; the rotor area is clearly identified, as the wake effect and in general the impact on the flow field.

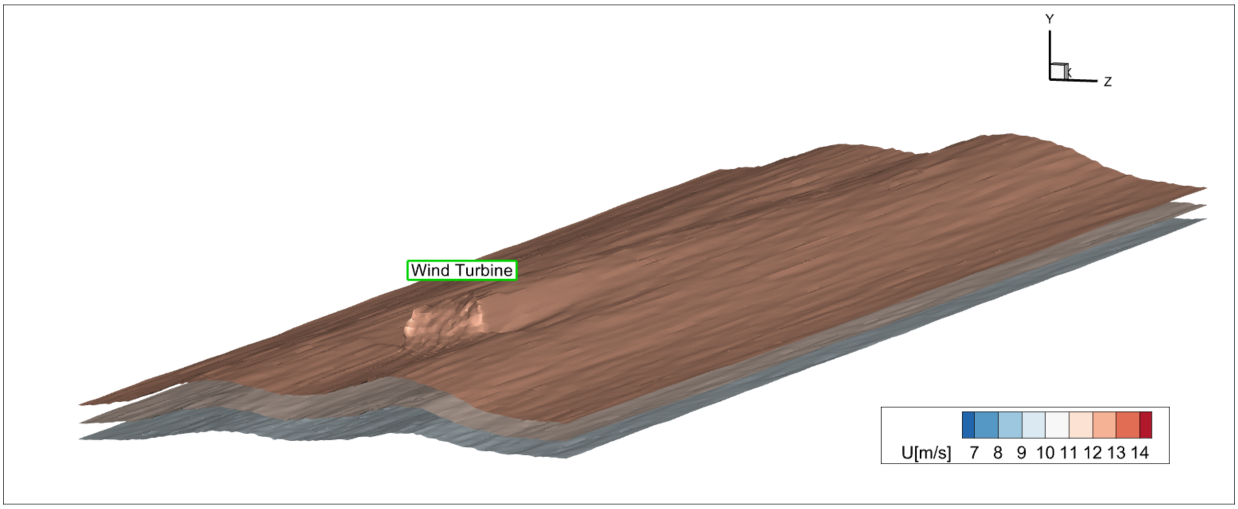

Figure 1: iso-surface for the streamwise velocity, averaged in time, at three different values.

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- Stevens, R.J.A.M., Martinez-Tossas, L.A., Meneveau, C., 2018 "Comparison of wind farm large eddy simulations using actuator disk and actuator line model with wind tunnel experiments". Renewable Energy, 116, 470-478.
- Wu, Y., Porté-Agel, F., 2013, "Simulation of turbulent flow inside and above wind farms: model validation and layout effects", Boundary-Layer Meterol 146, 181-205.frontation about the hemodynamic indicators have thus advanced during my staying in Torino.

Approximate Deconvolution Leray (ADL) reduced order model

Anna Sanfilippo, Università di Trento qnd Università Cattolica del Sacro Cuore, Brescia, Italy

Galerkin reduced order models (G-ROMs) are often used to reduce the computational cost of full order models (FOMs) in the numerical simulation of fluid flows. However, in the under-resolved regime (i.e., when the number of ROM degrees of freedom is not enough to accurately represent the flow dynamics), G-ROM yields inaccurate results, usually in the form of numerical oscillations. To alleviate this numerical inaccuracy, several types of ROM stabilization techniques have been developed, e.g., regularized ROMs (Reg-ROMs).

During winter 2023 I visited the group of Prof. Traian Iliescu in a secondment within the ARIA project (through Università Cattolica del Sacro Cuore). In my secondment we worked on regularized ROM (Reg-ROM) for Navier-Stokes and Burgers' equations, setting up a collaboration between Dr. Francesco Ballarin & myself and Prof. Traian Iliescu & Mr. Ian Moore.

In particular, we formulated a new Reg-ROM, i.e., the approximate deconvolution Leray ROM (ADL-ROM) since to our knowledge ADL has been used only at the FOM level [2]. Our numerical investigation is meant to show that the new ADL-ROM is more accurate than the Leray ROM (L-ROM) [3] and the classical G-ROM.

