

ECCOMAS European Community on Computational Methods in Applied Sciences

6th International Workshop on Model Reduction Techniques MORTech 2023

École normale supérieure Paris-Saclay France - November 22-24, 2023

An IACM Special Interest Conference



MORTech 2023 | mortech2023.sciencesconf.org



Day 1 – Wednesday, November 22

07.20 09.20	Wolcome coffee + Perintration					
07:30-08:20 08:20-08:30	Welcome coffee + Registration					
06.20-06.30		Opening Plenary Session - Alain Aspect Auditorium - Chair H. Matthies				
08:30-09:00		hary session - Alam Aspect Additionant - chair 11. Mat	ancs			
00.30 03.00	Recent advances in thermodynamics-informed neural networks for the prediction of physical phenomena					
09:00-09:30						
	pectral embedding of digital twins for rom-nets					
09:30-10:00						
	Reduced-order models as enablers for design, control and predictive digital twins					
10:00-10:30		COFFEE BREAK				
	Plenary Session - Alain Aspect Auditorium - Chair A. Nouy					
10:30-11:00	Ladevèze Pierre					
	PGD in nonlinear computational solid mechanics: a general weakly invasive version					
11:00-11:30						
11:30-12:00	Maday Yvon					
	Some elements of analysis for nonlinear compressive	reduced basis approximation for PDE's				
12:00-12:30	Casenave Fabien	Casenave Fabien				
	AI4Design@Safran: learning physics simulations for in	nproving design processes				
12:30-14:00	LUNCH					
		Parallel Sessions				
44.00 44.00	Alain Aspect Auditorium - Chair T. Chacon	Simondon 1 Auditorium - Chair B. Peherstorfer	Simondon 2 Auditorium - Chair D. Ryckelynck			
14:00-14:30	Falco Antonio	Allery Cyrille	Quaini Annalisa			
	Can we perform Model Reduction Techniques by using a NISQ quantum computer?	POD-Galerkin reduced order model coupled with neural network to solve flow in porous media	Reduced Order Modeling and LES filtering			
14:30-15:00	Kvamsdal Trond	Shakoor Modesar	Chakir Rachida			
	Novel L2-Projection to achieve Minimally Intrusive Affine Reduced Order Models	Autoencoder-accelerated computational homogenization of unsteady flows in porous media	Model order reduction for the identification of the thermal resistance of highly Insulated walls			
15:00-15:30	Nikolic Mijo	Bucci Michele Alessandro	Leturcq Bertrand			
	Fracture propagation problems enhanced by	Complemented Deep - Reduced Order Model	A posteriori model reduction combining creep,			
	uncertainty propagation and Bayesian identification		contact and friction in a multi-scale simulation			
	of parameters					
15:30-16:00		COFFEE BREAK				
		Parallel Sessions				
	Alain Aspect Auditorium - Chair A. Falco	Simondon 1 Auditorium - Chair J. Yvonnet	Simondon 2 Auditorium - Chair E. Quaini			
16:00-16:30	Chacon Tomas	Veroy-Grepl Karen	Zhang Yancheng			
	On the relationship between supremizers and least-	Model Order Reduction in the Parametrized Multi-	Thermomechanical modeling of the Directed Energy			
	squares pressure computation in ROMs for incompressible fluids	Scale Materials Setting	Deposition (DED) additive manufacturing process: coupling the Inherent strain rate and POD-based			
			model reduction			
16:30-17:00		Hernandez Joaquin	Strobl Dominic			
	Stochastic model updating and identification for nonlinear aeroelastic systems	The Empirical Interscale Finite Element Method: A novel approach for modeling heterogeneous	Reduced Order Model for Temperature Field Simulation of Wire Arc Additive Manufacturing with			
		structures using localized dimensional	Domain Mapping			
		hyperreduction				
17:00-17:30	Ehrlacher Virginie	Gravouil Anthony	Haddad Mohamed			
17.00 17.30	Model-order reduction of optimal transport	A databased approach for micro-macro topology	Interaction based deep material network model			
	problems	optimization of micro-architectured materials	reduction technique for porous polymer structures fabricated using additive manufacturing			
17:30-18:00	Panda Nishant	Bertrand Fleurianne	Nijhuis Bjorn			
17.50-10.00	Learning How RoMs Propagate Uncertainties Using	Model order reduction for the finite element	Local model order reduction to accelerate additive			
	Physics Informed Normalizing Flows	approximation of eigenvalue problems	manufacturing simulations			
18:00-18:30	Plenary Session - Alain Aspect Auditorium - Presentation of posters: F. Chinesta					
18:30						
	Posters & Cocktails					
	See the Book of Abstracts for the full list of posters					

Only the speaker is indicated in the agenda. Please refer to the corresponding abstract for the list of all contributors.



Use this QR Code to download the Book of Abstracts (which also includes this agenda)

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AGENDA

Day 2 – Thursday, November 23

07:45-08:30	Welcome Coffee					
	Plenary Session - Alain Aspect Auditorium - Chair R. Ohayon					
08:30-09:00	Benner Peter					
09:00-09:30	A Posteriori Error Estimation for Model Order Reduction of Parametric Systems Rozza Gianluigi					
09:30-10:00	Reduced Order Modelling in Computational Fluid Dynamics: state of the art, challenges and perspectives Néron David					
	Model reduction for multi-query simulations in nonlinear solid dynamics					
10:00-10:30	COFFEE BREAK					
	Parallel Sessions					
10:30-11:00	Alain Aspect Auditorium - Chair T. Taddei Iollo Angelo	Simondon 1 Auditorium - Chair K. Veroy Perotto Simona	Simondon 2 Auditorium - Chair PA. Boucard Prudhomme Serge			
10.50 11.00	Model Reduction by Convex Displacement Interpolation	Recent progress in applying Hierarchical Model reduction techniques to applicative contexts	On an Efficient PGD Solver for Structural Dynamics Applications			
11:00-11:30	Er Guo-Kang	Cauvin Ludovic	Oulghelou Mourad			
	A Model Reduction Method and Its Applications in Nonlinear Random Vibrations of Structures	Model reduction in the context of polycrystalline plasticity	Approach to Discover Redued Order Dynamics from Parametric Data			
11:30-12:00	Schwarz Henning	Ghnatios Chady	Duhamel Denis			
	Comparison of LSTM and Koopman-Operator approaches for Predicting Transient Ditching Loads	Generating materials yield surface by combining analytical models, model reduction techniques and data-driven approach	Reduced model based time domain absorbing boundary conditions for finite element modeling of infinite periodic structures			
12:00-12:30	Wick Thomas	Suliman Ridhwaan	Mencik Jean-Mathieu			
	Space-time goal-oriented a posteriori error control and adaptivity for incremental POD-based ROM	A reduced-order modal method for non-linear structural mechanics	Model reduction based on matrix interpolation and basis enrichment for dynamic analysis of nearly periodic structures including substructures with geometric changes			
12:30-14:00						
	LUNCH					
	Alain Aspect Auditorium Chair M. Dillaud Friess	Parallel Sessions Simondon 1 Auditorium - Chair R. Codina	Simondon 2 Auditorium - Chair F. Casenave			
14:00-14:30	Alain Aspect Auditorium - Chair M. Billaud Friess Taddei Tommaso	Manzoni Andrea	Chevreuil Mathilde			
14.00 14.00	Registration-based model reduction of parameterized PDEs with spatio-parameter adaptivity	Deep learning for reduced order modeling	Monitoring of composite structures using reduced order models			
14:30-15:00	Zheng Zhibao	Nardoni Chiara	Atak Onur			
	Model order reduction for nonlinear stochastic problems via stochastic LATIN methods	An energy-based approach to approximate the solution of PDEs using neural networks	An overview of ROM methods: An industrial point of view			
15:00-15:30	Dubreuil Sylvain	Navarro-Jimenez José Manuel	Bettinotti Omar			
	POD bases interpolation by Gaussian Process, benefits and difficulties	Combined Data Driven Convolutional-Recurrent Neural Networks methodology for accelerating the 2-level topology optimisation process	Surrogate Modeling for Multi-Physics General- Purpose Software			
15:30-16:00		COFFEE BREAK				
		Parallel Sessions				
	Alain Aspect Auditorium - Chair A. Iollo	Simondon 1 Auditorium - Chair C. Allery	Simondon 2 Auditorium- Chair M. Chevreuil			
16:00-16:30	Billaud-Friess Marie Probabilistic reduced basis method for solving parameter-dependent problems	Peherstorfer Benjamin Neural Galerkin schemes for model reduction of transport-dominated problems	Chamoin Ludovic Hybrid twins for the effective monitoring of real-life engineering systems: application to additive manufacturing processes and dynamics tests on			
			shaking tables			
16:30-17:00	Ramière Isabelle	Staber Brian	Srinivasan Shriram			
	On the Hyper-Reduction of variational inequalities. Application to contact mechanics problems.	MMGP: a Mesh Morphing Gaussian Process-based machine learning method for physical problems under non-parameterized geometrical variability	Reduced order models for the problem of optimal operation of natural gas flow networks			
17:00-17:30	Touzé Cyril	Phan Anh-Vu	Meunier Raphael			
	Reduced order modeling of finite element structures using invariant manifold theory	Eigenvalue Analysis in Confined Electron States of Quantum Wires	Application of Zonal Reduced-Order-Modelling to tire rolling simulation			
17:20 10:00	Plenary Session - Alain Aspect Auditorium - Chair P. Ladevèze					
17:30-18:00	Farhat Charbel (Videoconference) Assessment of Projection-Based Model Order Reduction for a Benchmark Parametric Hypersonic Flow Problem					
18:00-19:00	FREE TIME					
19:00	Bus to the Banquet					
	Banquet					

Return to ENS Paris-Saclay or Massy

Only the speaker is indicated in the agenda. Please refer to the corresponding abstract for the list of all contributors.

AGENDA

Day 3 – Friday, November 24

07:45-08:30	Welcome Coffee					
	Plenary Session - Alain Aspect Auditorium - Chair L. Chamoin					
08:30-09:00	Nouy Anthony					
	Optimal sampling for linear and nonlinear approximation					
09:00-09:30	Matthies Herrmann					
	Parameter dependent reduced order models, conditional expectation and machine learning					
09:30-10:00	Yvonnet Julien					
	Reduced order models for fracture and path-dependent multiscale simulations: Macro Clustering and data-driven approaches					
10:00-10:30	Chinesta Francisco					
	Recent advances on intrusive and non-intrusive separated representations					
10:30-11:00	COFFEE BREAK					
	Parallel Sessions					
		Simondon 1 Auditorium - Chair G. Rozza	Simondon 2 Auditorium - Chair E. Cueto			
11:00-11:30		Hoareau Christophe	Bergmann Michel			
		Parameterized reduced order model of linearized structural vibrations around a nonlinear static prestressed state due to follower forces	POD-assisted computations of incompressible fluid flows: applications to marine energy			
11:30-12:00		Placzek Antoine	Rohan Eduard			
		Nonlinear structural ROM for aeroelastic problems with large displacements	Two-scale modelling of fluid saturated electroactive porous media - nonlinear phenomena and computational homogenization			
12:00-12:30		Azaiez Mejdi	Ferrier Renaud			
		Certified Reduced Order Method for the Parametrized Allen-Cahn Equation	POD model order reduction for transient biphasic flows in porous media based on steady-state snapshots			
12:30-13:00	Plenary Session - Alain Aspect Auditorium - Conclusion					
13:00-14:00		LUNCH				

Only the speaker is indicated in the agenda. Please refer to the corresponding abstract for the list of all contributors.

Practical information

The Alain Aspect, and Simondon I & 2 Auditoriums are located on level I. Coffee breaks will be held at level 0. The Posters & Cocktails Session will take place on level 0. Finally, lunches will be taken at level 0.



For your presentation, a computer is available in each Auditorium. Please bring your presentation material with USB memory device and install it on the computer before the beginning of the session.

You can use your own computer as soon as you have ensured that it is working properly on the beamer: you must have a wifi connection (see below) and Intel Unite installed (see https://unite.ens-paris-saclay.fr/ to download and install it: accessible only when you are connected to the local wifi network).



Oral presentations will be 30 min long, including 5 minutes of discussion.

Session Chairs will strictly enforce these times and stop presentations that run over time.

Eduroam wifi access is available everywhere. If you do not have access to Eduroam, you can contact the Workshop reception desk, who will provide you with a login/password for the ENS-INVITES wifi network valid for the 3 days of the Workshop.

Posters & Cocktails Session

Don't miss the Wednesday evening session! See the Book of Abstracts for the full list of posters.



To Coffee brea

Simondon 1 & 2 Auditoriums

LEVEL 1

Alain Aspect

Main entrance (level 0)

ABSTRACTS

Day 1 – Wednesday, November 22

Morning sessions

Recent advances in thermodynamics-informed neural networks for the prediction of physical phenomena

Quercus Hernandez , Beatriz Moya , Carlos Bermejo , Francisco Chinesta , and Elias Cueto $^{\ast 1,2}$

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Abstract

Allowing an artificial inteligence (AI) to "understand" the physics of the surrounding environment is a challenging task with applications in many different fields. Among them, we can cite the development of an AI able to construct world models, or simply the development of engineering analysis systems that could potentially overcome the results of existing ones. But one of the most fundamental questions we must tackle is that of avoiding black-box approaches to the problems. These are weakly generalizable, prone to significant and unpredictable errors and not easily verificable. To evercome these difficulties, several approaches have tried to employ inductive biases, a set of rules that may guide the AI towards the right prediciton. In recent years, we have explored the possibility of employ, in the absence of any other information, the laws of thermodynamics as one of such inductive biases.

In this presentation we will discuss the state of the art in the field and present some new results that show the potentiallity of this technique.

SPECTRAL EMBEDDING OF DIGITAL TWINS FOR ROM-NETS

David Ryckelynck^{*1}

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Abstract

Data complexity and dimensionality are usually high in digital images of mechanical components. Hence, the mechanical models based on these images also exhibit high complexity. Manifold learning has the desirable property of extracting the main features from a set of training data involving both images, mechanical predictions, and other multimodal data for each instance of a mechanical component. In this work, a spectral embedding of asmanufactured geometries enables us to train a ROM-net (1) that captures a reduced latent space hidden in multimodal data. The training set is composed of Digital Twins (DT) and augmented data.

A Digital Twin is an ultra-realistic model with geometric details, including manu- facturing anomalies, or with specific material properties, specific to an instance of a real mechanical component. More precisely, when considering model-based engineering systems, a DT integrates ultra-high fidelity simulations, maintenance history, and all available historical data. With the development of Non-Destructive Testing (NDT) in the manufacturing industry, we can expect a growing activity on image-based DT (2) for accurate descriptions of as-manufactured geometries and microstructural properties

of structural components (3). Unfortunately, image-based twining in material science is so complex and time-consuming that, in practice, this task does not scale with the frequency of quality inspection in manufacturing. This is a major scaling issue for online DT of asmanufactured structural components when the lifetime or other functionalities of components are strongly affected by geometrical defects. However, new margins of tolerance to defects are certainly identifiable with a better modeling of part functionality in relation to defects. Another issue is the curse of dimensionality related to the dimension of the geometrical ambient space, i.e., the space that contains all geometries under consideration, so that a dense sampling of this ambient space is unaffordable. Thus, learning regressions for lifetime predictions from observational data may not be relevant for such image-based modeling. We think that a better approach is to consider a sparse latent space equipped with categories of data. So we can augment multimodal data in each cluster in order to train a ROM-net (1) that includes a classifier. In a ROM-net, input data feed a classifier that forecasts the label of a local reduced-order model, which is used for mechanical predictions.

In this work, we consider Real Instances of Mechanical Components (RIMC) that undergo mechanical or thermo-mechanical loadings in an experiment that reflects what materials have to support in extreme loading conditions. We focus on surface defects, unlike (2) where volume defects were considered. The as-manufactured geometries are observed by X-Ray Computed Tomography (CT) that generates 3D accurate digital images of RIMC with high

^{*}Speaker

complexity. Meshes of real geometries are extracted from X-Ray CT. The surface of the DT is a graph extracted from its surfacic mesh. Because of the variety of graphs we obtain, machine learning tasks using real geometry as input data are not trivial, especially when learning a manifold for nonlinear model order reduction. We propose two different ways to build a common embedding of the digital twin's geometries. One proposal is to deform a CAD mesh related to an ideal geometry in order to fit each DT's mesh, up to a given tolerance. Such a common embedding facilitates the computation of similarity matrices between mechanical predictions related to different digital twins, as proposed in (?). Unfortunately, the CAD mesh is a high dimensional object.

The mesh deformations are performed by using a spectral embedding of the graph related to the surfaces of the meshes. This spectral embedding gives a spectral clustering of the geometries. We show that the medoids (geometrical cluster centers) obtained by spectral clustering are good candidates for a reduced embedding of digital twin's geometries. The smaller the dimension of the input space, the smaller the number of augmented data we need to train an accurate classifier. Once this classifier is trained, the overall result is a ROM-net, that takes as input the reduced geometrical coordinates of digital twin, and forecast related reduced order predictions.

REFERENCES

(1) Daniel, T., Casenave, F., Akkari, N., and Ryckelynck, D. Model order reduction assisted by deep neural networks (ROM-net). Advanced Modeling and Simulation in Engineering Sciences 7, (2020).

(2) Launay, H., Willot, F., Ryckelynck, D., and Besson, J. (2021b). Mechanical assessment of defects in welded joints: morphological classification and data augmentation 11., (2021).

(3) Aublet, A., Rambaudon, M., NGuyen, F., Ryckelynck, D., Remacha, C., Cariou, R., et al. Mechanical fatigue testing under thermal gradient and manufacturing variabilities in nickel-based superalloy parts with air-cooling holes, (2022).

Reduced-order models as enablers for design, control and predictive digital twins

Karen Willcox*1

¹University of Texas at Austin – United States

Abstract

Reduced-order models play a critical role in achieving design, control and uncertainty quantification for complex systems. They are also a key enabling technology for predictive digital twins. Operator Inference is a scientific machine method that learns predictive reduced-order models from data. The method targets the derivation of a reduced-order model of an expensive high-fidelity simulator that solves known governing equations. Rather than learn a generic approximation with weak enforcement of the physics, as in other machine learning approaches, we learn low-dimensional operators of a dynamical system whose structure is defined by the physical problem being modeled. These reduced operators are determined by solving a linear least squares problem, making Operator Inference scalable to high-dimensional problems. The method is entirely non-intrusive, meaning that it requires simulation snapshot data but does not require access to or modification of the highfidelity source code. This talk will highlight successful application of Operator Inference for large-scale engineering problems in rocket combustion, additive manufacturing and materials modeling.

PGD in nonlinear computational solid mechanics: a general weakly invasive version

Pierre Ladevèze^{*1}, Ronan Scanff¹, and David Néron¹

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Abstract

The aim is to provide engineers, through industrial finite element analysis software, with new tools that are reduced solutions or reduced computational models in Nonlinear Solid Computational Mechanics. Model Order Reduction methods have now demonstrated their great strength and interest in reducing complexity. Unfortunately, today these methods are not fully integrated into the engineering tools of general industrial finite element analysis software.

The work presented here is an attempt to answer this question. To do this, we revisit the LATIN-PGD method, for which we present a version that is slightly less efficient than the current version but which is very general and not invasive regarding industrial finite element calculation software. General means compatible with all non-linear material models included in industrial finite element analysis software and, in particular unilateral contact models and all this in large displacements. The only restrictions we have for the actual implementation (1) in the Simcenter Samcef software are: quasi-statics conditions and loadings free of instabilities

The LATIN method is an iterative solver for non-linear time-dependent problems whose primary characteristic is that it is non-incremental. At each iteration, the histories of the various quantities are calculated over the entire time interval, which can be as large as desired. (2). The LATIN-PGD method allows the separation of the time variable from the space variable. For problems with parameters, the separation uses a remarkable property of LATIN-PGD: the initialization of the iterative process is arbitrary, and therefore, the calculation over the parameter surface is easily carried out from step to step.

To further improve performance, we introduce a hyper reduction technique, also weakly invasive, to reduce the computational time spent on the integration of constitutive laws, which is currently an important part of the computational time. It belongs to what is called shallow learning.

Finally, we give a number of illustrations that show the great possibilities and also the gains that we have with this new weakly invasive version of the LATIN-PGD.

(1) R. Scanff, D. Néron, P. Ladevèze, P. Barabinot, F. Cugnon, J.-P. Delsemme, Weaklyinvasive LATIN-PGD for solving time-dependent non-linear parametrized problems in solid mechanics, CMAME, 396, 2022.

(2) P.Ladeveze On reduced models in nonlinear solid mechanics, European Journal of Mechanics A/Solids 227-237, 2016.