We worked mainly on the numerical aspects of the proposed research by testing the proposed ROMs in different settings, especially concerning different 2D domains for the Navier-Stokes equations (flow past a cylinder and backward facing step). Moreover, we analyzed the differences between the approximate and the exact deconvolution [1] and investigated the sensitivity of the results to model coefficients such as filtering radius and Lavrentiev parameter. For all the numerical simulations, we used the RBniCSx software. RBniCSx [4] is an open-source FEniCSx-based software and contains several implementations of reduced order modelling techniques – e.g., Certified Reduced Basis method and Proper Orthogonal Decomposition-Galerkin methods, and will be the successor to RBniCS.

Some preliminary results showed that in the under-resolved ROM regime employing ADL at the reduced level can be beneficial in terms of accuracy in comparison to the G-ROM and L-ROM solutions without increasing the computational costs. These investigations can be the first steps towards more complicated applications of interest in the ARIA project context.

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.

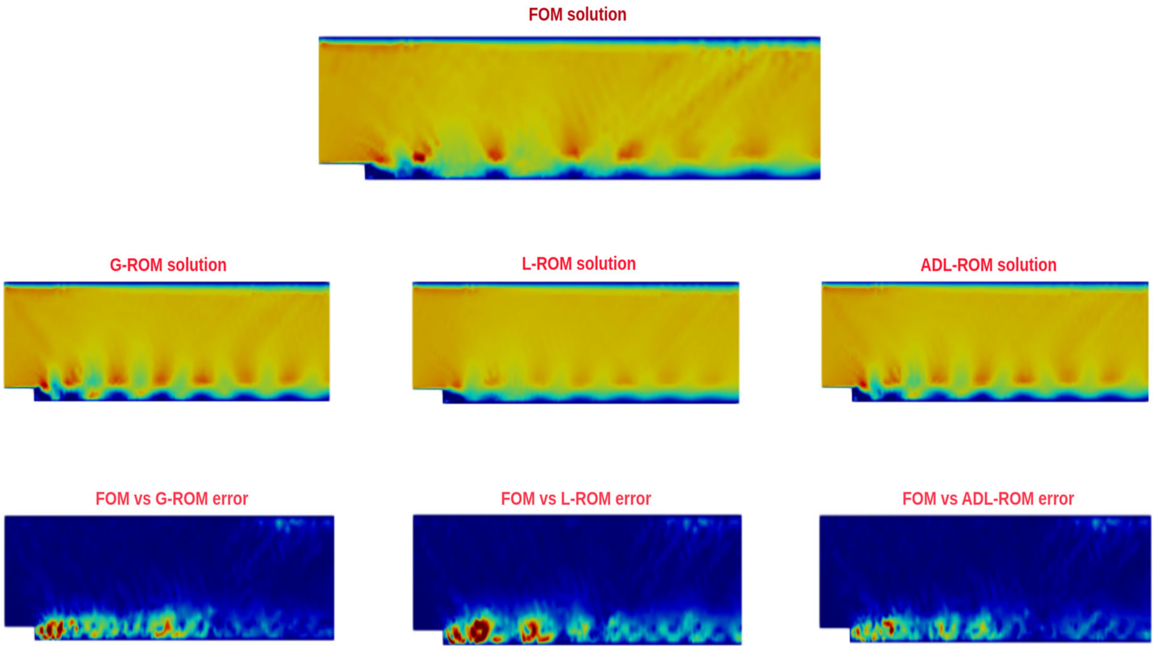

Figure 1: ROM solutions and pointwise errors w.r.t. FOM solution

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Research secondment of Luca Muscara (Politecnico di Torino) at Nurea

The simulation of turbulent flows in complex geometries presents notable challenges, primarily attributed to the presence of complex phenomena like laminar-turbulent transition and separation. These phenomena have a substantial influence on the performance of the system being studied. To accurately capture these important physical phenomena while minimizing the need for extensive modeling, scale-resolving simulations like Large Eddy Simulations (LES) and Direct Numerical Simulations (DNS) are employed. However, the high computational cost associated with scale-resolving simulations limits their practicality for evaluating numerous geometrical configurations during the design process. Indeed, the Reynolds-Averaged Navier-Stokes (RANS) models remain widely used, particularly for industrial purposes, due to their computational efficiency compared to scale-resolving simulations.