^{*}Speaker

Applications of Artificial Neural Networks in the design of Reduced Order Models: accuracy enhancement and improvement of hyper-reduction techniques

Ramon Codina^{*1}, Zulkeefal Dar¹, and Joan Baiges¹

¹Universitat Politecnica de Catalunya – Spain

Abstract

Reduced Order Models (ROM) in computational mechanics aim at solving problems approximating the solution in spaces of very low dimension. We shall concentrate on the case in which the Full Order Model (FOM) is solved by means of a Finite Element (FE) method and the ROM is obtained from a Proper Orthogonal Decomposition (POD) of a series of 'snapshots'. This way, the ROM solution can be considered to belong to a subspace of the FOM FE space.

The first purpose of this talk is to explain why the Variational Multi-scale (VMS) strategy can be applied quite naturally to the ROM approximation when this is based in a FE method to approximate flow problems. This yields a stable ROM problem.

The second objective of the talk is to explain two applications of Artificial Neural Networks (ANN) in the context of ROM. The first is the improvement in accuracy. An additional correction term can be added to the final discrete problem, and this is trained by the condition that the ROM solution at the time steps at which the snapshots are available be as close as possible to these snapshots. The second application is related to hyper-reduction of nonlinear problems. In this case, ANN can be used to choose the optimal sampling points in a classical greedy algorithm such as the Discrete Empirical Interpolation Method (DEIM).

Some elements of analysis for nonlinear compressive reduced basis approximation for PDE's

Yvon Maday^{*1}

¹Laboratoire Jacques-Louis Lions – Sorbonne Universite, Centre National de la Recherche Scientifique, Université Paris Cité – France

Abstract

Linear model reduction techniques design - off-line - low-dimensional vector subspaces suitable for approximating the solutions of a parametrized partial differential equation, with the aim of performing numerical simulations - on-line - with few degrees of freedom and therefore very fast. These methods, such as the Proper Orthogonal Decomposition (POD) or the Reduced Basis (RB) method, are very effective when the family of solutions has fastdecaying Karhunen-Loève eigenvalues or Kolmogorov m-widths, reflecting the approximation by linear spaces with small dimension. On the other hand, they become inefficient when these quantities have slow decay, particularly for families of solutions for transport problems with parameter-dependent fronts. The aim of this work is to explore the ability of nonlinear model reduction to circumvent this particular situation via nonlinear reconstruction. Based on the recent paper (2), we first review the various notions (linear and nonlinear) of m-widths for compact sets, and in particular the Kolmogorov m-width and the Gelfand m-width. Based on these notions, which can be very different, we then propose a new nonlinear approach (1)to take advantage of Gelfand's small m-width in a context where Kolmogorov's m-width is large. To maintain efficiency, algorithms must have complexity related to the first of these dimensions while minimizing that involving the second. We will present some recent developments in the analysis of such algorithms.

REFERENCES

(1) Barnett, J. L., Farhat, C., & Maday, Y. (2023). Mitigating the Kolmogorov Barrier for the Reduction of Aerodynamic Models using Neural-Network Augmented Reduced-Order, Models. In AIAA SCITECH 2023 Forum (p. 0535).

(2) Albert Cohen; Charbel Farhat; Yvon Maday; Agustin Somacal. Nonlinear compressive reduced basis approximation for PDE's. Comptes Rendus. Mécanique, Online first (2023), pp. 1-18. doi : 10.5802/crmeca.191.

AI4Design@Safran: learning physics simulations for improving design processes

Fabien Casenave^{*1}, Christian Rey¹, and Frédéric Feyel¹

¹Safran Tech – Safran Tech, Rue des Jeunes Bois - Châteaufort – France

Abstract

The project AI4Design at SafranTech, the corporate research center of Safran Group, aims to leverage AI technologies to improve the design processes that rely on the numerical simulation of physics phenomena. These improvements contain the derivation of fast and reliable surrogates for various physics, the construction of new models and certification algorithms, as well as the publication of available codes and databases for the community to use.

In this talk, we start by presenting the motivations for an industrial group like Safran to construct such a project, before shortly listing the activities of AI4Design. Then, we provide more details for three activities: (i) an open source numerical experiment platform called Lagun, providing tools for computing workflows involving Design of Experiment, meta-modelling optimization and visualization for scalars input-outputs, (ii) an open-source library called genericROM for non-intrusive physical reduced-order modeling of non-linear structural mechanics and thermal analysis, and (iii) experiments with convolutional graphneural networks applied to the construction of surrogates for stationary compressible flows. Information on the published codes and databases is provided for each subject. Finally, we present some outlook for this project.

Two other talks at MORTech 2023 present methodologies for learning physics simulations under non-parametrized geometrical variability: (i) using a variational auto-encoders for producing physical reduced-order models of unsteady and convective 3D flows, with predictive uncertainties, and (ii) using classical machine learning tools thanks to nonlinear deterministic dimensionality reduction (involving morphing and principal component analysis) and Gaussian process regression, with predictive uncertainties.

ABSTRACTS

Day 1 – Wednesday, November 22

Afternoon sessions

Can we perform Model Reduction Techniques by using a NISQ quantum computer?

Antonio Falco^{*1}

¹University CEU Cardenal Herrera (UCHCEU) – C/San Bartolome 55, Alfara del Patriarca (Valencia), Spain

Abstract

The aim of this talk is twofold. First, we will introduce quantum computers and their current capabilities. We will also compare these quantum devices to their classical counterparts, highlighting the differences in their formal languages. In the second part, we will explore two alternatives for utilizing this new class of computers.

(i) The deterministic approach involves extending the quantum version of our existing algorithms, which were originally designed for classical computer frameworks.

(ii) The stochastic approach, although still under development, holds the potential to efficiently implement stochastic differential equations.

POD-Galerkin reduced order model coupled with neural network to solve flow in porous media

Cyrille Allery^{*1}, Claudine Béghein, Claire Dubot, and Fabien Dubot

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Abstract

Flows in porous media have been encountered in various applications (water infiltration in the soil, flows in biomaterials, geothermal energy production, etc.). Numerical simulation of flows in porous media using classical approaches requires long computation times and significant storage capabilities. To overcome these difficulties, we propose in this paper to use model reduction techniques, which involve constructing a reduced spatial basis and projecting the governing equations of the problem onto this basis, to obtain a system of ordinary differential equations of small size that can be solved quickly. In the few existing works dealing with model reduction techniques applied to flows in porous media, flows were described by Darcy's law and the non linear Forchheimer term was neglected. This last term cannot be expressed in reduced form during the Galerkin projection phase. Indeeed, at each new time step, the norm of the velocity needs to be recalculated and projected, which significantly increases the computational cost, rendering the reduced model inefficient. In this work, we propose to model the projected Forchheimer term with artificial neural networks. To do that, a low order dynamical system, based on Proper Orthogonal Decomposition, was built. Performing a Galerkin projection of the Navier-Stokes equations onto the most energetic modes yields the following reduced equations: $d\mathbf{a}/dt = \mathbf{F}(\mathbf{a},\alpha) + \mathbf{R}\mathbf{f}(\mathbf{a},\alpha) + \mathbf{R}\mathbf{p}(\mathbf{a},\alpha) + \mathbf{R}\mathbf{u}(\mathbf{a},\alpha)$

where $\mathbf{a}(\mathbf{t},\alpha)$ represents the coefficients of the POD model, depending on time t and parameters α (the Reynolds number in this work). F includes convection and diffusion terms. Rf represents the projected term associated to the Forcheimer term, Rp the projected term associated to the neglected pressure and \mathbf{Ru} the influence of the unresolved scales. Instead of separately modeling each of these terms, they were combined into a single term **R**, which was modeled, depending on coefficients $\mathbf{a}(\mathbf{t},\alpha)$, using a neural network. It can be noticed that the presence of the Forcheimer term, which cannot be directly reduced by POD, makes difficult the application of Physics Informed Neural Network (PINN) (1) coupled with ROMs for solving problems in porous media. This study aims at taking into account the reduced residuals \mathbf{R} to improve the results of the low order dynamical system. To do that, the computed snapshots provided a data set associating the exact temporal coefficients **a** with the residuals \mathbf{R} , and the multilayer perceptron method (MLP)(2) was then employed. This method was applied to compute flow around and through a porous square obstacle in an unconfined channel for three Reynolds numbers Re=(120, 140, 160). The proposed ROM MLP method successfully evaluates the residuals in a low order reduced model. Moreover, the ROM MLP method improves, compared to the standard POD ROM Galerkin appropach,

^{*}Speaker

the prediction of flow for Reynols numbers that are included or not included in the sampling and for times longer than sampling times.

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. *Journal of Comp. Physics*, 378:686–707, 2019.
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Reduced Order Modeling and LES filtering

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Abstract

We will discuss the development of reduced order models (ROMs) for the incompressible Navier-Stokes equations (NSE) and the quasi-geostrophic equations (QGE). The commonality between these sets of equations is that in certain regimes (i.e., large Reynold number for the NSE and QGE and large Rossby number for the QGE) they require very fine meshes to compute accurate solutions. To circumvent this need, we adopt nonlinear filter stabilization as an efficient Large Eddy Simulation technique. For the realization of this stabilization, we combine a three-step algorithm called Evolve-Filter-Relax (EFR) with a computationally efficient finite volume method for both the NSE and the QGE.

The main novelty of our ROM for the NSE lies in the use within the EFR algorithm of a nonlinear, deconvolution-based indicator function that identifies the regions of the domain where the flow needs regularization. The ROM we propose is a hybrid projection/data-driven strategy: a classical Proper Orthogonal Decomposition Galerkin projection approach for the reconstruction of the velocity and the pressure fields and a data-driven reduction method to approximate the indicator function used by the nonlinear differential filter. This data-driven technique is based on interpolation with Radial Basis Functions. The EFR approach is used as a regularization for ROMs for the QGE to increase the accuracy when the Proper Orthogonal Decomposition modes retained to construct the reduced basis are insufficient to describe the system dynamics.

For both sets of equations, the accuracy of the ROMs is assessed through several benchmark tests.

Novel L2-Projection to achieve Minimally Intrusive Affine Reduced Order Models

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Abstract

Reduced Basis Methods (RBMs) promise fast solutions of parametrized problems arising from a wide variety of backgrounds. Such methods can be used to enable real-time response, control and efficient algorithms for inverse problems.

Although the solution stage of an RBM is fast, a great deal of care must be taken to ensure fast assembly. In particular the problem must be fully or approximately affine in the parameter space. Ensuring this is generally a process that involves expert knowledge not only of the specific problem and the parameters under consideration, but also of the full-order model (FOM) being used to construct the RBM. This process is rarely generalizable and highly intrusive. See for example (2).

We present AROMA (3) - a general framework for nearly non-intrusive RBMs for building re-usable joint component models (1) for jacket structures. Such components are generally highly geometrically variable, and thus almost never affine. By computing a least-squares fit of system matrices in the parameter space we are able to achieve appreciable accuracy without impacting speed.

To achieve rapid deployment in industry applications, a core aim for this work has been mimimal intrusiveness. To this end, AROMA only requires knowledge from the FOM about the system matrix and load vector, as well as information about which degrees-of-freedom are fixed. These data are generally readily available from most FOM software (even proprietary) as debug output. Therefore AROMA can be made to work with most such software with little effort.

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^{*}Speaker

Autoencoder-accelerated computational homogenization of unsteady flows in porous media

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Abstract

As an alternative to empirical approaches such as Darcy's law and its extensions, a computational homogenization approach has recently been developed for modeling flows in porous media (1,2). In this approach, equations of Navier-Stokes type are solved using the Finite Element (FE) method at the coarse scale of the domain instead of Darcy's law. These equations involve force and stress derivatives tensors instead of the permeability tensor. In the steady case, these tensors can be computed beforehand in a pre-processing step using simulations at the fine scale of the porous medium. In the unsteady case, fine scale domains are introduced at each point of the coarse scale domain, and simulations at the two scales are strongly coupled. The resulting FExFE or FE² scheme entails a significant computational cost. It has the advantage, however, of predicting simultaneously the flow at the two scales. This approach has been demonstrated to be reliable and robust, especially for problems involving a very small pore characteristic length and a Reynolds number below 100. It has been shown to be interesting for modeling unsteady flows in porous media as well as flows involving both a porous part and a purely fluid part such as a channel.

These results are promising for applications to reservoir engineering or composites manufacturing. The associated computational cost, however, is limiting. In this work, a nonlinear Reduced Order Model (ROM) inspired from a previous work on brittle fracture (3) is developed for solving the fine scale problems. The dimension of the fine scale velocity fields is reduced using an autoencoder, which is a specific kind of deep neural network that is tailored for nonlinear dimension reduction. A recurrent neural network is then developed to predict the fine scale flow in the reduced space. This recurrent neural network is integrated in an FExROM multiscale scheme where the coarse scale problem is still solved using the FE method, but all fine scale problems are solved using the nonlinear ROM combining an autoencoder and a recurrent neural network.

This presentation will introduce this original approach for modeling unsteady flows in porous media, with an emphasis on the nonlinear ROM. The integration of this ROM within the multiscale FE code will be detailed, especially regarding the computation of the derivatives tensors. The capabilities of the proposed FExROM multiscale method will be demonstrated for problems of increasing size.

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^{*}Speaker

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Model order reduction for the identification of the thermal resistance of highly Insulated walls

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Abstract

In a context of energy and environmental renovation, major advances are expected and necessary in the Building sector. For existing buildings, the reduction of energy consumption requires a better assessment of the energy performance of buildings and their improvement through rehabilitation actions. A particular attention has to be paid to in-situ evaluation and control of the thermal performance of the buildings before and after a rehabilitation action in order to prevent any defect and thus to obtain a building with the expected performances. In this work, we propose an inter-disciplinary technical solution combining physical modelling, statistical modelling and measurements for a better in-situ characterization of the energy performance of walls.

Simplified physical model like RC or 1D heat equation are not suitable for an accurate identification of the thermal resistance for highly insulated walls and for some wall typologies. This is due to the fact that transverse heat fluxes in the wall are not taken into account in these models. More sophisticated physical models are to be considered such has 2D/3D thermal simulations and hygro-thermal physical models.

As the considered models can be costly in terms of computational time, we propose to accelerate the identification method by using model order reduction approach. Projection techniques such as Reduced Basis Methods which are well adapted to unsteady thermal equations, will enable real-time calculations of the model solutions. Concerning the identification process, it will be based on Bayesian framework. The main goal is to develop a multi-fidelity approach using notably Gaussian process and meta-modeling to select the the appropriate model for a given wall typology in view of identifying its thermal resistance, to propagate uncertainty in the costly inversion model and to derive a robust confidence interval for the identified thermal resistance.

The numerical methods will be tested first on numerical benchmarks where the sensor outputs are numerically generated from a reference model.

Fracture propagation problems enhanced by uncertainty propagation and Bayesian identification of parameters

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Abstract

Fracture propagation simulations are highly sensitive to material and model parameters and can often produce uncertain results. In this work we exploit the Bayesian approach to consider uncertain parameters in fracture simulations. We also show the uncertainty propagation procedure in macro and mesoscale computations of cementitious materials. Two fracture models are considered in this work. One is based on enhanced solid elements with embedded strong discontinuity represented with discontinuity line in the element interior. The other one is an efficient discrete lattice fracture model with embedded discontinuities. The latter is improved by Bayesian identification of parameters in order to show how discrete models can be calibrated for proper representation of materials.

Complemented Deep - Reduced Order Model

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Abstract

Reducing simulation time is critical for applications such as closed loop control or iterative design optimisation. In this context, model reduction techniques have become a growing area of research in the last decades. While research efforts have mainly been centered around feature based approaches like POD, BPOD or DMD, direct approaches leveraging Deep Neural Networks have been proposed in recent years with great success. Despite these promising results, neural network architectures provide little to no physical guarantees, and have limited interpretability. On the other hand, feature based methods often reconstruct the final solution through a linear combination of modes embedded with physical constraints. However, this often comes at the cost of loss of information and increased error rates. POD-Galerkin models are a perfect example of this trade-off between physical guarantees and performance loss. These models have been shown to be very efficient for the reduction of linear systems, but they are extremely limited when applied to nonlinear systems such as the Navier-Stokes equations. To address these shortcomings, we propose to add a closure term to POD-Galerkin models to correct their dynamics. We use simple neural networks in combination with delay differential equations to reconstruct the required correction. We show that a satisfactory model can be trained through the Neural ODE framework to learn a memory based correction from simulation data. We preserve the simple structure and low computational cost of Galerkin models while improving their performance.

A posteriori model reduction combining creep, contact and friction in a multi-scale simulation

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Abstract

Multi-physics and multi-scale models are becoming increasingly common, with the corollary of high computing costs related to their dimension and presence of non-linear phenomena. This is particularly the case for simulating the irreversible deformations that gradually appear in the fuel assemblies inside a nuclear reactor core when they undergo intense irradiation, creep, internal contacts and friction as well as fluid-structure interactions. In this particular case, the topology and characteristics are well known and stable for a great number of studies, for this reason an *a posteriori* reduced order model is indicated for its better computing performance.

A general strategy combining Domain Decomposition and Nonuniform Transformation Field Analysis (NTFA) (1) is proposed herein for the simulation of nuclear fuel assemblies at the scale of a full nuclear reactor. The model at subdomain level (one fuel assembly) solves the full elastic problem but with a reduced nonlinear loading, based on simplified boundary conditions which operate on a POD basis (2). The NTFA idea is to define a reduced evolution law acting in an orthogonal basis of internal variables. This method has been adapted to a representative elementary volume of slender structure without scale separation, in order to obtain a reduced model for the creep of the fuel assembly with heterogeneous and time varying material characteristics.

In this framework, the model reduction of the contact problem calls on a NMF basis (3) to represent the Lagrange multipliers for contact and reduce the number of Signorini conditions. These are expressed in a specifically constructed basis of contact opening modes.

Finally, the reduction of the Coulomb friction model takes advantage of a POD basis of sliding modes and uses the normal forces solution of the previous contact problem. The threshold vector of the friction forces are approximated at any time thanks to a superposition of the criterions associated to each normal force amplitude. A spherical interpolation of the sliding direction with respect to the modal directions then gives the current modal friction forces. A penalization facilitates its implementation. In the end, the different test-cases show speed-ups ranging from 40 to 1000 with a reasonable accuracy. (1) Michel, J.C., Suquet, P., 2003. Nonuniform transformation field analysis. Int. J. Solids Struct. 40, 6937–6955. https://doi.org/10.1016/S0020-7683(03)00346-9

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^{*}Speaker

On the relationship between supremizers and least-squares pressure computation in ROMs for incompressible fluids

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Abstract

In this talk we afford the recovery of the pressure from weakly divergence-free basis functions in ROMs for incompressible fluids. We propose a recovery procedure by least-squares minimisation of the residual dual norm. We prove that this procedure provides a unique solution whenever the full-order pair of velocity-pressure spaces is inf-sup stable. We also prove that this least-squares recovery of the pressure is equivalent to solving the

reduced mixed problem with reduced velocity basis enriched with the supremizers of the reduced pressure gradients. A similar result holds for the full-order mixed problem.

We prove error estimates for the least-squares recovered pressure for general incompressible flow equations. We finally present some numerical results for transient Navier-Stokes equations, showing a spectral convergence, in good agreement with the theoretical expectations

Model Order Reduction in the Parametrized Multi-Scale Materials Setting

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Abstract

Two-scale simulations are often employed to analyze the effect of the microstructure on a component's macroscopic properties. Understanding these structure–property relations is essential in the optimal design of materials, or to enable (for example) estimation of microstructure parameters through macroscale measurements. However, these two-scale simulations are typically computationally expensive and infeasible in multi-query contexts such as optimization and inverse problems. To make such analyses amenable, the microscopic simulations can be replaced by inexpensive, parametric surrogate models. In this talk, we (1) present some recent work on a non-intrusive reduced basis method to construct inexpensive surrogates for parametrized microscale problems, and (2) highlight difficulties for model order reduction presented by nonlinear constitutive relations in (multi-scale) problems in mechanics.

^{*}Speaker

Thermomechanical modeling of the Directed Energy Deposition (DED) additive manufacturing process: coupling the Inherent strain rate and POD-based model reduction

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Abstract

The Directed Energy Deposition (DED) processes are additive manufacturing processes in which focused thermal energy is used to fuse materials by melting as they are being deposited. To optimize the process parameters in terms of distortion and stress prediction, numerical thermo-mechanical modeling is a good approach, as it allows for minimizing expensive and time-consuming experiments. However, the non-linear thermomechanical calculation is costly.

In this work, we focus on the complexity reduction of the macroscopic thermomechanical modeling of DED processes under the frame of the finite element method. As the plastic deformation is mainly localized within a small region near the deposition, this makes possible a linearization of the initial elastic-viscoplastic mechanical resolution. In practice, a prediction correction algorithm is developed. The predictor step consists of the linearized mechanical resolution, in which the generalized plastic strain rate is deduced from the previous resolutions. This is why the method is named "inherent strain rate". The corrector step consists of a local (e.g. in each finite element) reconstruction of the effective stress field by solving a local non-linear scalar equation. This predictor/corrector strategy is employed to deal with the dynamic evolution of strain rates and stress, in which the two situations of deposition on the one hand and dwell time on another hand are treated differently. With the above method, a time gain of around 5 is obtained, while the results (distortion and stress) of the full non-linear thermomechanical resolution are replicated with excellent accuracy.

To further reduce the computational cost, POD-based model reduction is proposed to couple the Inherent strain rate method. The primary purpose of this step is to reduce the number of degrees of freedom of the equilibrium equation to be resolved. Finally, a time gain of around 30 is achieved by maintaining the prediction quality for both distortion and stress. By coupling the Inherent strain rate and POD-based model reduction, the two-step reduction method provides an efficient solution for parametric analysis for DED processes.

Keywords: Inherent strain rate, POD-based model reduction, Directed Energy Deposition (DED) process

^{*}Speaker

Stochastic model updating and identification for nonlinear aeroelastic systems

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Abstract

With the growing integration of complex systems to improve efficiency and sustainability in aviation, nonlinearity is becoming increasingly present in many forms of aerospace engineering structures. The effects of these nonlinearities on dynamics and control can be very significant such as changing futter boundaries in tiltrotor systems leading to complex limit cycle oscillations. The objective of this work is to develop a probabilistic model updating the framework to efficiently identify the parameters and models of general nonlinear aeroelastic systems based on LCO experimental data obtained from control-based continuation testing. The Bayesian interface is applied to stochastically update the nonlinear aeroelastic systems using the noise and uncertain data directly from the nonlinear testing. Advanced Kriging algorithm is used to construct surrogate models for nonlinear aeroelastic systems with the databases from harmonic balance method-based bifurcation analysis. Three types of sampling methods, namely Markov Chain Monte-Carlo, Transitional Markov Chain Monte-Carlo and Sequential Monte-Carlo, are implemented into Bayesian model updating. The proposed methodology provided up to 20% improvement in accuracy compared to conventional deterministic methods with Transitional Markov Chain Monte-Carlo as the optimal choice of the sampling method. In selecting alternative nonlinear models, multi-modal solutions were identified that provided a closer representation of physical behaviour.

The Empirical Interscale Finite Element Method: A novel approach for modeling heterogeneous structures using localized dimensional hyperreduction

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Abstract

This study proposes an innovative Finite Element (FE) technology known as the Empirical Interscale FE method, designed specifically for modeling heterogeneous structures in the small strain regime. This method combines a domain decomposition framework, featuring interface conditions established through "fictitious" frames, with dimensional hyperreduction at the subdomain level.

Similar to other multiscale FE methods, the structure is divided into coarse-scale elements, each equipped with a fine-scale subgrid. The displacements of the coarse-scale element boundaries are described using standard polynomial FE shape functions. The distinguishing feature of the proposed method is its "interscale" variational formulation, which directly relates coarse-scale nodal internal forces to fine-scale stresses. This unique characteristic eliminates the nested local/global problems typically encountered in other multiscale methods, particularly in the nonlinear regime.

Additionally, the method incorporates hyperreduction schemes for nodal internal and external body forces, utilizing a continuous version of the Empirical Cubature Method previously proposed by the first author. These schemes greatly facilitate the implementation of the proposed formulation in existing FE codes for solid elements. By adjusting the location, weights, and empirical values of integration points, as well as the shape functions and strain-displacement "B"-matrices derived from appropriate computational experiments, the method can be seamlessly integrated into existing FE codes for solid elements.

The effectiveness of this formulation is demonstrated through several examples. Firstly, we demonstrate that the elements resulting from this method are not affected by volumetric locking, making them suitable for modeling nearly-incompressible materials. Furthermore, the method successfully handles non-matching fine-scale grids and curved structures. Lastly, for periodic structures, we show that the proposed method converges to the solution obtained through classical first-order computational homogenization as the mesh is refined. This capability allows the method to represent solutions even in cases without a distinct scale separation, as long as sufficiently small coarse-scale elements are employed.

^{*}Speaker

Reduced Order Model for Temperature Field Simulation of Wire Arc Additive Manufacturing with Domain Mapping

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Abstract

Additive manufacturing (AM) has revolutionized the manufacturing industry, offering a new paradigm to produce complex geometries and parts with customized properties. Among the different AM techniques, the wire arc additive manufacturing (WAAM) process has gained significant attention due to its high deposition rate and low equipment cost. However, the process is characterized by a complex thermal history making it challenging to simulate it in real-time for online process control and optimization.

In this context, a reduced order model (ROM) using the proper generalized decomposition (PGD) method (1) is proposed as a powerful tool to overcome the limitations of conventional numerical methods and enable the real-time simulation of the temperature field of WAAM processes. These simulations use a moving heat source leading to a hardly separable parametric problem, which is handled by applying a novel mapping approach (2). This procedure makes it possible to create a simple separated representation of the model, which allows to simulate multiple layers.

In this contribution, a PGD model is derived for the temperature field simulation of the WAAM process. A good agreement with a standard finite element method is shown. The reduced model is further used in a stochastic model parameter estimation using Bayesian inference, speeding up calibrations and ultimately leading to a calibrated real-time simulation.

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Model-order reduction of optimal transport problems

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Abstract

The aim of this talk is to present some recent results about the development of new reduced-order models for optimal transport problems. Optimal transport arise in a wide variety of applications: crowd motion, economy, quantum chemistry... In the most simple case, the aim is to find the optimal joint law of two random variables, for which we know their marginal laws, so that the variance of the difference between these two random variables is as small as possible. Our aim here is to propose a numerical method in order to accelerate parametric studies of optimal transport problems, where the marginals are parameter-dependent. While the set of solutions of the primal problem (in Kantorovich form) cannot be easily reduced by means of standard linear reduced-order models, the situation is different when one considers the solution of the dual problem, called the Kantorovich potential. Our strategy then consists in introducing a reduced-order model, inspired from the Reduced Basis method, where the Kantorovich potential is approximated in a small-dimensional vector space. This results in an approximate primal problem which reads as a Moment Constrained Optimal Transport problem, the solution of which is proved to be very sparse. We then exploit this sparsity pattern in order to propose an efficient numerical method to solve the obtained reduced-order model.

A databased approach for micro-macro topology optimization of micro-architectured materials

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Abstract

With respect to increasing industry demands for predictable computer simulations, the development of numerical methods in structural design has received considerable attention over the past few decades. Among them, the optimization of the topology has proven its effectiveness for the design of complex structures with requirement of specific mechanical properties. The latest advances in 3D printing processes allow today to manufacture of sophisticated structures and micro-architectural materials. This work presents an original approach for the design of compliant mechanisms integrating micro-architectured materials based on a multi-scale strategy. The underlying idea is that micro-architectured materials may exhibit more complex behaviors compared to standard materials. Therefore, adding those materials in the design of compliant mechanisms can lead to better performance. The method used replaces the standard density distribution used in common topology optimization methods, such as SIMP or levelset methods, by a distribution of material properties. Once the optimization has converged, a material map of the properties in the design domain are obtained and the corresponding microstructures are designed a posteriori by inverse homogenization. However, the computational cost associated with such a method can become exorbitant, especially if the number of micro-architectured materials to be designed is substantial. A databased approach is studied to reduce these computational efforts. An optimized catalog of micro-structured materials covering a wide range of different mechanical behaviors is calculated a priori. The catalog is then consulted to extract the microarchitectured materials as closely as possible, in terms of mechanical behaviors, compared to what is required for the compliant mechanism. References

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Interaction based deep material network model reduction technique for porous polymer structures fabricated using additive manufacturing

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Abstract

Additive manufacturing techniques offer new opportunities to produce new structure with enhanced performances. Particularly, the selective laser sintering (SLS) is widely used in the industry to fabricate polymer-based structures with high printing quality and properties. Recently, the SLS technique has been employed to produce lattice structures intended for shock absorbing applications, such as cycling helmets.

However, the structural responses of printed parts pose several challenges. In fact, microscopic tomographic images demonstrated the presence of porosity after polymer powder sintering during the process. This porosity is variable and has significant impact on the overall behavior of printed parts. Conventional multiscale techniques such as mean field and computational homogenization cannot be envisioned to addressee those issues due to different reasons. First, polymer behaviors are generally nonlinear and require considerable computational resources. Secondly, the assessment of the variabilities caused by the microstructure porosity on the structural behavior requires enormous evaluations of RVE models.

In this research paper, we present an extension of a model reduction technique known as interaction-based deep material network (IB-DMN) to porous polymer microstructures exhibiting ViscoElastic-ViscoPlastic behavior. The IB-DMN method aims to simplify the geometric complexity of the RVE by representing it using a deep physical network structure. This network consists of nodes and interactions characterized each by a set of parameters. The determination of optimal reduced representation of the microstructure is performed once for all during an offline step. It involves collecting the effective responses of the RVE under random loading conditions, considering only simple material models such as linear elasticity. The data base of simulations is then used to tune network parameters during a training phase. Once trained, the tuned parameters of the IB-DMN can be used in the multiscale modeling approach to replace the real RVE FE model.

The IB-DMN was also extended to be microstructurally guided to account for the RVE variable porosity. Toward this end, a limited number of base IB-DMN with known porosity level were constructed. The parameters of these base IB-DMNs were then interpolated to compute the parameters of a new microstructure without requiring additional offline training.

The developed model reduction technique demonstrated a good ability to be extrapolated to new material behavior, even when the training process employs different material models. The accuracy of the results is almost similar to computation homogenization when the

network structure is sufficiently dense. Moreover, the new method is able to considerably reduce the computational cost by at least two orders of magnitude. The extension of the IB-DMN to enable stochastic multiscale modeling makes it more affordable computationally, since it utilizes pre-determined base DMNs.
Learning How RoMs Propagate Uncertainties Using Physics Informed Normalizing Flows

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Abstract

Most Reduced Order Models (RoMs) for dynamical system can be casted as evolution equation on a lower dimensional manifold. However, how do these RoMs propagate uncertainty? For the particular case of an uncertain initial condition, we will derive propagation of uncertainties on the reduced manifold on which the RoM evolves. In particular we will show that this uncertainty is given by a pushforward map that evolves according to the liouville equation. We will develop physics informed Normalizng flows that learn this evolution equation.

Model order reduction for the finite element approximation of eigenvalue problems

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Abstract

We consider model order reduction methods for the approximation of the eigensolutions with the finite element method. In particular, time continuation techniques are used and a corresponding fictitious time parameter is introduced. We present some theoretical results associated to a POD approach showing how to choose the optimal dimension of the POD basis. The results of our computations confirm the optimal behavior of our approximate solution.

Local model order reduction to accelerate additive manufacturing simulations

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Abstract

Conventional transient mechanical FE simulations of large-scale metal additive manufacturing (AM) processes, such as wire-arc additive manufacturing or laser metal deposition, are computationally demanding. A local model order reduction (MOR) method has been devised to accelerate such simulations by using the characteristics of the process in an advantageous manner. In large-scale metal AM, nonlinear material behaviour is typically confined to a relatively small zone around the moving heat source, whereas material far away from the heat source remains elastic and experiences loading of repetitive character.

The FE model is decomposed into multiple subdomains using the dual-primal FETI (FETI-DP) method (1). Subdomains that behave nonlinearly are modelled full-order. Adjacent linear subdomains are grouped into a single reduced-order region and all their nodes are designated as primal nodes. The deformation of these nodes is approximated using novel covariant modes (2). These are based on local POD modes, capable of accurately representing local deformation characteristics, which are extended such that the entire reduced-order region deforms along with these local POD modes in a compatible manner. The POD modes are generated from displacement snapshots obtained while solving a representative set of simulation steps with the full-order model.

Because all nodes of reduced-order subdomains are primal nodes and due to the global nature of the covariant modes, the contribution factors of these modes become primal degrees of freedom. The deformation of the entire reduced-order region is then fully determined after solving the FETI-DP interface problem. This omits the need to locally solve the FE-equations for the displacements of reduced-order subdomains during the iterative solution of this interface problem, thereby accelerating the solution process.

The proposed local MOR method is applied to the mechanical additive manufacturing simulation of the model shown in **Figure 1a**. A 150x9x50 mm3 thin straight wall consisting of 25 two-track layers is deposited onto a 200x100x12 mm3 substrate. The substrate is clamped as a cantilever. The material is S355 structural steel. The deposition direction is alternated between layers. The geometry is decomposed into 176 subdomains, which are grouped into four regions. As shown in **Figure 1b**, region 1 is reduced from the start of layer 5, regions 1+2 from the start of layer 12 and regions 1+2+3 from the start of layer 20. In the final cooling stage (after layer 25), only region 1 is reduced. Covariant modes that span the entire reduced-order region are formed from POD deformation modes of interfaces between the subdomains in that region upon a change in the size of the reduced-order region. The POD

^{*}Speaker

modes are computed from the displacement snapshots saved during the four most recently computed layers. Deposition of layers 11 and 19 is solved full-order to enhance the quality of the deformation modes.

ABSTRACTS

Day 2 – Thursday, November 23

Morning sessions

A Posteriori Error Estimation for Model Order Reduction of Parametric Systems

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Abstract

We will review a posteriori error estimation for model order reduction of parametric systems, including linear and nonlinear, dynamical and static systems. We focus on the development of error estimators we have proposed in the past few years and compare them with other error estimators found in the literature, mostly from the reduced-basis-method community. Some new developments for our error estimators are explored. In particular, we suggest a new error estimator for nonlinear evolution systems. Our recent work on multi-fidelity error estimation will also be briefly discussed. Finally, we derive a new infsup-constant-free output error estimator for nonlinear time-dependent systems. Numerical results will be used to illustrate the robustness of our error estimators.

^{*}Speaker

Reduced Order Modelling in Computational Fluid Dynamics: state of the art, challenges and perspectives

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Abstract

We provide the state of the art of Reduced Order Methods (ROM) for parametric Partial Differential Equations (PDEs), and we focus on some perspectives in their current trends and developments, with a special interest in parametric problems arising in offline-online Computational Fluid Dynamics (CFD). Recent developments involve a better integration of emerging topics with model reduction, such as high performance computing (HPC), uncertainty quantification (UQ), data science (DS), machine learning (ML) in a data driven perspective, in order to allow a better exploitation of digital twins. All the previous aspects are quite relevant – and often challenging - when well integrated also in CFD problems, including turbulence, to focus on real time simulations for complex parametric industrial, environmental and biomedical flows, or even in a flow control/inverse problems setting with data assimilation. Crucial aspects to be addressed are related with uniqueness, stability, accuracy, as well as reliability of solutions. Some model problems will be illustrated by focusing on few benchmark study cases, for example on fluid-structure interaction problems and/or on shape optimisation, applied to some industrial and applied science problems of interest.

Model reduction for multi-query simulations in nonlinear solid dynamics

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Abstract

Simulating a complex structure subjected to a family of loadings is a recurring challenge in predicting service life and taking hazards into account. This is particularly the case when trying to predict the risk of failure of a structure subjected to seismic hazard, which often requires numerous costly computations. When computing fragility curves, for instance, the nonlinear damageable behavior of structures needs to be considered, and the dynamics response of the latter must be computed for a wide range of likely ground motion inputs. In this context, model reduction techniques are the strategies of choice, allowing us to take advantage of computational similarity to speed up the sequence of calculations. The LATIN-PGD method, proposed in (1), enables the non-linear aspects of the problem to be handled efficiently, while the handling of a parametric problem can be made very efficient by constructing a reduced basis shared by all the problems (2).

This work extends the method to the case of dynamics problems and proposes a new approach to deal efficiently with the case where the family of loadings cannot be parameterized. To this end, a space-frequency PGD is introduced when solving the dynamics aspect of the history-dependent nonlinear problem, thus coupling the efficiency of model-order reduction with the numerical benefits of frequency computations (3). The modes generated by the PGD technique are compared with the modes obtained using a modal approach, showing that the reduced PGD basis is particularly optimized to represent a given solution. In order to handle multi-query aspects, a new approach is also introduced, which allows a very efficient chaining of the computations. The final computational cost is significantly lower than the cumulative cost of independently performing the different cases.

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^{*}Speaker

Model Reduction by Convex Displacement Interpolation

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Abstract

Nonlinear interpolation of scalar fields is the focus of this talk. In particular, an extension to the multiparametric case of the technique known as convex displacement interpolation (CDI) is presented. The extension is based on i) the notion of probabilistic models of the solution features and ii) the projection of the resulting mappings onto the space of admissible applications preserving certain bijectivity constraints. Several numerical examples show that the fields obtained through convex displacement interpolation are inherently accurate compared to high-fidelity solutions. Furthermore, in the case of projection-based model reduction, the numerical illustrations show that the solutions obtained through convex displacement interpolation are an inexpensive and effective means of locally enriching the projection space, while still relying on an affine representation of the solution.

Introduction

Model reduction is based on exploring the parameter space of physical models described by a partial differential equations (PDEs) through numerical simulation.

Once a sufficiently rich database has been collected, principal component analysis or Gram-Schmid orthogonalization is performed in order to determine a vector subspace of reduced dimension that optimally reconstructs the starting database.

The sampling density of the parameter space depends strongly on the nature of the data. If the class of solutions being studied shows marked variability of compact support features such as solution singularities, then the density of the sampling and hence the dimension of the optimal reduced subspace increases to such an extent that the use of reduced models might become impractical.

In the literature, this problem is addressed using a variety of approaches that essentially make use of the notion of a mapping. The idea of introducing an appropriate mapping in order to improve the reproduction accuracy obtained with an optimal base of given size is very natural. A first approach is to settle for a non-intrusive prediction of the nonlinearly

interpolated field. Examples of such an approach will be detailed. However, it is not obvious how to subsequently use the mapping in a simple and effective way to devise a projection based reduced model. Some approaches for example integrate the parameters of the mapping into the residual minimization procedure with respect to the latent variables of the reduced model, others reformulate the problem in a reference domain according to a classical Lagrangian method. Appropriate reference to these methods will be given.

Main results

CDI is exact for some standard cases, it is symmetric, it respects positivity and a maximum principle. Moreover it can be extended to a multidimensional parametric spece. CDI can be used to locally enrich the projection space, while still relying on an affine representation of the solution. These results will be discussed in relation to the body of more recent contributions in this direction.

Recent progress in applying Hierarchical Model reduction techniques to applicative contexts

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Abstract

Hierarchical Model (HiMod) reduction has been conceived to describe flows in pipes, where a privileged dynamics aligned with the centerline of the pipe is locally modified by secondary dynamics evolving along the transverse sections (1). The modeling heterogeneity along the different directions finds a counterpart in the diverse discretization adopted along the mainstream and the transverse direction, consistently with a separation of variables paradigm. Standard choices include an isogeometric or a finite element approximation along the centerline, enriched by a (Fourier) modal expansion to describe secondary dynamics. HiMod showed a significant improvement in reducing the computational cost and simulation time, while providing an informative solution. So far, HiMod reduction has been essentially employed for the modeling of the blood flow in arteries affected by pathologies (such as severe stenosys or aneurisms), with excellent results (2).

Aim of this presentation is to highlight some of the most recent advances introduced for a HiMod reduction, both from a methodological and an application viewpoint.

In particular, it will be introduced a specific method to model flows in pipes characterized by a geometric setting inherently excluded by the theoretical formalization of HiMod, such as branches in hemodynamics. As possible instances of applicative contexts alternative to hemodynamics where HiMod reduction can be successfully applied, we will focus on the modeling of acoustic wave propagation in deformed pipelines (3) as well as of the transport of a solute in porous media.

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^{*}Speaker

On an Efficient PGD Solver for Structural Dynamics Applications

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Abstract

The talk will discuss the recent development of a Galerkin-based Proper Generalized Decomposition (PGD) solver for the simulation of low frequency responses in mechanical structures. Significant progress has been achieved on PGD solvers using separated representations with respect to the space and frequency variables(1,2), which allow one to take into account the parametric variability of a system (material properties, geometry, etc.). However, the space-frequency formulation does not necessarily provide direct insights into the transient behavior of the system. While it can determine its response at specific frequencies, it may fail to accurately capture time-dependent loadings or dynamical events. Alternatively, space-time formulations are usually preferred, but early results using the PGD framework were often unsatisfactory. One reason is that the fixed-point algorithm employed by Galerkin-based PGD solvers tends to exhibit poor convergence, if it does converge at all (3). It has even been questioned whether the PGD framework using space-time separability is suitable for solving the wave equation, or more generally, second-order hyperbolic problems.

The new PGD solver is based on the Hamiltonian formalism, which leads to an algorithm that was shown to be more stable (4) than classical approaches. Procedures to enforce orthogonality have also been implemented in the solver so that linear independence of the modes and stability of the reduced-order model are ensured while progressively computing the new modes. The Aitken transformation (5) has subsequently been introduced to accelerate the convergence of the fixed-point algorithm. All these techniques allow one to significantly reduce the number of required iterations for convergence. Yet, the computational cost of such solvers mainly depends on the problem with respect to the spatial variable, which needs to be assembled and factorized at each fixed-point iteration. An original approach has been developed to avoid having to repeatedly invert matrices. It consists in pre-processing the eigen-pair approximations of the operators, namely the Ritz pairs (6), that provide a subspace in which the problem in space remains diagonal throughout the fixed-point iterations. All computations are then carried out in the subspace provided by the Ritz vectors (7), hence drastically decreasing the computational burden while capturing using only a small number of modes most of the information from the full model.