However, RANS models face challenges when dealing with complex phenomena like laminar-turbulent transition and separation induced by shock-boundary layer interactions. These phenomena are inherently difficult to capture accurately using traditional RANS models, which rely on turbulence closure models and assumptions. The limitations of RANS models in handling such complex phenomena have motivated ongoing research to improve their predictive capabilities.

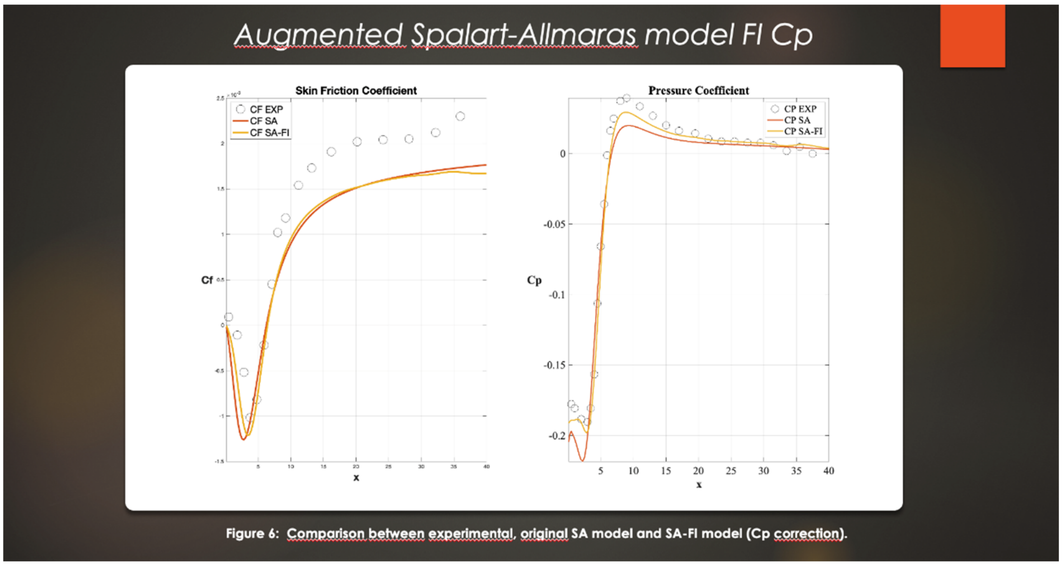
The use of data-driven algorithms is being explored to incorporate correction terms into RANS models, leveraging high-fidelity data from experiments or scale-resolving simulations to better account for complex phenomena. One promising data-driven approach that has demonstrated positive outcomes in enhancing RANS models is the Field Inversion and Machine Learning (FIML) paradigm. FIML is an optimization procedure that aims to solve an inverse problem by utilizing measurements to derive an accurate representation of the underlying physical field. This process involves two key steps.

In the first step, the optimization problem is solved by evaluating the gradient of the objective function with respect to the correction parameters using the adjoint solver. This step relies on the adjoint equation to calculate the sensitivity of the objective function with respect to the correction parameters.

In the second step, the inverse problem is solved for multiple test cases, creating a dataset that can be used with machine learning algorithms, such as neural networks. The dataset is constructed to establish a general expression that correlates the correction field with fluid dynamics variables, which are selected as inputs for the neural network. The choice of inputs is not standardized and depends on the specific case at hand. It is crucial to carefully select the inputs as they play a vital role in accurately predicting the correction field.