The methodology has been straightforwardly extended to viscoelastic systems modeled with Rayleigh damping, allowing for the construction of a parametric reduced-order model with respect to the Rayleigh damping coefficients. In the case of other classes of parameters, associated for instance with the material properties of the system or the geometry of the problem, it will be shown that the method can still be of interest if combined with dynamic substructuring. Several numerical examples dealing with the dynamical behavior of 3D structures

^{*}Speaker

will be presented in order to demonstrate the efficiency of the proposed approach.

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A Model Reduction Method and Its Applications in Nonlinear Random Vibrations of Structures

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Abstract

The effectiveness and efficiency of state-space-splitting (SSS) method which is a model reduction method and the exponential-polynomial-closure (EPC) method have been examined in analyzing the probabilistic solutions of the random vibrations of some strongly nonlinear structures, such as the random vibrations of strongly nonlinear beam systems, cable systems and plate systems formulated by Galerkin method. The SSS-EPC method was extended recently for analyzing the probabilistic solutions of the random vibrations of the geometrically nonlinear beam and plate systems formulated by finite difference method. In this presentation, the numerical analysis by SSS-EPC method will be summarized and numerical results will be presented about the probabilistic solutions of the above mentioned structures when they are excited by Gaussian white noise or filtered Gaussian white noise, such as the seismic ground motion. The numerical results show that the probabilistic solutions of deflections of the strongly nonlinear structures obtained by SSS-EPC method are close to Monte Carlo simulations (MCS) even in the tails of the probabilistic solutions when the structures are excited by Gaussian white noise or filtered Gaussian white noise. The computational effort needed by SSS-EPC method is much less than that needed by MCS for strongly nonlinear systems. Some future research topics about the investigation and applications of the SSS method and EPC method will also be briefed.

Model reduction in the context of polycrystalline plasticity

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Abstract

The plastic behavior of polycrystalline metals is highly influenced by the initial texture of the material and its evolution during loading and/or forming processes (1). Transmission electron microscopy (TEM) investigation and electron backscatter diffraction (EBSD) analysis are commonly employed to examine the textures of polycrystalline materials using pole figure illustrations. However, the increasing volume of experimental data, such as crystallographic observations stored in ODF files, necessitates improved data processing techniques. Indeed, to better understand material behavior, multi-scale experimental characterization is more and more common, especially in academic studies and in the context of new manufacturing processes like additive manufacturing.

In the field of reduced-order modeling, Proper Orthogonal Decomposition (POD) offers a powerful approach to handling high-dimensional data and uncovering its underlying dimensionality (2). This communication aims to introduce a novel application of POD for representing polycrystalline textures in the context of data-driven simulation (3). By applying POD to a set of texture snapshots acquired at different stages of mechanical tests, it is possible to extract the lowest-dimensional basis that captures the primary modes of variation in the data. This basis can then be used to generate an admissible random texture for the same test, significantly reducing the problem's dimensionality. Since ODF files typically describe the orientation of crystals within a specimen using Euler angles, performing POD on periodic data becomes necessary. Different strategies can be considered to deal with periodic data, such as representing one snapshot on a unit sphere and using distance functions. The specific aspects of linear algebra operations on periodic data will be illustrated through various examples, including synthetic ODF files.

The presented results are part of a broader effort (4) to implement model-order reduction in multiscale data-driven simulations with the objective of incorporating experimental information on polycrystalline textures into simulation and design processes.

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Approach to Discover Redued Order Dynamics from Parametric Data

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Abstract

The aim of this talk is to present a regression approach to approximate the dynamics of physical data that are parametric and time dependant. The underlying problem is formulated as a regularized minimization problem for which the stationary points are represented as a sequence of generalized Sylvester equations. We show that the solution of this problem can be efficiently determined by approximation on Krylov subspaces, and demonstrate its potential on the problem of Ahmed body flow with variable rear slant angle.

^{*}Speaker

Comparison of LSTM and Koopman-Operator approaches for Predicting Transient Ditching Loads

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Abstract

This research is concerned with building machine learning (ML) models to predict dynamic ditching loads on aircraft fuselages. The employed learning procedure is structured into two parts, the reconstruction of the spatial loads using a convolutional autoencoder (CAE) and the transient evolution of these loads in a subsequent part. Both parts are simultaneously (jointly) learned in a global network.

To predict transient load evolution, the CAE is combined with either different long shortterm memory (LSTM) networks (1, 2, 3) or a Koopman-operator based method (4, 5, 6, 7). To this end, both approaches advance the solution in time based on information from two previous and the present time step.

The training data is compiled by applying an extension of the momentum method of von-Karman and Wagner (8, 9) to simulate the loads on a generic D150 fuselage (10) model at various approach conditions.

Results indicate that both baseline methods, i.e., the LSTM and the Koopman-based approach, are able to perform accurate ditching load predictions. Predictive differences occur when looking at the different options to capture the temporal evolution of loads and will be outlined in greater detail.

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Generating materials yield surface by combining analytical models, model reduction techniques and data-driven approach

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Abstract

Obtaining a three-dimensional yield surface from several laboratory testing points is a challenging issue to tackle with several solutions proposed in the literature. In fact, obtaining testing points is often expensive. Moreover, only few loadings' combinations are accessible through direct experimentation. Despite these difficulties, several analytical yield functions were developed, including description of the anisotropy in plastic properties While these analytical yield functions do capture accurately the materials behavior, generating the entire data set necessary for parametrization may be expensive. Moreover, obtaining a reliable parametrization may require experience in generating the cost function. This work proposes the use of model order reduction techniques to address efficiently the construction of a reduced basis for the yield surface of various materials from the analytical yield surface of a specified material. Specifically, a machine learning algorithm based on spectral neural network and trained on this dataset is used to generate the yield surface of a new material using very few laboratory tests. The NR is built such as to automatically fulfill both the yield surface symmetries restrictions related to the intrinsic material anisotropy and convexity requirements. To be noted that once the laboratory testing results are available for a new material, the computing time required to determine its yield surface is reduced to a few seconds.

Reduced model based time domain absorbing boundary conditions for finite element modeling of infinite periodic structures

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Abstract

A finite element (FE) strategy is proposed to compute the time response of infinite 1D periodic structures. These structures are composed of identical cells which can represent any arbitrary-shaped 2D or 3D substructures. Typical applications may concern railway tracks under dynamic loadings (trains) or resonant metamaterial beams. To express absorbing boundary conditions (ABCs) for periodic structures in the time domain, they are first described in the frequency domain in terms of impedance matrices via the wave finite element (WFE) method. For complex substructures such as those involved in the modeling of railways tracks or metamaterial structures with heterogeneous cells, the computation of the impedance matrices turns cumbersome. To solve this issue, a Craig-Bampton reduction of the number of internal degrees of freedom (DOFs) together with a reduction of the number of boundary DOFs of a substructure can be considered. For reducing the number of boundary DOFs, the displacement vector at each substructure boundary is expressed in terms of a few number of orthogonalized eigenvectors that represent the solution of a boundary eigenproblem. This leads to computing a few number of propagation constants and wave modes and, also, expressing reduced impedance matrices for describing the ABCs. Then, these reduced impedance matrices can be approximated via rational functions in terms of poles and matrices of residues. It is shown that the resulting ABCs can be expressed in terms of polynomials of the frequency $i\omega$ up to the order two using vectors of supplementary variables. In this way, the ABCs can be formulated by considering a classical dynamic equation involving boundary mass, damping and stiffness matrices for the displacement vectors and the vectors of supplementary variables. Following the FE assembly procedure, a classical dynamic matrix equation for a finite periodic structure subjected to ABCs can be proposed which involves the usual vectors of displacements, velocities and accelerations, as well as vectors of supplementary variables. To couple the dynamic equations describing the ABCs with the dynamic equation of the periodic structure, the displacement and force vectors at the boundaries of the structure have to be expressed on a reduced basis encompassing some orthogonalized eigenvectors, in the same way as the substructure boundaries. Finally, a second-order time differential reduced equation for a finite periodic structure with ABCs can be proposed which can be integrated into a Newmark's algorithm. Numerical experiments are proposed which highlight the efficiency of the approach in terms of computational times. Also, the accuracy of the proposed reduced modeling (ABCs) is discussed through an error analysis.

^{*}Speaker

Space-time goal-oriented a posteriori error control and adaptivity for incremental POD-based ROM

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Abstract

In this presentation, the dual-weighted residual (DWR) method is applied to obtain a certified incremental proper orthogonal decomposition (POD) based reduced order model. A novel approach called MORe DWR (Model Order Reduction with Dual-Weighted Residual error estimates) is being introduced. It marries tensor-product space-time reduced-order modeling with time slabbing and an incremental POD basis generation with goal-oriented error control based on dual-weighted residual estimates. The error in the goal functional is being estimated during the simulation and the POD basis is being updated if the estimate exceeds a given threshold. This allows an adaptive enrichment of the POD basis in case of unforeseen changes in the solution behavior which is of high interest in many real-world applications. Consequently, the offline phase can be skipped, the reduced-order model is being solved directly with the POD basis is being enriched on-the-fly during the simulation with high-fidelity finite element solutions. Therefore, the full-order model solves can be reduced to a minimum, which is demonstrated on numerical tests for the heat equation and elastodynamics.

A reduced-order modal method for non-linear structural mechanics

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Abstract

This work details an extension and enhancement of the standard modal decomposition technique for linear structural analysis, for the purpose of modelling elastic structures undergoing large deflections that extend beyond the linear regime. By extending the standard linear modal decomposition technique, the governing equations and boundary conditions are updated to account for the leading-order non-linear terms and a new modal formulation with quadratic modes is derived. The quadratic modal approach is tested on standard benchmark problems of increasing complexity and compared with analytical and full non-linear numerical solutions.

Model reduction based on matrix interpolation and basis enrichment for dynamic analysis of nearly periodic structures including substructures with geometric changes

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Abstract

The dynamic behavior of nearly periodic structures with disordered substructures is investigated. This may concern 2D or 3D substructures subjected to geometric changes which can result from manufacturing process (variability), or design requirement for systems exhibiting particular properties (e.g., energy localization) and low vibration levels. These geometric changes can represent any classic parametric variations (thicknesses) or mesh changes where the nodes of a baseline substructure mesh are moved using shape functions and mesh parameters. The mesh parameters are different between the substructures and, therefore, they can be chosen in a random way to generate different substructures.

Reduced order models of substructures can be formulated with the Craig-Bampton (CB) method in the framework of which the displacement vectors for the internal nodes are expressed in terms of static modes and a reduced set of fixed interface modes. Within this framework, reduced mass, damping and stiffness matrices of substructures are obtained via Galerkin projection of the finite element (FE) matrices onto component modes (static and fixed interface modes). To quickly recompute the reduced substructure matrices, for any new geometric variation, they can be interpolated over a parametric space. This strategy requires the reduced matrices to be expressed at interpolation points (e.g., some distorted FE meshes) in compatible coordinate systems, e.g., via modal assurance criterion (MAC) analysis. To improve the efficiency of the interpolation strategy, an interface reduction (between the substructures) for modeling a nearly periodic structure can be considered where the projection basis consists of the interface modes of an equivalent purely periodic structure.

Although efficient, the aforementioned interpolation strategy is prone to numerical limitations and lack of accuracy, however. First, to express the reduced substructure matrices in compatible coordinate systems, only a few low-order fixed interface modes must be kept in the CB basis. Indeed high-order modes are usually associated with irregular shapes which make them difficult to correlate between several interpolation points. Next the proposed interface reduction for modeling a nearly periodic structure considers the interface modes of a purely periodic one, which as such cannot account for geometric modifications. Thus the interpolation strategy is likely to suffer from lack of accuracy, especially at high frequencies.

To solve these issues, two basis enrichment techniques are proposed whose key steps can be detailed as follows:

^{*}Speaker

- Enrichment of the CB basis of the substructures using high-order static modes. Prior to any matrix interpolation, these modes are orthogonalized and transformed using a MAC-based correlation criterion. Then, a reduced set of these high-order static modes are used to enrich the CB basis at the interpolation points.

- Enrichment of the basis of interface modes using static correction vectors. The strategy consists in adding to the interface modes a set of static response vectors resulting from parametric changes, i.e., those induced by the perturbations of the stiffness matrices of the substructures.

Numerical experiments are carried out where the advantages of the interpolation strategy with basis enrichment over the classic interpolation strategy are clearly highlighted. Nearly periodic structures with 2D substructures whose FE models depend on two and three parameters are considered. The case of 3D substructures involving FE models of relative large sizes and three mesh parameters is also discussed.

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ABSTRACTS

Day 2 – Thursday, November 23

Afternoon sessions

Registration-based model reduction of parameterized PDEs with spatio-parameter adaptivity

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Abstract

We propose an automated nonlinear model reduction and mesh adaptation framework for rapid and reliable solution of parameterized advection-dominated problems, with emphasis on compressible flows. The key ingredients of the method are threefold: (i) a metric-based mesh adaptation technique to generate an accurate mesh for a range of parameters, (ii) a general (i.e., independent of the underlying equations) registration procedure for the computation of a mapping that tracks moving features of the solution field, and (iii) an hyper-reduced least-square Petrov-Galerkin reduced-order model for the rapid and reliable estimation of the mapped solution. We discuss the problem of registration in complex geometries: we introduce a class of compositional maps that enable non-trivial deformations over curved boundaries of the domain; we develop a thorough analysis of the proposed ansatz for polytopal domains and we discuss the approximation properties for general curved domains. We discuss a general paradigm — which mimics the refinement loop considered in mesh adaptation to simultaneously construct the computational mesh, the mapping and the reduced-order approximations; finally, we discuss actionable strategies to accelerate the offline phase.

Deep learning for reduced order modeling

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Abstract

Reduced order modeling (ROM) techniques, such as the reduced basis method, provide nowadays an essential toolbox for the efficient approximation of parametrized differential problems, whenever they must be solved either in real-time, or in several different scenarios. These tasks arise in several contexts like, e.g., uncertainty quantification, control and monitoring, as well as data assimilation, ultimately representing key aspects in view of designing predictive digital twins in engineering or medicine. On the other hand, in the last decade deep learning algorithms have witnessed dramatic blossoming in several fields, ranging from image and signal processing to predictive data-driven models. More recently, deep neural networks have also been exploited for the numerical approximation of differential problems yielding powerful physics-informed surrogate models.

In this talk we will explore different contexts in which deep neural networks can enhance the efficiency of ROM techniques, ultimately allowing the real-time simulation of large-scale nonlinear time-dependent problems. We show how to exploit deep neural networks (like, e.g., convolutional autoencoders) to build ROMs for parametrized PDEs in a fully non-intrusive way, ultimately yielding deep learning-based ROMs (DL-ROMs) and their further extension to POD-enhanced DL-ROMs (POD-DL-ROMs). Moreover, we will show how the datadriven discovery paradigm relying on sparse identification of nonlinear dynamics (SINDy), combined with autoencoders, can be extended to the case of parametrized PDEs, yielding the possibility to identify the system dynamics at the latent level in the case of parametrized dynamical systems. Furthermore, we will also show how to improve a low-fidelity ROM through a multi-fidelity neural network regression technique that allows to merge low- and high-fidelity data, when dealing with both input/output evaluations and solution field approximations.

Through a set of applications from engineering including, e.g., structural mechanics and fluid dynamics problems, we will highlight the opportunities provided by deep learning in the context of ROMs for parametrized PDEs, as well as those challenges that are still open. This is a joint work with Stefania Fresca, Paolo Conti, Attilio Frangi (Politecnico di Milano), Mengwu Guo (University of Twente), J. Nathan Kutz and Steven Brunton (University of Washington).

Monitoring of composite structures using reduced order models

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Abstract

For robustness and performance concerns, composite materials are privileged in the design of naval structures. As they are exposed to various and complex loadings, these structures ought to be monitored in order to ensure the material health. Indeed damage can occur and there is a need for assessing the stress *in situ* in real time. This consideration raises some technological and numerical issues among which the instrumentation of the structure and the assimilation of the measured data in a model. Fiber optics are chosen to measure strains in wet environment. Reduced order model techniques, based on the empirical interpolation method and its generalized or regularized versions (1,2,3), are used both to optimize the positions of the sensors while considering technical constraints due to the use of fiber optics and to interpret the measurements to approximate the strain and stress fields. The idea is to build a reduced basis associated to an optimal set of sensors in an off-line phase and to reconstruct the strain field in a fast on-line phase. For the purpose of structural health monitoring, a modified empirical interpolation method is proposed to reconstruct the stress field which is not a linear function of the partially measured field. **REFERENCES**

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Model order reduction for nonlinear stochastic problems via stochastic LATIN methods

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Abstract

Model order reduction for nonlinear (high-dimensional) stochastic problems is prohibitively expensive due to the coupling of randomness and/or parameters, nonlinearity and large-scale spatial domains. Most of the current research focuses on dealing with randomness efficiently. To reduce the computational effort in nonlinear aspects, we extend the LATIN method to a probability framework in this research, called stochastic LATIN method. Although the LATIN method has been successfully applied to a variety of problems, there is still a gap in its extension to nonlinear stochastic problems. Similar to the classical LATIN method, the stochastic LATIN method involves a linear and deterministic global stage and a nonlinear and stochastic local stage. Efficient treatment of random and/or parametrized inputs is presented in both stages. Specifically, the stochastic solution is approximated by the sum of a set of products of triplets of spatial functions, temporal functions and random variables. Each triplet is then calculated in a greedy way using a stochastic LATIN iteration. The spatial function is solved by global and linear deterministic problems, and the temporal function and the random variable are calculated by local and nonlinear stochastic problems. The high efficiency of the proposed method relies on two aspects: The nonlinearity is efficiently handled by inheriting advantages of the classical LATIN method, and the randomness and/or parameters are effectively treated by a sample-based approximation of stochastic spaces. Further, the proposed method is not sensitive to the stochastic and/or parametric dimensions of inputs due to the sample description of stochastic spaces. It can thus be applied to high-dimensional stochastic and parameterized problems. 3D high-dimensional stochastic and parametrized elastoplastic problems demonstrate high efficiency and good accuracy of the proposed method.

An energy-based approach to approximate the solution of PDEs using neural networks

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Abstract

This contribution focuses on a new energy-based approach to approximate the solution of PDEs using neural networks. The general idea behind this approach is to minimize a loss function, i.e. the potential energy resorting from the underlying variational formulation, at specific collocation points in order to train a neural network. The proposed method can adress both unsupervised and supervised problems. A data-driven term can be added to the loss function whenever measurements from experiments are available. We will discuss some difficulties and challenges of the proposed approach such as numerical integration accuracy and exact imposition of essential boundary conditions. Eventually, we will illustrate the performances of the proposed approach on benchmark problems of interest in computational mechanics.

An overview of ROM methods: An industrial point of view

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Abstract

Accelerating the simulations via fast numerical methods has always been the ultimate target for the CAE world. While this requirement is as present as ever, the new trends in pushing the numerical models from design and validation phase to in-operation phase (as in Executable Digital Twins) are making this target even more urgent, while also bringing in additional requirements. Whereas majority of the past efforts focused on accelerating simulations in a single run, the current environments allow offline and online phases of calculations. It also puts an emphasis on packaging and deployment aspects and time-stable state-space forms. There is also a huge momentum behind Machine Learning/AI (data-driven) approaches as compared to physics-based methods and there is a need for good understanding of the positioning of different approaches.

Considering the recent shift of the requirements for fast simulations, this talk will give an overview of ongoing Reduced Order Modelling activities within Siemens Digitial Industries Software and will highlight the complementarity of different techniques. In particular, Modal Methods, Krylov Methods, Parametric Model Order Reduction Techniques, Fast Frequency Sweep algorithms will be discussed among other techniques. The positioning of data-driven and physics-based methods will be highlighted. Finally, future challenges will be laid out.

POD bases interpolation by Gaussian Process, benefits and difficulties

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Abstract

Construction of robust POD basis for the resolution of time dependent and/or nonlinear parameterized PDE has been widely investigated in the literature. Among the various proposed approaches this study focuses on the interpolation of POD bases. It is notable that since the original work from Amsallem and Farhat (1) on POD bases interpolation on Grassmann manifold, an important number of studies has been published, either to propose alternative interpolation schemes (e.g.(8)) or to study the properties of the interpolation (e.g. (5)). The general idea of these approaches can be described as follows. First, the High Dimensional Model (HDM) is sampled at a number of points over the parametric space and a POD basis is computed for each one of these points (classically by singular value decomposition of the snapshots matrix). This leads to the creation of a database, or a Design of Experiments (DoE), of POD bases. Then, for a new point in the parameter space, this DoE is used to interpolate the value of the corresponding POD basis. Several interpolation methods have been proposed and the one used in the present work will be further detailed. It is interesting to note that the sampling procedure, used for the construction of the DOE, is either random or constructed by a greedy procedure based on an accuracy criterion computed over the whole parametric space. Hence, the numerical cost of this sampling procedure (also known as the offline phase in the literature) is sometimes prohibitive and could annihilate the interest of model order reduction. This observation is the starting point of the present study and its objectives are, first, to propose a Gaussian Process (GP) interpolation of POD bases and, second, to discuss the opportunity for Bayesian approaches.

Indeed, since the pioneer work by Jones *et al.* on an Efficient Global Optimization algorithm (6), Bayesian approach has been successfully applied not only to optimization problem ((2) for example) but also to several other parametric problems such as reliability analysis (3), (4) etc. The keystone of the Bayesian paradigm is the construction of a stochastic approximation of the Quantity of Interest (QoI). The majority of the literature relies on Gaussian Process (GP) interpolation for this purpose and the present work is no exception. Indeed, by carefully using the stochastic information of the obtained approximation, it is possible to define enrichment criteria that allow an easy iterative construction of the GP interpolation. Several criteria have been proposed in the literature depending on the type of problem (e.g. expected improvement, probability of improvement for optimization purpose and probability of misclassification for reliability analysis). In many applications reported in the literature the use of these sampling criteria allow to focus the sampling (i.e. evaluations of the HDM) at relevant points of the parametric space (near the optimum in optimization or close to the failure limit state in reliability) leading to a drastic reduction of the computational budget compared to more conventional procedure. However this approach remains blind to the

^{*}Speaker

physics of the problem under study and consider the HDM as a so call *black box*. This could be considered as a weakness of the approach when the PDE under study is perfectly known and thus brings supplementary information that is ignored by the black box approach. Hence the idea of coupling the adaptive construction of GP approximation with the resolution of the parameterized PDE by POD.

Following this idea it is proposed in the present study to investigate the GP interpolation of POD bases on the Grassmann manifold. It should be noted that the use of GP to interpolate data on Riemaniann manifolds is proposed for example in (7) and that the particular case of POD bases interpolation is mentionned in (9). However, to the best of our knowledge, the stochastic properties of the GP interpolation has not been yet exploited to construct adaptive sampling strategy. Our interpolation approach, inspired by the work of (7) and adapted to our context, could be summarized as follows.

- Choose a prior base-point. This prior could be constant (the Frechet mean of the POD bases DoE or a particular point in this DoE for example) or it could depend on the parameter point.

- Use the logarithmic mapping of the Grassmann manifold at the base-point to obtain the tangent vectors of each POD bases. Note that each tangent vector is associated to a parameter point.

- Construct a basis of a subspace of the tangent plane (in practice we use a SVD of the tangent vectors) and express the coordinates of the tangent vector in this basis.

- For a new parameter point, interpolate the values of the coordinates in the basis of the subspace of the tangent plane to obtain an approximation of the tangent vector. In practice, each coordinate is independently interpolated using a GP. Note that the interpolated tangent vector is thus a Gaussian random vector which takes value into the tangent space of the Grassmann manifold at the base-point (more precisely into the subspace of the tangent plane previously defined).

- Construct the interpolated POD basis using the exponential mapping of the Grassmann manifold at the base-point. One could note that, even if the interpolated tangent vector is a Gaussian vector, the exponential mapping being non-linear, the resulting random POD basis is non-Gaussian. However its distribution could be easily sampled (by sampling the Gaussian tangent vector and applying the exponential mapping to each sample) which allows to easily set up Monte Carlo estimation when needed.

Using this approach, the first numerical experiment proposed is to set up an EGO-like optimization strategy. The main difficulty to handle is the non-Gaussian approximation QoI in the estimation of the expected improvement criterion. However, in the investigated numerical experiments, a simple Monte Carlo estimation appears to be efficient enough (alternative estimation procedure could be proposed). So far this EGO-like strategy has been applied to the resolution of an inverse problem in the context of a linear dynamical structural mechanic PDE with a single parameter. From this first numerical experiment the following advantages are highlighted. First, the adaptive sampling strategy is efficient and the sample locations proposed by the algorithm are indeed in subsets of the parametric space relevant for optimization. Hence, the proposed approach outperforms, in terms of HDM evaluations number, the classical greedy procedure for this optimization problem. Second, it appears that the proposed approach is also much more efficient than the classical EGO applied to the same problem but with a black box paradigm (i.e. adaptive construction of a GP surrogate model of the QoI directly). This is explained by the regularity of the field to interpolate compared to the regularity of the QoI. Indeed, in this application, the regularity of the displacement field to approximate (with respect to the parameter) seems higher than the one of the QoI. This behavior explains that the GP interpolation is more prone to accurately interpolate the POD basis rather than the QoI directly. Even if this behavior is difficult, if not impossible, to generalize, it seems likely to be encountered in practice when the QoI is a non smooth function such as the extreme values of a field (which is often the case in optimization problems constrained by PDE or reliability problems).

The next steps of this study are, first, to confirm that the proposed approach presents the two highlighted advantages on different and more challenging application examples. An optimization problem constrained by a geometrically non-linear structural mechanic PDE is currently under study. It should also be noted that the potential of the proposed approach is probably not limited to Bayesian optimization. An interesting perspective is to adapt GP based reliability algorithms to our framework.

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Combined Data Driven Convolutional-Recurrent Neural Networks methodology for accelerating the 2-level topology optimisation process

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Abstract

In recent years, the use of methods from the artificial intelligence field in topology optimisation schemes has been an active area of research. These machine-learning-based models have mainly been applied to create direct optimised designs or accelerate these procedures. One of the main challenges in this field is improving the multiscale resolution of structural problems. This study presents a new methodology to accelerate the topology optimisation process at the mesoscale by using neural networks. The multiscale topology optimisation process involves solving a global topology optimisation process for material distribution. Then, the macro problem is divided into cells or regions where the resolution is improved by applying mesoscale topology optimisation in each cell. Since the number of cells can be significant, the computational cost of such an algorithm is expensive. Then, taking advantage of both, the repeated structure of the cells and that the load applied to each cell can be defined with a reduced number of parameters, a neural network-based topology optimization algorithm is trained to obtain the topology of each cell with a small computational cost. This is feasible since there exists a small latent topology space.

In this work, we present a hybrid approach for the mesoscale topology optimisation process consisting of two steps: i) the topology of the firsts iterations is predicted by a convolutional neural network (U-Net architecture) while ii) the remaining steps are predicted with a recurrent neural network (Long Short Time Memory architecture).

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Surrogate Modeling for Multi-Physics General-Purpose Software

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Abstract

As system controls and design exploration require a dramatic reduction in computing costs of high-fidelity multi-physics simulations, surrogate modeling technologies are today the most relevant solution. Due to the multiple directions that research is taking in the field, it is quite challenging today to implement general-purpose software. A possible classification of existing surrogate modeling technologies consists in a subdivision into two main subsets: Machine Learning (ML) modeling and Reduced Order Modeling (ROM). Within the latter, Craig-Bampton reduction (1) has reliably been covering linear structural simulations for decades, Proper Orthogonal Decomposition technology coupled with hyper-reduction techniques (2,3) has been proposed as an accurate and more generic tool for non-linear simulations in structural mechanics and fluid dynamics, Proper Generalized Decomposition technology (4,5) has been proposed as valid online-only alternative. Within the ML subset, traditional statistical learning techniques (e.g. polynomial response surfaces, radial basis functions, Gaussian processes) interpolate scalar quantities over a design space with acceptable accuracy, whereas more advanced Deep Learning techniques based on Neural Networks, for instance the ones proposed in (6), are better positioned to recover the full history of transient quantities or full 3D fields.

The authors are currently exploring two parallel directions of research and development, one in ML modeling, the other in ROM. Since the beginning, developments have been proceeding at different pace. ML techniques have emerged as less intrusive techniques, performing well in terms of computing times with GPU architectures and in terms of accuracy for a wide range of design exploration space (geometric, material and load parametrizations), with slight algorithmic distinctions for the different types of procedures such as quasi-statics and transient dynamics. ROM techniques, although requiring intrusive access to modeling data during the online phase, offer an effective alternative, possibly less demanding in terms of amount of training data.

As developments are currently ongoing, fully open questions remain regarding potential synergies between ML and ROM techniques and the industrial interests in the overall workflow, starting from a single fully parametrized model of a given product or family of products or from the full history of data of an engineering team. With this presentation, the authors would like to share the status of their prototyping efforts for a variety of test cases, ranging from quasi-statics to transient dynamics and multi-physics applications.

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Probabilistic reduced basis method for solving parameter-dependent problems

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Abstract

Probabilistic variants of Model Order Reduction (MOR) methods have been recently proposed to improve stability and computational performance of classical approaches. In this talk, we particularly focus on the approximation of a family of parameter-dependent functions by means of a probabilistic Reduced Basis (RB) method in the line of (3,4).

In this contribution (see (2), for more details), we propose a RB using a probabilistic greedy algorithm using an error indicator that can be written as an expectation of some parameter-dependent random variable. Here, practical algorithms relying on Monte Carlo estimates of this error indicator can be considered. In particular, when using Probably Approximately Correct (PAC) bandit algorithm (1), the resulting procedure is proven to be a weak greedy algorithm with high probability. Applications concern the approximation of a parameter-dependent family of functions for which we only have access to noisy pointwise evaluations. Especially, we consider the approximation of solution manifolds of linear parameter-dependent partial differential equations with a probabilistic interpretation through the Feynman-Kac formula.

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Neural Galerkin schemes for model reduction of transport-dominated problems

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Abstract

Nonlinear parametrizations such as deep neural networks can circumvent the Kolmogorov barrier of classical model reduction methods that seek linear approximations in subspaces. However, numerically fitting ("training") nonlinear parametrizations is challenging because (a) training data need to be sampled (residual evaluations) to estimate well the population loss with the empirical loss and (b) training errors quickly accumulate and amplify over time. This work introduces Neural Galerkin schemes that build on the Dirac-Frenkel variational principle for training nonlinear parametrizations sequentially in time. The accumulation of error over the sequential-in-time training is addressed by updating only randomized sparse subsets of the parameters, which is motivated by dropout that addresses a similar issue of overfitting due to neuron co-adaptation. Additionally, an adaptive sampling scheme is proposed that judiciously tests the residual so that few residual calculations are sufficient for training. In numerical experiments with a wide range of evolution equations, the proposed scheme outperforms classical linear methods, especially for problems with transportdominated features and high-dimensional spatial domains.

^{*}Speaker

Hybrid twins for the effective monitoring of real-life engineering systems: application to additive manufacturing processes and dynamics tests on shaking tables

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Abstract

The real-time monitoring of real-life engineering systems, by coupling simulation tools and observed data (Dynamic Data Driven Application Systems – DDDAS), is made very difficult in practice due to several issues. In particular, the complex nonlinear multiscale phenomena which are involved may be associated with computationally intensive simulations (hardly compatible with real-time) which requires reduced order modeling and/or model coarsening. In addition, the problem is plagued with model bias, uncertain environment, and measurement noise, which need to be taken into account for robust data assimilation, accurate diagnosis and prognosis, and safe decision-making. An appealing trend is to refer to hybrid techniques, in which an a priori physics-guided model is updated and enriched with data-based information (1), thus making benefit of all knowledge available.

In this context, we present two methods for the construction of such hybrid twins, with practical applications on the online monitoring of engineering systems. The first application deals with transient thermal analysis in LPBF additive manufacturing processes, in which a hybrid twin is built from a time-dependent version of the Parametrized Background Data-Weak (PBDW) method (2,3). PBDW is a non-intrusive, reduced-basis, real-time and in-situ data assimilation method whose key idea of the formulation is to seek an approximation of the true state by employing projection-by-date, with a first contribution from a background estimate computed from a reduced-order method (ROM) on a surrogate model, and a second contribution from an update state informed by the experimental observations (correction of model bias). We here investigate the use of PBDW for thermal state reconstruction and prediction-in-time purposes, at the scale of the melting pool or of the manufactured part, by means of high-fidelity and high-frequency camera-based data.

A second application deals with the on-the-fly monitoring of vibratory dynamics tests on damageable buildings placed on shaking tables and submitted to low-frequency seismic loadings (4,5,6). Here, experimental data is given by sparse accelerometers, and the hybrid twin representing damage effects is constructed from the modified Constitutive Relation Error (mCRE) concept. This energy-based concept is driven by reliability of information, with

^{*}Speaker

regularization from physics and natural quantification and localization of modeling error. The mCRE concept is moreover coupled with Kalman filtering to address sequential data assimilation, with enhanced robustness to highly noisy measurements. We show how the strategy effectively permits the online process of data obtained from the SMART2013 experimental campaign at CEA.

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On the Hyper-Reduction of variational inequalities. Application to contact mechanics problems.

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Abstract

This work deals with efficient reduced order modeling for variational inequalities treated by a mixed formulation. The problem arising for the High Fidelity (HF) formulation is then a saddle-point problem implying positive Lagrange multipliers. To overcome the issue of finding an accurate positive reduced basis for the Lagrange multipliers, the Hybrid Hyper-Reduction (HHR) method has been recently introduced (2, 5). It relies on a Reduced Integration Domain (RID) (6), a primal POD reduced basis and a restriction to the RID of the HF dual basis. These choices ensure the reduced HHR saddle-point problem to respect the non-linearity constraints.

We show in this contribution that thanks to the hybrid formulation with respect to the truncated Lagrange multipliers basis, Céa's a priori primal error bounds can been derived with respect to a Finite Element HF solution. Hence, we have sharpened bounds depending on the primal reduced basis only, compared to Brezzi's mixed error bounds classically obtained for Reduced Basis Methods (RBM) (3). The Petrov-Galerkin feature of the HHR method enables us to further obtain an a priori

bound on the whole initial computational domain. Furthermore, this work also provides new insights on the relation between the HHR inf-sup constant and the dual error precision. This confirms the importance of enriching in a smart way the primal reduced basis to obtain accurate dual solutions, as numerically introduced in (5).

A posteriori bounds confirm the potential of the HHR approach implying also sharpened bounds compared to RBM methods (4). These bounds however depend on the RID interface residual between HF and HHR primal solutions, which highlights the interest of an error indicator based on the prediction of the HF primal solution on the RID interface as previously suggested in (2). Numerical results on academic and industrial mechanical contact test problems prove the accuracy of

the proposed error bounds on parametric spaces.

The capabilities of the HHR method being demonstrated, we propose an extension of this method to non-conforming contact surfaces meshes. Up to now, the contact was treated by a node-to-node algorithm (2, 5), leading to a classical block-symmetric saddle-point problem. Due to the Petrov-Galerkin projection nature of the HHR method, the node-to-surface contact algorithm induces a change of formalism for the discrete HHR model that results

^{*}Speaker

in a generalized (non block-symmetric) saddle-point formulation (1). Once both stability conditions respected, we show the good accuracy of the

generalized HHR method for such kind of complex contact geometries. Thanks to the mesh sampling techniques, the HHR method is well suited to reduce the computational effort of this kind of locally highly non linear problems. Speed-ups between 5 and 20 have been obtained. Extension to non-linear material behaviors is also presented.

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MMGP: a Mesh Morphing Gaussian Process-based machine learning method for physical problems under non-parameterized geometrical variability

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Abstract

This work deals with the construction of surrogate models that approximate quantities of interest related to the solution of physics problems, under variability of the geometry of the support.

Classical regression techniques like Gaussian Process Regression are successful when the geometry is parametrized and the quantities of interest are scalars. In this work, we assume that the parametrization of the shape is not available in the inference stage: we only have the mesh at our disposal, and we are interested in fields supported on this mesh. Hence, learning some shape embedding and comparing fields of interest associated to different samples is not straightforward. Recent techniques based of graph neural networks have proved to be successful under these assumptions, but they usually need large datasets, are hard to train for large meshes, and efficiently providing predictive uncertainties is still an open question. We propose a machine learning methodology based on classical technologies to address these challenges. Our two principal ideas consist in using a mesh morphing pretreatment with finite element interpolation to handle complex shape variations with fixed topology, and building a shape embedding by dimensional reduction of the mesh vertex coordinates considered as continuous fields over the geometrical support. These respectively prevent the machine learning task from having to handle variable size samples and learning implicit shape embedding. With reduced dimensional inputs and outputs, small Gaussian Process Regressors can be trained.

Our methodology, that we call MMGP (Mesh Morphing Gaussian Process), can easily handle large meshes without parametrization of the shape and provides predictive uncertainties with marginal additional cost. In our numerical experiments, MMGP is competitive with respect to our implementation of graph convolutional neural networks (GCNN), for both efficiency of the training and accuracy of the predictions. In two datasets constructed for this work (a 3D RANS CFD setting and 2D elastoviscoplatic solid mechanics simulation), MMGP features better Q2 regression coefficients than our GCNN implementation for all scalars and fields of interest. In a third experiments, we applied MMGP to the AirfRANS dataset produced in (1). In all experiments, we illustrate MMGP predictive uncertainties. In particular on scalars of interest for the AirfRANS dataset, 95

Reduced order models for the problem of optimal operation of natural gas flow networks

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Abstract

Natural gas is the second most consumed primary energy source in the United States. Most natural gas production sites are in remote locations and need to be transported to the customer sites through a pipeline network with a variety of physical components like compressors, valves, regulators etc.

Optimal transportation of natural gas using these pipeline networks is of great interest due to both economic and reliability reasons. The physics that governs the flow of natural gas through various components in a pipeline network is governed by nonlinear and non-convex equality and inequality constraints and the most general problem takes the form of a Mixed Integer Nonlinear Program (MINLP).

The ability to determine global optimal solution or bounds to the global optimal solutions of the MINLP quickly for different consumer profiles plays a key role in day-to-day operations.

Consequently, it is imperative to develop reduced-order models (ROMs) of the nonlinear constraints and governing equations. Currently, there are either no reduced-order models of certain components or current ROMs do not scale well to networks that span 1000s of miles.

In the optimization community, such ROMs usually take the form of "relaxations". In this work, we leverage the recent advancements in polyhedral relaxations for univariate and bilinear functions and develop Linear Programming (LP)- and Mixed Integer Linear Programming (MILP)-based ROMs for the MINLP. We further apply techniques such as variable bound tightening to improve the quality of these relaxations. We demonstrate the quality of these relaxations through extensive numerical simulations on small, medium, and large-scale test instances.

Reduced order modeling of finite element structures using invariant manifold theory

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Abstract

Summary.

The direct parametrisation method for invariant manifolds (DPIM) is a simulation-free reduction technique that allows computing the reduced dynamics along the invariant manifolds associated to the linear eigenspaces in a direct manner, from the finite element mesh. Converged solutions thanks to arbitrary order asymptotic expansions are achievable, leading to drastic reductions in the computing time for the steady-state nonlinear vibrations of geometrically nonlinear structures. The method is briefly recalled and exemplified on two different structures: a MEMS (Micro-Electro Mechanical System) micromirror and a rotating twisted plate.

The direct parametrisation method for invariant manifolds (DPIM)

The DPIM as a reduction technique is specially well suited for computing the nonlinear vibrations of lightly dampedgeometrically nonlinear structures. The review article (1) recalls some historical background and provides comparisonswith other methods such as implicit condensation and modal derivatives. The considered invariant manifolds are tangent the origin to the linear vibration modes. The reduced invariant subspace on which the dynamics is projected is thusoften referred to as Nonlinear Normal Mode (NNM) in the literature, and can be seen as a direct extension of the linearmodes to the nonlinear range. Thanks to the invariance property, the reduced subspace contains the solutions of the fullorder model, hence ensuring maximal dimensionality reduction.

Recent developments have adapted the parametrisation method, developed in e.g. (2), in a general framework to vibratingstructures with geometric nonlinearity, also making clear the link with previous developments that used either a centermanifold technique to define the manifold as a graph over the modal coordinates (3), or the normal form theory (4). Twoimportant contributions have been considered. First, arbitrary order expansions are computed,

^{*}Speaker

such that the reduced-ordermodel can be made converged by increasing the orders. This is a key feature, for example in cases where full-ordersolutions are out of reach. Second, the method is direct and can be applied to the finite element mesh, thanks to anaugmentation procedure which is needed to solve singular problems. The method is fully described in (5, 6, 7). In short, the method relies on computing a nonlinear mapping that relates the original problem to a reduced dynamics, expressed with normal coordinates, along the embedding acting as invariant manifold. Both the nonlinear mapping andthe reduced dynamics are unknowns, and are solved iteratively up to an arbitrary order, by sequentially solving thehomological equations. As a result, the user obtains a severely reduced ROM containing only a few master modesnonlinearly interacting together and reproducing the original dynamics up to the selected accuracy of the asymptotic pansion.