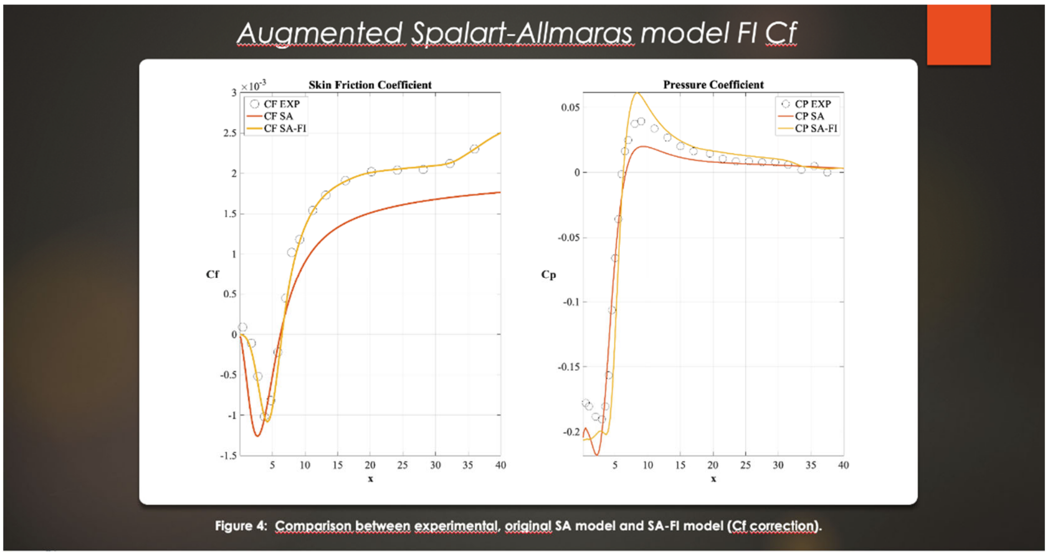
By incorporating additional information from experiments or simulations, FIML improves the prediction of turbulent flows. This approach enhances the capabilities of traditional models by leveraging machine learning to refine and correct the models based on high-fidelity data, leading to improved accuracy in predicting turbulent flow behavior.

As part of my research, I focused on implementing the method into a parallel computational fluid dynamics (CFD) solver that I am currently working on. This implementation aimed to harness the capabilities of the method while also understanding its limitations. During the past few months, I had the opportunity to undertake my secondment at Nurea. Their expertise in data-driven algorithms proved to be invaluable in expediting the implementation process and gaining a deeper understanding of the algorithm itself. Their knowledge and guidance significantly aided in accelerating my progress and expanding my knowledge and expertise in utilizing data-driven methods effectively for turbulence modeling.



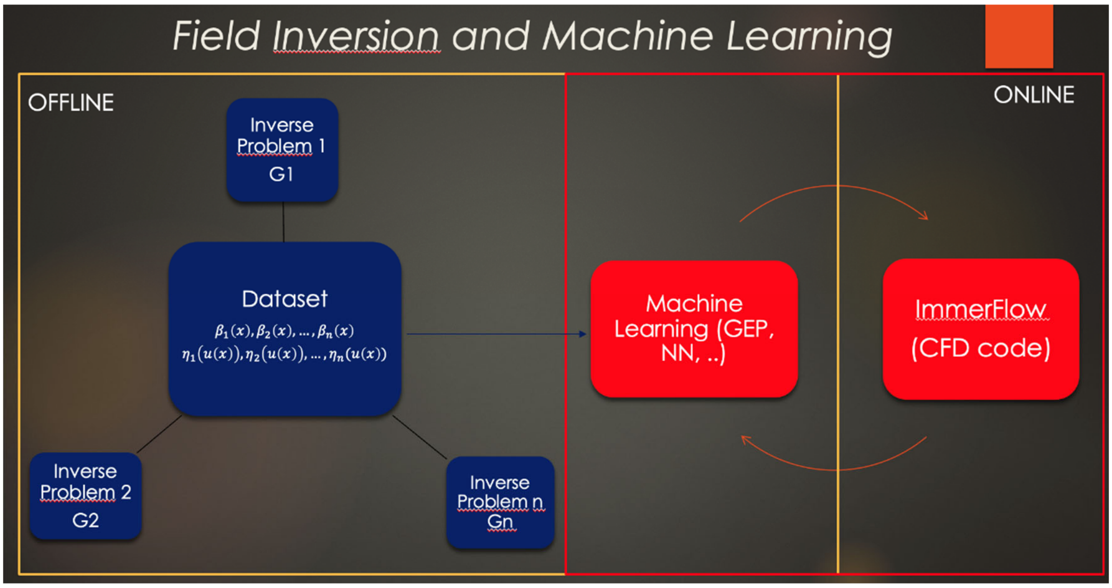
Augmented Spalart-Allmaras model FI Cp

Figure 6: Comparison between experimental, original SA model and SA-FI model (Cp correction).



Augmented Spalart-Allmaras model FI Cf

Figure 4: Comparison between experimental, original SA model and SA-FI model (Cf correction).