Numerical results

In order to illustrate the capabilities of the reduction technique, two examples are selected. The first one is a MEMSmicromirror, whose geometry and functioning mode is shown in Fig. 1(a). The finite element (FE) mesh contains 9732dofs. The nonlinear oscillations of this mirror, involving large rotations and geometric nonlinearity, displays a softeningbehaviour, as highlighted by the frequency-response curve (FRC) plotted in Fig. 1(c), where the normalised amplitude(corresponding to the modal amplitude divided by the radius of the center mirror) is shown as a function of the normalized excitation frequency (eigenfrequency of the considered mode being 0.1839 rad/ μ s2). A reference solution is computed with a direct application of the Harmonic Balance Method (HBM) to the FE mesh (HBFEM solution). A solution with 7harmonics is taken as reference, resulting in a computing time of 2 days. On the other hand, the ROM is constructed in 3minutes (offline time) and less than one minute is needed to continue the FRC (online time).

The second example is a rotating twisted plate, used to illustrate how the method can deal with the centrifugal effect fora structure mimicking the geometry of a fan blade (8). The blade is 1 m long, 20 cm wide and has a thickness of 1.5 cm,see Fig. 1(b). The axis of rotation is shifted from a distance of 30 cm from the foot. The FE mesh has 4095 dofs. Withincreasing rotation, the centrifugal effect that is dominating here has two main consequences. First a stretching effectleads to a new position at rest that needs to be computed before addressing the nonlinear vibrations around this state. Then the nonlinear oscillations are turning from hardening to softening when increasing the rotation speed. This is shownin Fig. 1(d) that reports two FRCs for the nonlinear vibrations along the fundamental bending mode, with two differentrotation speeds: 0 and 2000 rpm. Without rotation the blade has a hardening behaviour, whereas the change to softeningoccurs around 2000 rpm. The HBFEM reference solution needs one day of computation. On the other hand, the ROM isbuilt in a few minutes and then each FRCs is computed in a few seconds.

Conclusions

The DPIM is a powerful technique that provides efficient ROMs for systems with geometric nonlinearity. It is particularly suited to compute the steady-state dynamical solutions of nonlinearly vibrating structures. It offers a simulation-freetechnique that accounts for the curvature of the invariant manifolds that expresses the nonresonant couplings, which arecomputed automatically. Converged solutions (thanks to arbitrary order expansions), directly applicable to FE problems, are now readily available. Current development considers extending the formulation to take into account other nonlineari-ties occuring in MEMS physics (e.g. piezoelectric coupling (9)), and comparison to deep learning based approaches (10).

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Accelerated Boundary Integral Technique for Energy Eigenvalue Analysis in Confined Electron States of Quantum Wires

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Abstract

In the realm of quantum mechanics, the behavior of particles within confined structures often leads to intriguing and complex physical phenomena. The study of energy eigenvalues in such systems is not only an intriguing exercise in mathematical physics but also holds significant implications for the design and understanding of nanoscale devices and quantum structures.

It is essential to note that directly formulating the eigenvalue problem for the determination of energy eigenvalues proves to be a complex task. Consequently, the approach of scanning the energy variable E within a specified interval, in order to locate local minima of the eigenvalue determinant, as obtained through boundary element analysis (BEA), has emerged as a practical solution. While this search method exhibits a straightforward approach, it is not without its limitations. Notably, because the determinant is a function of the energy variable E, employing this method necessitates the complete repetition of the BEA for each value of E. This approach, though conceptually simple, incurs a substantial computational burden.

This presentation introduces a novel and efficient approach for the computation of energy eigenvalues in bound electron states of quantum wires. Accurate determination of the electronic states in these structures is crucial for understanding their optical and electronic properties, rendering this a fundamental problem in semiconductor physics. The proposed method is based on utilizing series expansions of zero-order Bessel functions to produce a set of fundamental functions that are independent of the energy E. The resulting coefficient matrix in the system of boundary element equations takes the form of a polynomial matrix in terms of the parameter E. This characteristic enables a significantly expedited search for eigenvalues across a specified range of E values.

To validate the effectiveness of this technique, it was employed to issues previously explored by other research groups. The results unequivocally showcase the computational efficiency and high precision of the proposed approach. This technique offers a notable advantage through a substantial reduction in computational time when compared to the conventional method for searching the energy eigenvalues in quantum wires.

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Application of Zonal Reduced-Order-Modelling to tire rolling simulation

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Abstract

Physical simulation remains a key enabler for real-world ever-growing complex industrial systems especially when crucial decisions are needed. While classi- cal approaches have proven their accuracy and robustness over the years and come with a rich mathematical foundation, they suffer from several limitations depending of the underlying physics and use cases. For instance, especially concerning the resolution of Partial Differential Equations (PDEs), classical approaches are known to be computationally expensive. However, it turns out that simple pure data-driven approaches, while much more efficient from a computational point of view, do not necessarily hold up well regarding physical considerations. In this work, our aim is to investigate the tradeoff between accuracy and computational cost to design efficient physical simulation methods. We propose to hybridize a standard FEM physical simulation with a zonal ROM approach for an industrial usecase provided by Michelin: the tire rolling.

The aim is to assess the behavior of the tire during an idealized straight rolling on a nondeformable ground at constant speed. The inherent complexity (hyper-elasticity, contact...) of the problem results on a high computational cost that can make prohibitive the use of classical methods. An order of magnitude acceleration with acceptable accuracy would enable the use of such models in real-world industrial applications. In practice, the computation of the tire state, involving the displacement and the contact stress arising from the contact conditions on the discretized domain (i.e. the mesh), is performed based on the resolution of a set of PDE through Finite Element (FE) formalism. As such, the solution for the displacement is evaluated at all the nodes of the domain's mesh, whereas it is evaluated at the nodes on the contact boundary for the contact stress. In these PDEs, several physical considerations are involved such as: the behavior law, the motion law, frictional contact conditions. These problems are strongly nonlinear due to the nonlinearity of the underlying behavior law, the large deformation framework and the frictional contact conditions. In order to estimate the displacement and the stress, the FE solver Getfem (1) is used. Note that, while the displacements and contact stresses at the contact boundary are the actual unknowns of the problem, they may not represent all the required measures depending on the use case. Some physical quantities relevant to a given application can be computed as a post-processing of the unknowns.

As a consequence, we are interested in numerical methods which provide the best trade-off between execution time and physical meaningfulness. In this spirit, we divided the domain of interest in two zones:

• The contact zone, close to the ground, where the numerical method should be very accurate

^{*}Speaker

• the complementary zone, close to the rim, where precision is not that critical but computations have to be really fast

It should also be noted that we are only interested, in this study, in accelerating one simulation: No offline training is used, the training is encompassed in the rolling simulation. Because when running their simulations, tire designers want to have their results as fast as possible, the training time of our method should be negligible. This constraints motivates the usage of a special kind of Reduced Order Models (ROM), inspired from the zonal POD method of (2) and denoted as Fast Zonal ROM in the following. Fortunately, a tire tread presents patterns that repeat. We take advantage of this property: Only a few simulation time steps might be necessary to understand the tire behavior and then predictions can be made accurately even for multiple wheel spins.

To assess the results, we consider classical numerical indicators (Mean Square Error, Mean Absolute Error...), and specific meaningfull physical criteria (such as contact patch size and contact patch pressure). We also compare our approach with other literature approaches. It turns out that the Fast Zonal ROM shows consistent performances on those indicators while halving the computational time.

As future work, we plan to investigate the robustness of our process by assessing the method interoperability (solver agnostic) and introducing more physical complexity (multi materials and 3D tire tread sculpture).

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Assessment of Projection-Based Model Order Reduction for a Benchmark Parametric Hypersonic Flow Problem

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Abstract

Computational fluid dynamics (CFD) is essential for assisting in the aerodynamic design of a hypersonic vehicle, predicting its performance, and complementing or assisting in its flight testing. However, parametric, high-dimensional, high-fidelity, viscous CFD can be prohibitively expensive. Projection-based model order reduction (PMOR) followed by hyperreduction is a candidate mathematical technique for greatly alleviating the computational cost of parametric CFD, while maintaining a desirable level of accuracy. In recent years, the least-squares Petrov-Galerkin (LSPG) method has emerged as a state-of-the-art nonlinear PMOR method for realistic, convection-dominated, and challenging CFD applications. Its parametric performance is assessed here for the numerical prediction of a variable speed hypersonic flow past a double-cone obstacle, which is a benchmark problem in hypersonic CFD. Present in the steadystate solution of the flow are attached and detached shocks; a separation shock; a transmitted shock; multiple shock-shock interactions; a recirculation region at the intersection of the conical surfaces; and a shear layer of supersonic shock and expansion wave reflections along the rear cone surface. Each of these flow features challenges PMOR. First, a high-dimensional, highfidelity, viscous flow model (HDM) is constructed for this application, verified, and validated. Next, its dimensionality is reduced using LSPG and three different approximation manifolds: an affine one; a quadratic one; and an arbitrarily nonlinear manifold constructed using a deep artificial neural network. Each resulting global, projection-based reduced-order model (PROM) is hyperreduced using the ECSW method and transformed into a hyperreduced PROM (HPROM); and each PROM/HPROM is trained in a high-Mach rangeusing an adaptive sampling procedure. Finally, the accuracy of each trained PROM/HPROM is assessed for the numerical prediction of various quantities of interest and contrasted with that achieved using snapshot interpolation. For this purpose, three different error measures are considered, contrasted, and discussed in the context of shock-dominated flow problems. Wall-clock time and CPU time speedup factors are also reported. Overall, it is shown that using a relatively small set of training data, all constructed global, viscous, CFD-based LSPG PROMs and HPROMs are nonlinearly stable, real-time capable, and highly predictive, despite the complex nature of the flow; and that the LSPG HPROM variant constructed using the arbitrarily nonlinear manifold grounded in a deep artificial neural network is in this case the most computationally efficient.

^{*}Speaker

ABSTRACTS

Day 3 – Friday, November 24

Morning sessions

Optimal sampling for linear and nonlinear approximation

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Abstract

We consider the problem of approximating functions from point evaluations, using linear or nonlinear approximation tools. For linear approximation of functions in L^2 , recent results show that weighted least-squares projections allow to obtain quasi-optimal approximations with near to optimal sampling budget.

This can be achieved by drawing i.i.d. samples from suitable distributions (depending on the linear approximation tool) and subsampling methods.

After reviewing different strategies based on i.i.d. sampling, we will present alternative strategies based on repulsive point processes that allow to achieve the same task with a reduced sampling complexity.

Then, we show how these methods can be used to approximate functions with nonlinear approximation tools, in an active learning setting, by coupling iterative algorithms and optimal sampling methods for the projection onto successive linear spaces. We particularly focus on the approximation using tree tensor networks, whose architectures allow for an efficient implementation of optimal sampling procedures within coordinate or gradient descent algorithms.

These are joint works with R. Gruhlke, B. Michel, C. Miranda and P. Trunschke.

PARAMETER DEPENDENT REDUCED ORDER MODELS, CONDITIONAL EXPECTATION AND MACHINE LEARNING

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Abstract

Many times one treats systems which have parameters, which may be parameters which one can control and serve to optimise or control the system, or they may be imposed from outside, and could be following some probability distribution. This last case may be taken as the "Leitmotiv" for the following. The reduced order model (ROM) is produced from the full order model (FOM) by some kind of projection onto a (relatively) low-dimensional manifold – like low-rank tensors – or even subspace. The parameter dependent ROM reduction process produces a function of the parameter set into the ROM manifold which in some way approximates the FOM state for that parameter value. It is now of interest to examine the relation between the FOM state and the ROM approximation for all possible parameter values of interest.

In the field of machine learning, also a function of the parameter set into the ROM manifold – the image space of the machine learning model – is learned. This is done on a training set of samples, typically minimising the mean-square error. The training set may be seen as a sample from some probability distribution, and thus the training is an approximation computation of the expectation. This thus produces an approximation to the conditional expectation. The conditional expectation is a special case of an Bayesian updating, where the Bayesian loss function is the mean-square error. This offers the possibility of having a combined look at these methods, and also introducing more general loss functions.

Reduced order models for fracture and path-dependent multiscale simulations: Macro Clustering and data-driven approaches

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Abstract

Multi-scale fracture modelling is a key issue in engineering to understand the fracture mechanisms in new advanced materials such as 3D printed meshes, high performance composites or concretes, as well as to provide guidelines for the design of these materials. In this work, two approaches using Reduced-Order Models (ROMs) are presented in the context of multi-scale fracture modelling, and more generally of non-linear multi-scale simulation involving path-dependent behaviors (damage, plasticity, viscoelasticity).

First, a method using unsupervised machine learning (k-means clustering) is developed (1,2) to reduce the computational costs in nonlinear multiscale simulations (FE2). To this end, a k-means clustering algorithm is used to classify Gauss points with close mechanical states in the macro mesh. In contrast to micro-scale ROM techniques, the ROM here is constructed at the macro-scale by appropriately selecting the macro Gauss points and avoiding redundancy in the non-linear Representative Volume Elements (RVE) calculations.

Secondly, a data-driven method is proposed (3,4) to perform sequential (non-simultaneous) simulations of multi-scale fractures. This method, called Data-Driven Harmonic Damage Analysis (DDHAD), involves several steps. First, off-line fracture simulations (phase field) are performed in RVE of the material. During this step, a computational homogenization is performed to evaluate the evolution of the effective elastic tensor, which may eventually evolve to an arbitrary anisotropy. Then, a harmonic analysis of the elastic tensor is performed to define the appropriate internal variables defining the anisotropic damage. Finally, a Proper Orthogonal Decomposition (POD) is employed to define a small set of internal variables.

The proposed techniques are illustrated by applications involving fracture in civil engineering materials and 3D printed lattices, as well as the prediction of the behavior of complex elastoplastic, viscoelastic and quasi-fragile composites.

Keywords : Fracture, phase field, multiscale methods, nonlinear problems, path-dependent problems, clustering, data-driven.

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Recent advances on intrusive and non-intrusive separated representations

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Abstract

Separated representations at the heart if the so-called Proper Generalized Decomposition -PGD- experienced recently many new developments for addressing several simulation challenges.

This contribution revisits some of the most recent and powerful proposals, embracing:

- Multi-time separated representations for simulating aging and fatigue
- In-plane-out-of-plane separated representation empowered by machine learning techniques
- Geometry separation enabled by the NURBS geometry parametrization
- Lego-like PGD for elastic and inelastic behaviors in complex multicomponent systems
- Multi-parametric surrogates
- Parametric optimal transport
- Hybrid Twins

Parameterized reduced order model of linearized structural vibrations around a nonlinear static prestressed state due to follower forces

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Abstract

The study is motivated by the computation of parameterized hydroelastic vibrations of liquid propeller tanks around a prestressed state using reduced order model (ROM). The prestressing is due to the liquid and gas pressurization considering geometrical nonlinearities and follower forces which lead to a change of the natural eigenfrequencies of the system. In (1,2), the effect of prestressing has been considered in the coupled problem using appropriate structural bases, to avoid prohibitive computational cost of the hydroelastic high-dimensional model (HDM). Those bases are generated by the calculation of the dry structural eigenmodes around a nonlinear static prestressed state. Only a parameterized ROM of the structural vibrations around prestressed states is investigated in the following.

The objective of this presentation, as an extension of (3), is to compute the eigenmodes of three-dimensional elastic structures around various nonlinear static equilibrium configurations. The HDM is based on two steps using the Finite Element Method (FEM). At first, we compute the displacement fields from a static problem with geometrical elastic nonlinearities (i.e. Saint-Venant Kirchhoff constitutive equations) depending on parameterized static load amplitudes. Then, the second step consists in evaluating the eigenmodes and eigenfrequencies around a known operating point. We recall that this HDM approach is time consuming due to the nonlinearity nature of the prestressing for parametric investigations. The goal here is to construct two ROM. The first ROM (static nonlinear ROM) is devoted to evaluating efficiently prestressed states for parameterized affine static load cases. Here, the nonlinear part of the internal and external load vectors are nonlinear cubic polynomials functions of the static unknown displacements. In (3), the approach has been demonstrated successfully for one parameter and with a precomputed ROM obtained by projection on POD modes (4). This approach has limitations due to the polynomial nature of the nonlinearity (5). As described in (6), we will use here hyperreduction techniques to accelerate the computation of the nonlinear part of the static ROM. Either approximate-then-project methods as DEIM (7) or UDEIM (8) or project-then-approximate methods as ECSW (9) has been considered. The second ROM (linearized vibration ROM) necessitates the computation of a tangent stiffness matrix based on the prestressed configurations. This matrix is an operator with a quadratic dependence on the static nonlinear solutions and can be precomputed. Those precomputed operators are then projected on selected linearized structural prestressed modes.

Numerical examples will be presented. Advantages and drawbacks with respect to speed

^{*}Speaker

up and accuracy will be discussed.

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POD-assisted computations of incompressible fluid flows: applications to marine energy

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Abstract

We are interested in numerical modeling of complex flows. The complexity may come from the geometry of the domain or from the inherent multiscale behavior of the flows under consideration. A typical example is a wave energy converters farm, where both complex geometry and multiscale phenomena are present. Full order numerical simulations of such problems are very difficult to perform because of the computational costs involved.

We thus propose to couple a Full Order Model (FOM) with a Reduced Order Model (ROM). The FOM (or high order model) is only used in regions where ROM give poor results, especially in highly non-linear regions like the neighborhoods of the obstacles. The ROM can be used elsewhere. These ROMs can be also viewed as propagation models of the main information between several obstacles (wave energy converter farms).

We will describe the Galerkin Free Proper Orthogoal Decomposition (POD) ROM used in this study. In an optimization-based process (maximize the power extraction), the model has to be accurate for the input parametre space under consideraton (the ocean wave intensity, direction, etc.), at least on the trajectory to reach the optimum. It is thus necessary to obtain a POD subspace that is robust enough with respect to the input parameter space. We thus propose 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. We will show that this metric performs better than classical ones like PABS or Grassmann geodesics.

Nonlinear structural ROM for aeroelastic problems with large displacements

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Abstract

Aeronautical structures are inherently flexible and have to sustain various aerodynamic loads in their operating range. Future designs, like high aspect ratio wings or highly loaded open fan of large diameter which are currently investigated, involve lighter and slender structures with the aim of reducing environmental impact. This results however in even more flexible structures that undergo large static but also possibly dynamic displacements. The design of such structures requires appropriate numerical methods to properly capture these nonlinear effects. The purpose here is to have a sufficiently rich model of the structural behavior, which can be easily coupled with another model providing the aerodynamic forces, so that coupled aeroelastic phenomena involving nonlinear structural effects can be accurately predicted.

We focus here on the structural model and we assume that the aerodynamic loads are obtained with a computational fluid dynamics code providing an accurate solution for the flow considered (possibly viscous and transonic). A coupled partitioned procedure is traditionally used to couple the fluid and the structure for aeroelastic problems involving a linear structural behavior, where the structure's dynamics is well captured by a small set of linear eigenmodes. This strategy is quite easy to implement as the CFD solver interacts with a very simple structural model, avoiding complicated data transfer processes with another Finite Element code for the structure. The use of a reduced order model for the structure is therefore appealing but taking into account nonlinear effects requires an enhanced formulation of the reduced order model.

The elaboration of the structural reduced order model has to face several practical constraints when dealing with industrial structures: first, the model has to be non-intrusive so that it is possible to use a commercial Finite Element code; then it has to be a standalone model, meaning that it does not require any interaction with the full order Finite Element model. The second point is particularly important in the context of a coupled partitioned procedure to ease the exchanges between the fluid solver and the structure.

Several approaches are possible to build a structural reduced order model in this context. The first method investigated here is based on the projection of the equation of motion on a suitable basis containing the usual linear eigenmodes and supplemented by dual modes (1). These additional dual modes are determined from a set a nonlinear static solutions resulting from different generic load cases. Residual vectors are then defined from the difference between these solutions and their approximation by the linear eigenmode basis and the missing

^{*}Speaker

contribution contained in these residuals is processed by a singular value decomposition to extract the most relevant features. A subset of the singular value vectors (called dual modes) is selected with a combination of criteria based on the associated singular values and the linearized strain energy. These modes include in particular membrane contributions that are often missing in the first linear eigenmodes. This enhanced projection matrix containing both linear and dual modes is used to project the equation of motion, including the nonlinear internal force term. This term is then approximated as a third order polynomial whose coefficients are identified with the Implicit Condensation method. This approach called ICDual is compatible with the use of a commercial Finite Element code to extract relevant data required to identify the polynomial coefficients. Finally, a reduced order model is obtained with very few degrees of freedom.

This first version of a structural reduced order model with dual modes has been investigated and compared to the classical Implicit Condensation and Expansion (ICE) method (2) where the projection basis include only linear eigenmodes but the expansion step provides a partial reconstruction of the missing contribution. For static loadings, both approaches are similar but in the dynamic case, the ICDual approach performs better on the cases investigated here.

Finally, another type of reduced order model has been considered. It is based on nonlinear normal modes that generalize the notion of linear eigenmodes. These modes can be computed with a parametrization of the invariant manifold and recent progresses have paved the way for a practical application of the approach on large systems with many degrees of freedom. The intrusive version of this approach exists, where the nonlinearity can be approximated with an arbitrary order. On the other side, a non intrusive approach has been derived to deal with black box Finite Element models, but a the price of a reduction to the third order for the approximation of the non linear term and the mapping (change of variable). This last approach from (3) is called Direct Normal Form (DNF) and has been compared here to the previous method and a simple test case.