Field Inversion and Machine Learning

OFFLINE

Inverse Problem 1
G1

Dataset
$\beta_1(x), \beta_2(x), \ldots, \beta_n(x)$
$\eta_1(u(x)), \eta_2(u(x)), \ldots, \eta_n(u(x))$

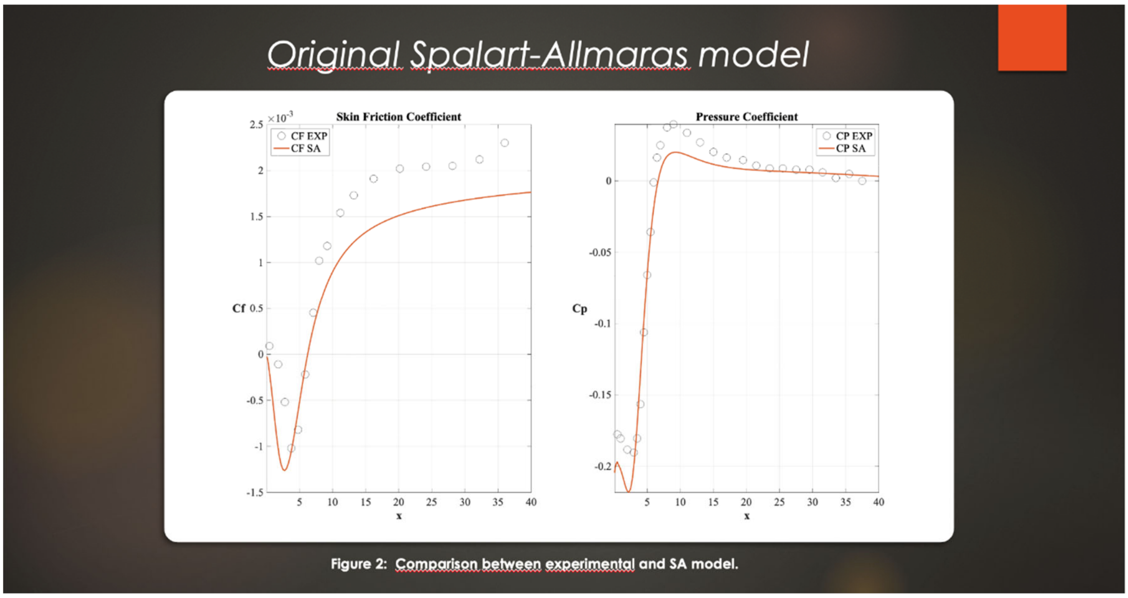
Inverse Problem 2
G2

Inverse Problem n
Gn

ONLINE

Machine Learning (GEP, NN, ..)

ImmerFlow (CFD code)



Original Spalart-Allmaras model

Figure 2: Comparison between experimental and SA model.

Mesh adaptation techniques for the VMS-SGS model

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Turbulence is a complex phenomenon that occurs in multidisciplinary fields, such as industrial, environmental, medical applications. The numerical simulation of such events represents one of the major challenges for the computational community, due to the inherent involved nature. Our research focuses on accurately simulating turbulent flows, with a specific interest in performance and efficiency aspects, which reveal to be crucial in different applications. For instance, in hemodynamics, the blood flow can be accurately modeled as a turbulent flow in certain artery districts. In solar panel technologies, the flow of fluid in pipes plays a crucial role in heat transfer processes.

To mathematically model turbulent flows, two main approaches are commonly employed: the Reynolds-Averaged Navier-Stokes (RANS) equations and the Large-Eddy Simulation (LES) model. We focus on the latter, which relies on the consideration that turbulence is characterized by multi-dimensional scales (i.e., vortices of different sizes). Due to energy dissipation, large scales are reduced into small scales. LES equations resolve the large scales (i.e., the so-called resolved field) up to a certain size, while surrogating the effect of the smallest ones (i.e., the unresolved field), which cannot be explicitly computed due to an intrinsic limit in the mesh resolution. For reproducing the effect of the unresolved field, we adopt the well-known Smagorinsky (SGS) model that resorts to an artificial turbulent viscosity ν_T. In particular, we enrich the Smagorinsky turbulence model with the Variational Multi-Scale method [1], which decomposes the resolved field into large and small scales. As a consequence, the overall flow turns out to be decomposed into three levels: the largest and the smallest resolved scales (VMS), and the unresolved ones, whose effect, acting only on the smallest resolved scales, is modelled through the Smagorinsky turbulent viscosity term. The resulting model is known in the literature as the Variational MultiScale - Smagorinsky (VMS-SGS) model (see, for instance, [2, 3]). In more detail, we focused on a finite element discretization of the VMS-SGS model.