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Two-scale modelling of fluid saturated electroactive porous media - nonlinear phenomena and computational homogenization

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Abstract

The conference paper is devoted the homogenization based modelling of locally periodic porous media featured by nonlinearities. Three particular but mutually tightly related topics are presented: peristaltic driven flow in an electroactive porous structures, unilateral (self) contact at the pore level of a poroelastic medium, and the electroactive large deforming porous inflatable medium. The homogenization is based on the asymptotic analysis of the micromodel equations using the periodic unfolding method.

The first topic, the peristaltic flow in deforming elastic scaffolds with embedded piezoelectric locally controlable actuators, shows the use of the homogenization to derive a metamaterial which enables to transport fluid against small pressure slope. The recent paper (1) is extended to treat dynamic problems. To explore functionality of such metamaterial structures, we developed multiscale computational tools using the homogenization of the fluid-structure interaction problem. Cell problems (at the microlevel) provide characteristic responses of the microstructures with respect to macroscopic strains, fluid pressure and electric potentials. The homogenized model is derived under the small deformation and linear constitutive law assumptions at the heterogeneity level. Within the homogenized model which in the structure is a modification of the Biot continuum due to the piezoelectric parts, the macroscopic nonlinearity is introduced using the first order expansions of the homogenized coefficients with respect to macroscopic variables. It appears that this feature is crucial to capture the pumping effect of the metamaterial. In the macroscopic model, the nonlinearity is introduced by deformation-dependent homogenized coefficients. For this, linear expansions based on the sensitivity analysis of the homogenized coefficients with respect to deformation induced by the macroscopic quantities are employed. This enables to avoid the two-scale tight coupling of the macro- and microproblems otherwise needed in nonlinear problems.

As an optional feature of the smart devices, distributed valves can be involved which strongly influence the macroscopic permeability of the material (the second topic). We confine to the case of closed pore microstructures with unilateral contact at the pore level, as considered in (2), but extended for inflatable porous structures. The homogenization procedure leads to a nonlinear elastic model at the macroscopic scale. An efficient algorithm for two-scale

^{*}Speaker

computational analysis is based alternating micro- and macro-level steps. A dual formulation of the pore-level contact problems in the local representative cells provides actual active contact sets which enable to compute efficiently consistent effective elastic coefficients at particular macroscopic points. At the macroscopic level, a sequential linearization leads to an incremental equilibrium problem which is constrained by a projection arising from the homogenized contact constraint. The stress-strain characterization of the homogenized unilateral contact interaction for specific elementary loading scenarios, can be used to construct efficient computational algorithms based on a precomputed database of responses parameterized by local macroscopic strains. However, such a kind of

the "model order reduction" is feasible as far as elastic materials and friction-less contact conditions are considered. In a "dissipative, rate-dependent case", internal variables would have to be involved. Nonetheless, the same computational scheme can be applied to the coupled micro-macro two scale computations.

The third topic shows the use of the homogenization to upscale the micromodel describing large deformations of a porous electroactive (electrostrictive (3), or piezoelectric (4)) polymeric inflatable structures. Using the concept of the locally periodic structures, cf. (5), the homogenization is applied to the incremental formulation arising due to linearization of the residual formulation in the Eulerian framework, such that the incremental scheme uses the updated Lagrangian approach. The material derivative with respect to a convection velocity field is used to differentiate the governing equations expressed in the spatial configuration. The linearized system is subjected to the two-scale homogenization and due to the proposed incremental scheme, the homogenized material coefficients can be computed for given updated microscopic configurations, as in the linear case. **References**

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Certified Reduced Order Method for the Parametrized Allen-Cahn Equation

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Abstract

In this contribution, we present a ROM-POD technique that uses time difference quotients as snapshots to provide fast solutions to the parameterised Allen-Cahn equations. We develop an error analysis that includes a specific use of the time difference quotients to improve the error estimates by an order of convergence with respect to the time step. And includes a series of numerical experiments that provide exhaustive tests of the theoretical error estimates. To conclude this investigation, we derive a new posteriori error estimate for the AC equation through residual error estimators that we evaluate thanks to several numerical examples.

^{*}Speaker

POD model order reduction for transient biphasic flows in porous media based on steady-state snapshots

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Abstract

Liquid Resin Infusion (LRI) processes are known as economic routes for manufacturing structural composite parts. They can be numerically simulated through an approach presented in (1, 2). It requires the resolution of a weakly-coupled problem between a biphasic fluid flow computation and the convection of the interface between those two phases.

The interface between air and resin is given by the zero iso-value of a level-set function. At each time step, the biphasic fluid flow problem (Darcy and/or Stokes equation depending on the scale of the study) provides a velocity field. The level-set function is then convected according to that velocity field in order to determine the shape of the interface at the next time step. Both PDEs (fluid motion and convection problem) are solved via P1 Finite Elements, with suitable stabilization approaches.

On complex and realistic geometries, the discretized systems have large numbers of degrees of freedom, and the above-described process may be computationally expensive. This contribution will hence address the feasibility of a non-intrusive Reduced Order Model (ROM) through POD-Galerkin (3) on such a complex geometry.

The POD method is applied to the fluid flow computation, which is the most computationally expensive step in the procedure, and more precisely to the biphasic Darcy equation, solved with a mixed velocity-pressure formulation. The reduced basis is built from snapshots obtained through a resolution of the steady-state biphasic equation for different positions of the interface.

Three main questions will be addressed. The first one is the influence of the choice of the interface positions used for computing the snapshots. It will be shown that a reliable way to obtain those positions is to run the transient problem on a coarse mesh.

The second point is the actual separability of time and space in this problem, evaluated through the decay of singular values. In connection with this question, the impact of the number of modes on the error of interface velocity (the main quantity of interest of this problem) will be empirically investigated.

The last question is the stability of the reduced problem. One can indeed show that, even if the underlying Finite Elements method is stabilized, there exists no stability guarantee for the reduced problem, what calls for an ad hoc stabilization approach.

^{*}Speaker

The gain in computational time in absence of any reduced integration method (like DEIM) will be evaluated. What is more, for this particular problem, insight will be given on how to save much computation time without the need to rely on such a reduced integration method, hence preserving the non-intrusive nature of the reduction approach.

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ABSTRACTS

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Coupling of Deep Learning on Graphs and Model Order Reduction for Efficient Preliminary Sizing of Mechanical Structures in Aircraft Crash Simulations.

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Nonlinear model order reduction with mesh adaptation for hyperbolic systems

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Schopper Sebastian

Removing Inconsistencies of Reduced Bases in Parametric Model Order Reduction by Matrix Interpolation

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Model reduction for non-linear structural problems with multiple contact interfaces: application to the modeling of mooring lines for floating offshore wind turbines

Model order reduction for inf-sup-stable problems using optimally stable discretization schemes

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Abstract

A known challenge in the field of model order reduction is the application of established techniques to hyperbolic problems. If we consider the linear transport equation with parametrized transport direction as a simple example, it has been shown that the approximability - measured by the Kolomogorov N-width - decays slowly and thus linear techniques are bound to perform poorly (1). However, in many real-world-applications the velocity field is often constant as it is either analytically known/measured or given as the solution to i.e. the Darcy- or the Navier-Stokes-equation. In particular, we examine the reactive transport of a substance in a catalytic filter where the velocity field is constant and given by a porous media equation (in our example Darcys law). One is now interested in solving the ensuing advection-reaction equation for a parametrized, spatially varying reaction coefficient. Using a generalization of the proof of exponential decay for symmetric and coercive variational problems (1) to inf-sup-stable problems and exploiting the structure of our parametrization we were able to also prove exponential approximability in our setting. Additionally, one obtains an interesting insight why a different parametrization (e.g. of the transport direction) might yield different rates.

Numerical experiments where we construct reduced spaces with a greedy-type algorithm confirm the exponential decrease of the approximation error. For the full order discretization we employ a numerical scheme based on the theory of optimal test functions. Initially formulated for the Discontinuous Petrov-Galerkin (DPG) method (2), continuous variants have been developed with model order reduction in mind (e.g. the double-greedy method (3)). We adapt the construction introduced by Brunken et al. (4) yielding an optimally-stable scheme using non-standard function spaces (5). The advantages of this approach for (localized) model order reduction, as well as its challenges will also be discussed.

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A computational framework for predictive digital twins of civil engineering structures

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Abstract

The digital twin concept represents the most appealing opportunity to move forward condition-based and predictive maintenance practices. Enabling such a paradigm shift for civil engineering systems would allow for reducing lifecycle (economic and social) costs and increasing the system safety and availability. This is nowadays possible as the installation of permanent real-time data collecting systems has become affordable, as well as thanks to the recent advances in learning systems and diagnostic activities.

This work proposes a predictive digital twin approach to the health monitoring, maintenance and management planning of civil structures. The asset-twin coupled dynamical system, and its evolution over time are encoded by means of a probabilistic graphical model. In particular, a dynamic Bayesian network equipped with decision nodes is adopted to rule the observations-to-decisions flow and quantify the related uncertainty. For diagnostic purposes, the dynamic Bayesian network is used to update and track the evolution of the structural health parameters comprising the digital state and describing the variability of the physical asset. The assimilation of observational data is carried out with deep learning models, useful to automatically select and extract damage-sensitive features from raw high-dimensional vibration recordings, and ultimately relate them with the corresponding structural state in real-time. The digital state is continuously updated in a sequential Bayesian inference fashion, and eventually exploited to inform an optimal planning of maintenance and management actions within a dynamic decision making framework. For prognosis purposes, the dynamic Bayesian network is used to forecast the future damage growth, according to control-dependent transition dynamic models describing how the structural health is expected to evolve.

The digital twinning framework is made computationally efficient through a preliminary offline phase that involves: (i) the population of training datasets through reduced-order numerical models, exploiting the physics-based knowledge about the system response. This is useful to overcome the lack of experimental data for civil applications under varying operational and damage conditions. (ii) the computation of a health-dependent control policy to be applied at each time step of the online phase. Such a control policy is then exploited to map the belief over the digital state onto actions feeding back to the physical asset.

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The strategy is assessed on the simulated monitoring of a cantilever beam and a railway bridge. The obtained results prove the capabilities of health-aware digital twins of accurately tracking the evolution of structural health parameters under varying operational conditions, and promptly suggesting the most appropriate control input with relatively low uncertainty. (1) L. Rosafalco, M. Torzoni, A. Manzoni, S. Mariani, and A. Corigliano. Online structural health monitoring by model order reduction and deep learning algorithms. Computers & Structures, 255:106604, 2021.

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A Hyperreduced Reduced Basis Element Method for Model Reduction of Component-Based Nonlinear Systems

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Abstract

Building on the principle that many engineering structures consist of identical or similar components, this work proposes a reduced basis element (RBE) method for model reduction of large, parametrized, component-based systems in continuum mechanics governed by nonlinear partial differential equations (PDEs). The present work extends upon previous works on RBE methods for linear PDEs (2,3). The key idea in RBE methods is to build a library of archetype components and their local RB in the offline phase, and, in the online phase, to construct a global RB model for the system by coupling the preconstructed local models. While some extensions of the concept to nonlinear PDEs have been sought, they have been constrained to systems with localizable nonlinearities (3) or have not accommodated online interchangeable components in the sense of those in component-based RBE methods for linear problems (4).

This study aims to overcome these limitations by presenting a hyperreduced RBE (HRBE) method. The developed approach extends the component-based formulation to parametrized PDEs that demonstrate general and non-localized nonlinearities. The primary ingredients of the method are as follows: an extension of the empirical quadrature procedure (5) to the component-wise construction of RBs and in particular hyperreduced components; a library of archetype components comprising HRBEs of varying RB and hyperreduction fidelities; adaptive online selection of HRBEs to assemble a global system that meets the user-prescribed error tolerance; and an application of the Brezzi-Rappaz-Raviart error estimation theory to the component-based context to inform the error control strategy. We assess the formulation using large nonlinear-thermal and hypereleasticity systems.

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A model order reduction technique for substructuring by mortar tied contact in nonlinear solid mechanics

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Abstract

This work is concerned with a model order reduction (MOR) technique for substructuring problems, in nonlinear solid mechanics, where the system is assembled from substructures. The computational effort to solve such systems is high. Therefore, each substructure is reduced separately by the proper orthogonal decomposition (POD) method. The reduced substructures are connected by a mortar tied contact formulation for non-matching interface meshes. The POD bases of each substructure are computed in an offline training stage by the method of snapshots and are independent of the global structure. The choice of these snapshots strongly influences the quality of the solution. Therefore, we present a method to compute significant snapshots from a specific set of boundary conditions to obtain POD bases that can be used in many different assemblies of the substructure. With this method, many different reduced structures can be assembled from a set of reduced substructures. Finally, the method is tested by numerical examples considering finite strains, hyperelasticity, and viscoelasticity.

A Non-Intrusive Physics-Informed Artificial Neural Network Hyper-Reduction approach for Nonlinear Structural Finite Element Formulations

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Abstract

Over the past decade, several nonlinear Model Order Reduction (MOR) schemes, such as the Proper Orthogonal Decomposition (POD) with Energy Conserving Sampling and Weighting (ECSW) approach(1), have been introduced to reduce the computational cost of nonlinear Finite Element (FE) analysis in structural systems. However, many of these Hyper-Reduction approaches have been found to be intrusive in nature, posing challenges when it comes to integration into simulation frameworks and existing commercial software.

Recently, several data driven Non-Intrusive Model Order Reduction (NIMOR) methodologies have been proposed for the (hyper-)reduction of nonlinear FE problems, many of which rely on the use of Artificial Neural Networks (ANNs) to approximate the (low-order) nonlinear operators(2). While these approaches are general and non-intrusive, they typically suffer from limitations such as overfitting, a reduced capacity to extrapolate and violation of key physics properties like energy preservation. The latter can lead to unstable behavior when employing the reduced nonlinear model in static or time-domain analysis.

This work proposes a data-driven, physics-informed ANN approach based on the Input Convex Neural Network (ICNN) architecture(3) for nonlinear structural FE formulations. This architecture has recently been applied to model constitutive laws of nonlinear elastic materials, which preserve fundamental principles of solid mechanics(4). The proposed approach combines stability-preserving properties of hyper-reduction approaches with the non-intrusive properties of data-driven approaches. More specifically, the proposed methodology approximates, i.e. hyper-reduces, the reduced nonlinear internal force term by means of identifying a nonlinear mapping between the reduced displacement field and associated strain energy. The corresponding reduced internal forces are computed by evaluating the partial derivatives of the network output (i.e. strain energy) with respect to the input (i.e. reduced displacements). Positive semi-definiteness of the Jacobian (i.e. stiffness matrix) of the approximated reduced nonlinear internal force term is a priori enforced by using the ICNN architecture. Therefore, the resulting (hyper-)reduced map possess the necessary

^{*}Speaker

stability-preserving properties to be successfully employed in numerical simulations.

The proposed approach is validated on a nonlinear static structural FE model of a cantilever beam undergoing nonlinear geometrical and material behavior. A POD reduced order basis is generated using a set of displacement field snapshots obtained from different loading conditions, whereas reduced internal force snapshots are used to train the proposed network. A comparison of a deep Fully Connected Neural Network (FCNN)(5) not enforcing the physical constraints and the proposed architecture is carried out. Even though both approaches provide a good approximation of the reduced internal forces, the FCNN architecture leads to inconsistent results when using the (hyper-)reduced map to compute the reduced order solution of the static equilibrium equations for different load magnitudes. The FCNN architecture does not ensure stability-preserving properties which leads to the observed unstable behavior and related convergence issues. The ICNN architecture however does guarantee the a priori enforcement of the physical constraints and therefore provides stable and consistent results when comparing the reduced order solution with the projected reference solution.

These results highlight the efficacy of the proposed approach in addressing static structural FE problems and showcase its potential for dynamic analysis, as well as applicability in more advanced parametric and multiphysics applications.

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A Reduced Order Model conditioned on limited measurements for structural health monitoring in parametric nonlinear systems

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Abstract

Nowadays the importance of Reduced Order Models (ROMs) is continuously increasing, allowing them to pose as an essential asset in many areas of engineering where computationally intensive numerical simulations are required. In this context, established physics-based approaches imprint a physical connotation on the ROM via the use of projection-based reduction to achieve high-accuracy estimates. However, popular Reduced Basis (RB) methodologies can become inefficient or fail in the case of multi-parametric or strongly nonlinear systems whilst no confidence bounds are provided for the estimation tasks. Such problems are typically tackled via a library of local reduction bases, and thus local ROMs, each of which represents a training realization of the parameter vector. The performance of such ROMs largely depends on the technique utilized to relate the parameter vector to the suitable local subspace, with clustering and interpolation strategies being used in consequence.

Our work employs Variational Autoencoders (VAEs) to perform a more accurate mapping, in place of the utilized clustering or interpolation. In addition, the proposed ROM assumes no knowledge of the actual parameter values after its deployment; rather it utilizes a conditional VAE component as a generative model which can infer the local basis corresponding to features extracted from the monitored response. The physical insights of a projection-based strategy are still retained by the derived ROM, allowing propagation of the dynamics forward in time. To accurately reconstruct the physics involved, an auxiliary task is introduced that makes use of the latent space of the VAE to carry out the parameter estimation task. At the same time, uncertainty quantification on the response estimates is injected into the ROM via the probabilistic treatment of the VAE representation. These components lead to an efficient and generalized ROM representation, with high utility for structural health monitoring tasks. The derived ROM is validated in case studies featuring damage in the form of stiffness reduction or hysteretic nonlinearities and multi-parametric dependencies.

A review of multi-fidelity surrogate models for high dimensional field outputs

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Abstract

In the field of computer experiments, analyses such as optimization and uncertainty quantification typically require many evaluations of a physical model simulator, which for practical reasons often needs to be seen as a black-box. In this work, we consider a simulation with an input that consists in a vector and an output that is a field discretized on a high-dimensional mesh (e.q.), a univariate physical quantity which is a function of time or spatial coordinates). For a high-fidelity simulation, a single run can induce a large computational cost, making a high number of evaluations unaffordable in practice. To tackle this issue, one classically relies on data-driven surrogate modeling to build an approximate mathematical model of the simulator. However, the high dimension of the output creates specific challenges. Indeed, building a classical surrogate model mapping the inputs to each output field local value leads to a prohibitive cost. Taking advantage of the strong spatial or temporal correlations of the output field, dimensionality reduction techniques can be used to map the high-dimensional output space to a lower dimensional latent space. The most widely used dimensionality reduction technique is the Proper Orthogonal Decomposition (5). Mapping the input vector to a lower dimensional latent space reduces the number of variables to predict, making the use of surrogate models possible. Then, combining the surrogate models and an inverse mapping from the latent space to the initial high dimensional output space, it is possible to predict fields. This global metamodel is much faster to evaluate than the exact simulator but has to be trained with snapshots of the output field obtained by repeated runs of the high-fidelity simulator for different input values. In the case when the computational cost of the simulator is too large to acquire enough snapshots for the dimensionality reduction and the surrogate model to be effective, multi-fidelity techniques may be used to get additional snapshots from lower fidelity models, which are cheaper to evaluate. For example, in Computational Fluid Dynamics (CFD), the high-fidelity model could be a CFD Reynolds-Averaged Navier-Stokes simulation while the low-fidelity one could be a CFD Euler simulation (*i.e.*, no viscosity and no thermal conductivity hypothesis). Several approaches combining dimensionality reduction, surrogate modeling and multi-fidelity have been proposed recently in the literature (1–4, 6–11) without a deep theoretical and numerical comparison between them.

The objective of this work is to describe the existing approaches with a unified formalism and to compare them on a common set of representative test cases. These approaches include linear and non-linear dimensionality reduction (3, 7), combined with various surrogate models

^{*}Speaker

(4, 6, 7). The specific capabilities and limitations of each approach are discussed (*e.g.*, the ability to fuse information issued from different meshes without interpolation, the need to evaluate the low-fidelity simulator to predict high-fidelity fields). Each of these approaches is tested on four test cases involving two simulator fidelities. The first two are the viscous free fall of a sphere with and without a ground (the former introducing discontinuities). Then, two aerodynamics test cases are considered. The first one is the prediction of the pressure field of the flow (spatial mesh in two dimensions) around a transonic airfoil (7). From the theoretical and numerical studies, pros and cons of each reviewed approaches are described and guidelines are discussed to help practitioners choose the appropriate technique for a given application.

Acknowledgements

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An adaptive finite elements - neural network method applied to parametric PDEs

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Abstract

A generic parametric partial differential equation

 $F(u(x;\mu);\mu) = 0 \quad x \in \Omega, \ \mu \in P,$

is considered, where Ω denotes the physical domain and P the parameters domain. In order to compute the solution corresponding to a given parameter μ in real time, we train, during an offline phase, a deep neural network using data from finite element simulations. Once trained, the network can be efficiently evaluated online and can then also be used, e.g., to solve inverse problems.