The mathematical tool that we exploit to reduce the computational effort characterizing the numerical simulation of a turbulent flow is an anisotropic mesh adaptation procedure. It is well-established in the literature that anisotropic meshes guarantee a user-defined solution accuracy with a considerably lower number of elements, when compared with uniformly refined or isotropic adapted grids [4]. This goal is reached by properly tuning the shape, the size and the orientation of the triangles constituting the computational mesh. There exist many criteria to drive the mesh adaptation and to generate application-tailored computational grids. We resort to a posteriori error estimator frequently adopted in the scientific community, namely the Zienkiewicz-Zhu (or recovery-based) error estimator (see [5, 6]). Such an estimator is used to control the error on the gradient of one of the physical (driving) quantities characterizing the problem at hand, such as the pressure or the velocity when dealing with a fluid dynamic context, the displacement or the stress for a linear elasticity problem. More in general, a recovery-based adaptive procedure consists of two steps, i) the definition of the so-called recovered gradient based on the discrete solution, and ii) the employment of the recovered gradient to estimate the error on the H1-seminorm associated with the driving quantity. The massive employment of recovery-based error estimators in scientific modeling can be ascribed to the several good properties they share. In particular, they are not confined to a specific problem, they are independent of the selected discretization, cheap to compute and easy to implement, and they work extremely well in practice. The anisotropic version of Zienkiewicz-Zhu error estimators adds to this list of smart features the richness of information typical of an anisotropic setting [7]. We have successfully employed the anisotropic error estimator to improve the discretization of the VMS-SGS model, by assuming the pressure and the velocity components (or a possible combination of these quantities) as the driver of the adaptive process. In particular, to carry out the mesh adaptation procedure, we have resorted to a metric-based approach, according to [8].

We have selected FreeFEM as software environment to implement the proposed technique, since representing an ideal setting both for a finite element discretization and a metric-based mesh adaptation procedure. So far, we have limited the numerical assessment to 2D test cases, in a stationary regime, starting from a comparison with an isotropic mesh adaptation approach driven by the residual-based error estimator in [9]. In more detail, we have selected the backward facing step and the cavity flow as benchmark configurations, when dealing with a moderate Reynolds number.

Figure 1 compares the adapted meshes (top row) and the associated velocity modulus (bottom row) for the cavity flow test case at Re=3500. The three grids have been obtained by exploiting different driving quantities, namely the horizontal (left) and the vertical (center) velocity components, and a combination of them (right). The three meshes consists of 4019, 4933, 4516 triangles, respectively and exhibit an alternance between equilateral and stretched elements, accordingly to the directional features of the flow. We observe that the meshes yielded by the single velocity components identify different flow features, which are simultaneously detected in the third mesh. The flow velocity modulus associated with the three meshes is very similar, while, in all the considered cases, the L2 norm of the error on the velocity components is below 1%, after assuming as ground truth, the finite element approximation associated with a uniform mesh consisting of 845000 triangles.

To better corroborate the advantages led by a discretization based on an anisotropic adapted mesh, we are generalizing the proposed approach to an actual unsteady turbulent regime, before moving toward 3D configurations. In particular, we refer to Figure 2 for a preliminary result associated with the cavity flow benchmark case at Re = 7000, when a combination of the velocity components is taken as driving quantity.

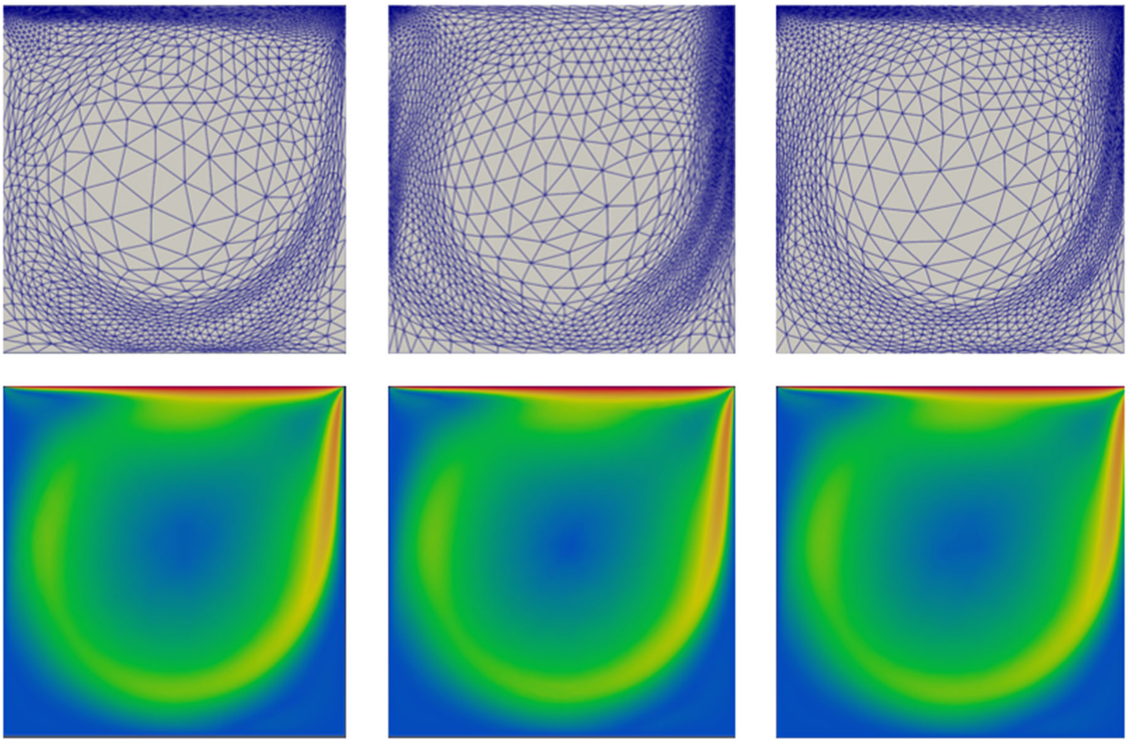

Figure 1: Cavity flow (Re = 3500): anisotropic adapted mesh (top) driven by the horizontal (left) and the vertical (center) velocity component, and by a combination of these (right); associated velocity modulus distribution (bottom). The meshes consist of 4019, 4933 and 4516 triangles (left-right).

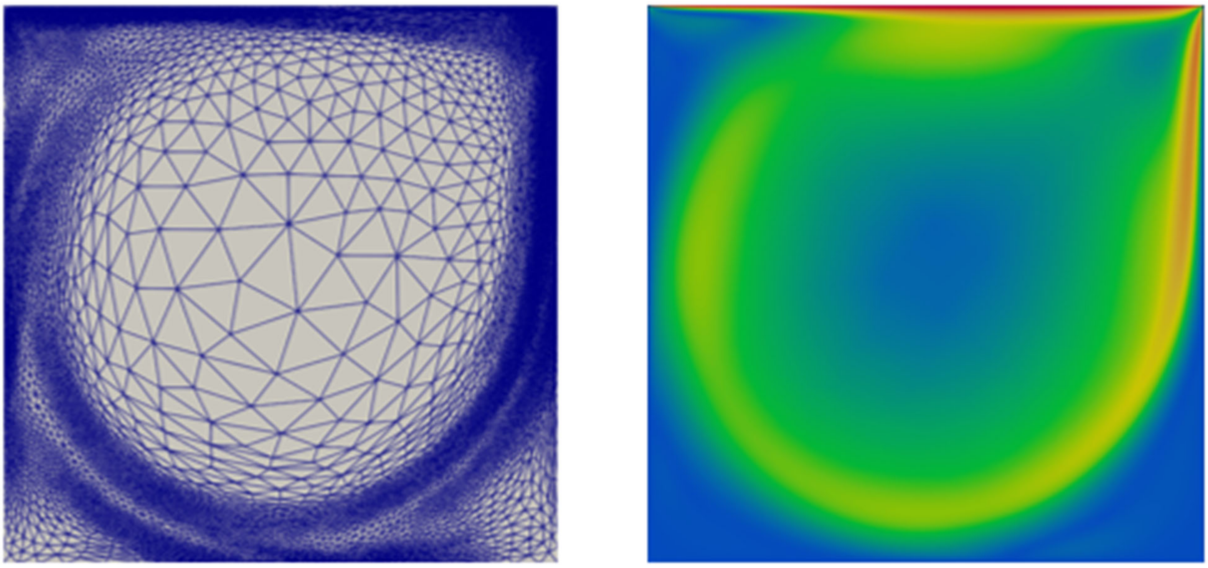

Figure 2: Cavity flow (Re = 7000): anisotropic adapted mesh (left) driven by a combination of the velocity components; associated velocity modulus distribution (right). The mesh consists of 60521 triangles.

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Adrian Ayala's Secondment (Virtualmechanics) at SISSA

Adrián Ayala (Virtualmechanics R&D manager) spent 18 days at SISSA, working on the topic of computational fluid dynamics in the group of Professor Gianluigi Rozza. The goals of this secondment were: 1) to present the activity of Virtualmechanics company, specially in the interplay of renewable energy and fluid dynamics; 2) to present a software tool implemented in Python/ParaView, for the visualization of thermal transport Reduced Order Models (ROMs); 3) to establish a frame of common interests for the collaboration of Virtualmechanics and Professor Gianluigi Rozza's group.

Concerning the second goal, Adrian gave a seminar entitled "A visualization tool for ROMs", where he focused on a software developed by Virtualmechanics. This software takes advantage of a python/ParaView interface, and implements methods of the EzyRB library (https://mathlab.github.io/EZyRB/).

The software is intended to derive non-intrusive ROMs from high-fidelity solver snapshots, by means of interpolation algorithms, and also to visualize the snapshots and the corresponding ROMs. The errors due to the choice of the snapshots are estimated using the k-fold method, available in EzrRB.

Graph quality is improve due to VTK library. The 'data-to-point' representation enables to set a variable like mesh or color map. Other important features are:

- color and mesh variables can be reassigned.
- Different styles, colors and orientations can be set.
- Opacities and point sizes can be changed.
- Good resolution and quality.

Adrián presented examples of the thermal transport inside the solar receiver cavity of a concentrating solar plant (Fig 2).

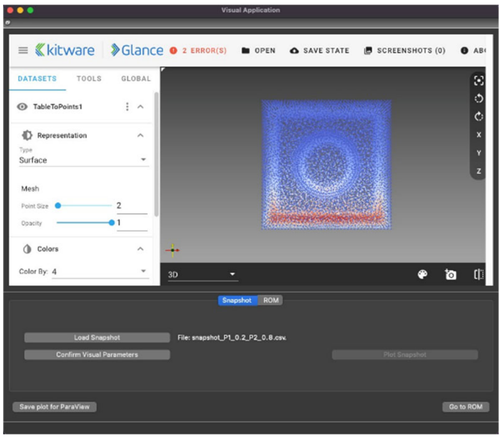

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Fig 1. ParaView interface to load snapshots

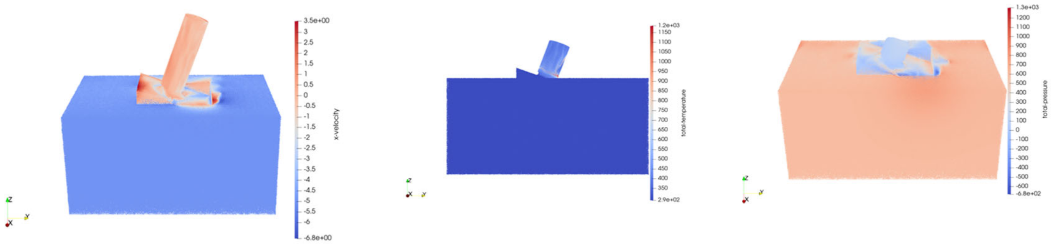

Fig 2. Visualization of a solar receiver cavity with the VM Visualization tool, showing the corresponding variable as heat map at each point. From left to right: x-velocity, total temperature, and total pressure.

The visualization tool is now under further development. In this moment, some pending tasks include adding features for the visualization of Neural Networks combined with POD (Proper Orthogonal Decomposition) methods.

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