In order to asses the accuracy of the network approximation u_N , we decompose the error between u and u_N as

 $||u - u_N|| \le ||u - u_h|| + ||u_h - u_N||,$

where u_h denotes the finite element approximation and || || denotes the L^2 -norm over $\Omega \times P$.

A way to estimate and possibly control the two error terms is discussed. For this purpose, adaptive finite element techniques based on a posteriori error estimates are in particular introduced. Numerical results are presented for different model problems. A way to use neural networks to solve an inverse problem is presented.

Keywords: Error estimates; finite element method; parametric PDEs; neural networks; adaptive mesh refinement.

An efficient physics based model order reduction technique applied to problems involving geometrical nonlinearity and moving load scenarios

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Abstract

Real-time analysis of complex problems like catheter-tissue interactions remains challenging despite computational advancements. Model Order Reduction (MOR) aims to address this issue by solving a reduced set of equations compared to the original complex problem, typically through projection. The data-based approach Proper Orthogonal Decomposition (POD) based MOR using Singular Value Decomposition (SVD) has shown promise in tackling various complex problems (Calberg et al 2011, Balajewicz et al 2016). However, a key limitation of these data-based approaches is their reliance on generating data by solving complex problems with varying parameters. An alternative approach, rooted in physics, avoids the need for solving the complex problems themselves. In (Idelson and Cardona 1985) the concept of modal derivatives is introduced to simulate nonlinear structural dynamics which has since evolved into linear and nonlinear projection-based model order reduction techniques (Tiso et al 2011, Jain et al 2017). Nevertheless, these methods have their own limitations, particularly the lack of orthogonality in the achieved projection, which can introduce stability and convergence issues. To enhance this physics-based approach, we propose incorporating the Gram-Schmidt process to ensure an orthogonal projection. This enhanced method Orthogonal Linear manifold (Orthogonal LM), also involves a greedy selection algorithm that constructs a projection function compromising only dominant modal derivatives and Eigenmodes. This approach will be advantageous in simulating moving load scenarios, a common occurrence in complex problems.

We assess the performance of the Orthogonal LM compared to the existing methods, namely POD-based MOR and Original LM in quasi-statics and finite strain formulation of the complex problem. For simple loading scenarios, the Orthogonal LM demonstrates equivalent or lesser cumulative displacement error compared to the Original LM while utilizing fewer basis functions. Both of these physics-based approaches, leveraging their respective greedy selection algorithms, outperform the data-based POD-based MOR, albeit with only minor differences. However, the Orthogonal LM's superior performance becomes evident in complex loading scenarios, exhibiting less cumulative displacement error and requiring a reduced number of basis functions to achieve it. Furthermore, Orthogonal LM achieves a computational time reduction of approximately 25-30 % compared to the original finite element calculation. To further demonstrate the effectiveness of Orthogonal LM, we employ moving load scenarios on the same examples. The results confirm the Orthogonal LM's superiority over existing MOR techniques in complex loading scenarios.

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Application of the direct parametrisation of invariant manifold to coupled electromechanical problems

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Abstract

Micro Electro-Mechanical Systems (MEMS) devices have gained significant attention due to their potential applications in various fields, including sensing, actuation, and signal processing. Understanding and accurately characterising the complex nonlinear electromechanical response of MEMS devices is crucial for optimising their performance and reliability. Despite the fact that computational resources are seeing a steady increase in performance, both in terms of power and of speed, the computation of accurate solutions for these devices by means of full order models is still prohibitive. Indeed, a large number of degrees of freedom is required for them to correctly capture the coupled phenomena up to the desired accuracy. Due to this, the search for a highly efficient reduced order model is thus critical: a faster simulation phase is the cornerstone on which a broader understanding of the coupled interactions can be constructed, leading to advances in both the industrial and the academic reality.

In this setting, nonlinear reduction techniques have recently become one of the major tools to develop efficient, converged and fast reduced order models. Among these, we focus on the Direct Parametrisation for Invariant Manifolds (DPIM), which is a simulation-free method directly applicable to the FE mesh of the structure (1, 2, 3, 4, 5). This technique computes a low-dimensional invariant subspace that is tangent to the linear vibration master nodes. As such it extends the notion of linear modes to the nonlinear range, such that these computed invariant manifolds are often referred to as Nonlinear Normal Modes (NNMs). By parameterising this manifold to increasing orders, one can obtain an arbitrarily accurate simulation-free reduced order model, leading to a remarkable reduction of the computational effort required.

First implementations of the method as reported for example in (2, 4, 5) considered geometric nonlinearity. The aim of the present work is to extend this formulation in order to tackle electro-mechanical problems arising in Micro Electro-Mechanical Systems (MEMS). More specifically, the vibrations of MEMS coupled to electrodes are considered. The electrostatic coupling, which makes appear a non-polynomial nonlinearity, is a key feature that needs to be addressed by the method. We propose a technique to deal with this provlem and show on simple MEMS the solutions obtained.

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Dictionary-based model reduction for state estimation

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Abstract

We consider the problem of state estimation from m linear measurements, where the state **u** to recover is an element of the manifold **M** of solutions of a parameter-dependent equation. The state is estimated using a prior knowledge on **M** coming from model order reduction. Variational approaches based on linear approximation of **M**, such as (3), yields a recovery error limited by the Kolmogorov **m**-width of **M**.

To overcome this issue, piecewise-affine approximations (2) of \mathbf{M} have also be considered, that consist in using a library of linear spaces among which one is selected by minimizing some distance to \mathbf{M} .

In this paper, we propose a state estimation method relying on dictionary-based model reduction, where a space is selected from a library generated by a dictionary of snapshots, using a distance to the manifold. The selection is performed among a set of candidate spaces obtained from the path of a **l1**-regularized least-squares problem.

Then, in the framework of parameter-dependent operator equations (or PDEs) with affine parameterizations, we provide an efficient offline-online decomposition based on randomized linear algebra (1), that ensures efficient and stable computations while preserving theoretical guarantees.

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ENABLING EXECUTABLE DIGITAL TWINS USING NONLINEAR MODEL ORDER REDUCTION

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Abstract

Modern model order reduction techniques serve as a key facilitator for executable digital twins. They reduce the computational costs of high-fidelity complex systems while capturing their essential behaviour. Linear model order reduction methods have been extensively utilized throughout the course of the last decades and they are nowadays considered to be reliable and well-established. However, a lot of industrial applications such as online monitoring of both thermal and mechanical behaviour of advanced technological systems, cannot be in general approximated with solely reduced linear models. Therefore, we present an adopted model reduction technique, which will allow to generate a fast approximate nonlinear reduced model applicable to such complex use cases. Even more, for profoundly nonlinear models, combining prominent reduction methods such as operator inference with an appropriate sparsity technique, provides a smaller subset of basic functions and can significantly decrease the size and the evaluation time of the resulting reduced order model.

Flexibility-based Reduced Order Models for damage feature inclusion without offline model evaluations

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Abstract

State-of-the-art (SOTA) approaches in structural health monitoring during damage in structural systems involve Reduced Order Models (ROMs) as low-order representations able to provide real-time inference on the system's behavior. In this context, fracture phenomena and localised damage features pose demanding and challenging requirements when deriving a high-precision ROM. Essentially, incorporating this type of effects at a ROM level has imposed certain limitations on projection-based SOTA frameworks. The resulting models either represent a narrow range of system configurations or require frequent computationally intensive model evaluations to update the low-dimensional spaces, in which solutions are sought. In this work, a novel methodology is introduced for deriving a high-precision ROM that accelerates the solution of structural dynamics systems in the presence of localised damage features, without the need for repeated full-order simulations. Specifically, the proposed approach relies on the initial system configuration, termed as healthy, to construct the low-order projection subspaces. In turn, these bases are enriched with appropriately selected columns of the flexibility matrix of the system for the ROM to be able to capture concentrated damage effects like cracks. It can be shown that the resulting enriched subspaces already contain and can fully represent the solution to the original problem including damage effects, while the retained ROM dimension is much smaller, thus achieving efficiency. However, to fully harvest the potential the derived ROM offers and enable the construction of ROMs for arbitrary localised features in an online manner, the full flexibility matrix of the system should be available. This imposes intractable computational storage and memory requirements, which are addressed here via a Hierarchical Off-Diagonal Low Rank (HODLR) representation. The implemented technique allows the computation and storage of the flexibility matrix in an efficient way and reduces the respective memory requirements. The resulting ROM delivers significantly accelerated model evaluations, without trading the accuracy or flexibility of the full-order representation. The performance and limitations of the approach are validated in a series of structural dynamics case studies.

Improvement of PODI-RBF solutions for real-time finite element simulations of indenter contact problems

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Abstract

The finite element method (FEM) has been widely used to solve a variety of problems in applied science and engineering. However, the high computational cost associated with FEM simulations of high-dimensional models poses significant challenges, particularly to realtime applications. To address this issue, model order reduction (MOR) methods have been developed to reduce the computational complexity while preserving the essential features of the system. One of the popular MOR methods is the proper orthogonal decomposition (POD) technique that constructs a reduced-order model (ROM) using a lower-dimensional space derived from solution snapshots obtained from full-order FE simulations.

In this study, we propose an improved POD with interpolation (PODI) method for real-time simulations of indenter contact problems. The key idea is to use a global-local approach by constructing a POD basis matrix for each training contact location. In the offline stage, solution snapshots from full-order FE simulations are collected, and POD basis matrices and coefficient vectors are separately extracted from the solution snapshots for training contact locations. In the online stage, the POD basis matrices and coefficient vectors are interpolated using a radial basis function (RBF) interpolation technique. The RBF interpolation allows for efficient and accurate approximation of the POD vectors and coefficients associated with a new contact location. By using the precomputed POD basis matrices and coefficient vectors, the computational cost can be significantly reduced in the online stage. In order to improve the accuracy of local deformations near the contact locations, the first POD basis vector is achieved by shifting the first basis vector to the closest training contact location. This approach enables a more precise representation of the PCB modes associated with new contact locatings in the online stage, enhancing the fidelity of the FE solutions.

The proposed global-local PODI-RBF method is evaluated through numerical examples of indenter contact problems. Numerical results demonstrate its effectiveness in obtaining realtime solutions with improved accuracy for local deformations near contact locations. The global-local PODI-RBF method offers an innovative approach to real-time FE simulations of indenter contact problems. By extracting POD basis matrices for training contact locations and shifting the first POD basis vector, the present method can achieve an improvement of local PODI-RBF solutions for real-time FE simulations of indenter contact problems.

^{*}Speaker

Multi-Fidelity Ensemble Kalman Filter with Non-Intrusive Surrogate Model based on Dynamic Mode Decomposition

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Abstract

The use of surrogate modeling techniques in combination with ensemble-based methods for estimating the state of systems described by partial differential equations has been of great interest in recent years in the data assimilation community. Methods such as the multi-fidelity ensemble Kalman filter (MFEnKF) (2) and the multi-level ensemble Kalman filter (MLEnKF) (1) have been developed and implemented in several papers and are recognized as state-of-the-art techniques. However, providing an accurate surrogate model at a reasonable computational cost represents a challenging task. The complexity of solvers used in real-life applications and the performance requirements make appealing the use of data-driven surrogate models. In our work, we investigate the use of the Dynamic Mode Decomposition (DMD) method (3), in a data assimilation context, for the construction of non-intrusive surrogate models. Using a sample of observed states of the system, this method provides a decomposition in: spatial modes, temporal modes and amplitudes. Then, only the information associated to dominant modes is retained to give a reliable estimation the whole system dynamic. A challenge for the method is combination with the ML/MFEnKF is the availability of training data only in the form of fragmented trajectories and the need to produce reliable solutions for a large range of initial conditions. We propose an implementation of the DMD which allows to tackle these issues and to directly provide an estimation of the state at the time of interest at a negligible computational cost.

Acknowledgments: This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (Grant agree- ment No. 818473).

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^{*}Speaker

Multi-fidelity reduced-order surrogate modeling

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Abstract

High-fidelity approximations of the solutions of partial differential equations (PDE) by means of accurate full-order models might require prohibitive computational costs. Commonly, computational restrictions only allow for a small number of high-fidelity evaluations at a limited set of parameter configurations and over a limited time window. By exploiting extra sources which provide less accurate data but at a lower cost, multi-fidelity surrogate modeling aims to enhance predictive accuracy when high-fidelity data are scarce. However, when we are interested in computing the full solution field on a fine spatial and temporal resolution, multi-fidelity techniques often suffer from the large dimensionality of solution space. To overcome this issue, we introduce a new strategy that combines reduced order modeling with multi-fidelity neural network surrogates. The core idea is to generate a set of spatial basis function by applying proper orthogonal decomposition (POD) to collected high-fidelity solution snapshots, and approximate the time-parameter-dependent expansion coefficients of POD basis using multi-fidelity long-short term memory (LSTM) networks. In particular, the LSTM network approximates the mapping from the low-fidelity POD coefficients to their high-fidelity counterpart, such that the proposed reduced-order surrogate model allows to efficiently recover high-fidelity full solution fields over time and parameter variation at the computational costs of computing low-fidelity data. The generality and robustness of this method is illusrated by a collection of parametrized, time-dependent PDE problems where the low fidelity can be defined by coarse meshes and/or time stepping, as well as by misspecified physical features.

Neural networks for large deformation plasticity. Towards real-time interactive simulations

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Abstract

1.Introduction

Due to strong material and geometric non-linearities, simulating large-transformation plasticity is time-consuming: it is a history-dependent process, the governing equations of which require dedicated and computationally-expensive numerical methods (1).

In this work, acceleration of the simulation is targeted through the use of neural networks, seen as a model reduction technique. The history-dependence of elasto-plasticity constitutive laws indicates that recurrent neural networks are well suited (2–4).

The main contribution of this work is the training of NNs for large transformation plasticity, when the state of the art is limited to NNs in small transformation. Results are exemplified on a paperclip. Three different existing network architectures are compared: two classical recurrent architectures (5–7) and TCN (8). Focus is made on in their ability to learn displacements resulting from loads imposed on the paperclip.

2.Dataset

To demonstrate and assess the capability of neural networks to learn elasto-plastic displacements in large transformations, we introduce a use case consisting in a paper clip undergoing large deformation under two simultaneous balanced mechanical loads.

Each mechanical load represents the action of someone manipulating the paperclip. The two loading points are selected randomly (uniform distribution along the paperclip).

The first point is subjected to a random force sequence F_1 and a random torque sequence M_1 , with $F_1 \leq 1.25$ N and $M_1 \leq 0.02$ N m.

The force F_2 and torque M_2 are selected such that the paper clip is globally balanced at each sequence step.

3.Results

All the tested architectures take the loading sequence as input and give the displacements as output.

They all have the same order of magnitude of parameters, and all manage to learn the problem correctly.

However, TCN performs slightly better. The results are given in table below.

-Network - RNN - LSTM - GRU - TCN - TCN-tf -

 $- \mathrm{prec} \ 1 \mathrm{mm} - 0.95 - 0.97 - 0.97 - 0.98 -$

-prec 0,5mm - 0,85 - 0,87 - 0,88 - 0,88 - 0.89 -

 $-{\rm MSE}\xi - 0.35{\rm mm} - 0.28{\rm mm} - 0.30{\rm mm} - 0.23{\rm mm} - 0.25{\rm mm} - 0.25{\rm mm} - 0.00{\rm mm} - 0.00$

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Non-Intrusive Coupling of Neural Network-Based Local Model and Explicit Dynamics Scheme: Application to Spot-Welded Plates under Impact

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Abstract

Solving large structural problems with multiple complex localized behaviours poses significant challenges, primarily due to the requirement of a fine mesh to capture local features and the need for a fine time step to satisfy the CFL condition. To address these difficulties, both intrusive and non-intrusive Domain Decomposition Methods (DDM) have been developed in the past, which involve solving the fine (local) and coarse (global) models separately at their respective time and space scales, with interface quantities exchanged between them. This study presents an innovative approach to further reduce computational time by replacing the Finite Element Model (FEM) at the local scale with a data-driven Reduced Order Model (ROM). The work consists of two main parts: developing a data-driven Reduced Order Model (ROM) at the local scale and formulating a non-intrusive local/global coupling (1) method to integrate the ROM with an Explicit solver. The ROM aims to establish an accurate and efficient mapping from interface velocities to interface forces, enabling the prediction of their temporal evolution. This paper proposes a modelling technique based on the Physics-Guided Architecture of Neural Networks (PGANN) (2), which incorporates physical variables beyond the input/output variables into the neural network architecture. The local/global coupling strategy relies on an iterative exchange of interface quantities between the global and local computations. An extended version, as proposed (3) for explicit dynamics problems, allows the global computation to be performed only once per global time step, while multiple solutions are required for the local problems. To achieve this, we propose replacing the FEM local problem with PGANN, significantly reducing computational time. To demonstrate the efficiency and robustness of the proposed approach, two examples will be presented: a 2D plate with a hole and a 3D case involving fast deformation of spot-welded plates.

^{*}Speaker

Reduced basis construction for PDEs with high-dimensional parameter spaces

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Abstract

In the last two decades, model order reduction has been established as an important tool for the solution of high-dimensional parametrized partial differential equations, particularly in the many-query contexts of optimization, control, uncertainty quantification, and inverse problems. However, even with the development and success of new methods that exploit machine learning tools, the problem of offline sampling — in which "data" from observations or simulations are used to train the surrogate model — remains. Most methods rely on a random sampling of the parameter space, which typically necessitates large amounts of training data, especially in the case of high-dimensional parameter spaces. In this work, we propose a novel method intended to drastically reduce the required number of samples in the construction of reduced bases in high-dimensional parameter cases. We introduce a method that splits the parameter space into polytopes and uses this division to determine where in the parameter space we should sample to get the best improvement in the construction of the reduced basis.

^{*}Speaker

Reduced order modeling for second-order computational homogenization

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Abstract

Computational homogenization is often employed to study the effect of microstructure on macroscopic behavior, resulting in a two-scale formulation, where the macro- and microstructure are separately modeled, discretized and solved concurrently in coupled manner. If scale separation can be assumed, i.e., the microstructural features are much smaller compared to the macrostructural size, then the effective behavior can be accurately approximated with first-order computational homogenization. However, in the case where the microstructure is of comparable size to the macrostructure, or non-local effects due to buckling, softening, etc., emerge, scale separation cannot be assumed and higher-order methods must be considered. One formulation is the second-order computational homogenization scheme (1), which contains the second gradient of the displacement field, making it possible to capture size and non-local effects. Solving such problems is currently computationally expensive and typically infeasible for realistic applications, which limits the applicability of this method. In this work, we develop a reduced order model for second-order computational homogeniza-

tion by employing the proper orthogonal decomposition combined with hyper-reduction. We discuss different examples in terms of training strategy, computational savings and accuracy as compared to the direct numerical simulation.

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Robust Learning of Non-linear Mechanics using Latent Energy-based Neural Networks

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Abstract

In recent years, Neural Networks have been widely used in the context of model order reduction in structural mechanics. Although some results are promising, neural networks often suffer from the lack of interpretability and are seen as "black boxes" compared to classical model reduction methods such as Proper Orthogonal Decomposition or Proper Generalized Decomposition (1). Many researches have been conduced to injecting physical knowledge in neural networks, with penalisation methods such as Physics Informed Neural Networks (2) or directly into the networks architectures such as with Lagrangian Neural Networks (3). In this work we propose a neural network architecture, referred to as Latent Energy-Based Neural Network (LEBNN), designed for model order reduction of non-linear hyperelastic problems addressing the interpretability issue and allowing the neural network to be reversible: the model is trained in forward mode (i.e. having to predict the loading vector f given the displacement field u of the structure) and can then be used in backward mode (i.e. predict u given f and a starting point u0) using a Newton algorithm in a low-dimensional latent space.

Traditional methods fail to provide reliable solutions in the backward direction due to the absence of an energy structure. In the absence of such a structure, there is no guarantee that non-physical mechanical equilibria will not occur outside of the range of the training data, leading the backward mode to often predict absurd unphysical displacement fields.

LEBNN overcomes this limitation by incorporating a latent energy structure within its neural network architecture. The network learns to encode the underlying energy function of the mechanics problem in a low-dimensional latent space, and looking at the local minima of this energy we can certify the absence of unphysical equilibrium outside forward training range, allowing accurate predictions in backward mode without any further training.

The interpretability of LEBNN arises from its ability to explicitly represent the energy structure within the network's parameters. By leveraging this structure, researchers and practitioners gain valuable insights into the mechanics problem being studied.

A non-linear static beam problem which a non-convex underlying energy is used to exemplifie the proposed approach. Comparative experiments were conducted using both the LEBNN

^{*}Speaker

architecture and fully-connected architectures. LEBNN is the only architecture leading to accurate results in backward mode while being trained only in forward mode, even when the error in forward mode is significantly higher than with the other architectures. LEBNN allows to visualize the underlying energy of the structure in a two-dimensional latent space, providing an intuitive understanding of the structure's behavior.

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Sensor monitoring and spatio-temporal (4D) interpolations for deep geological repository for radioactive waste using GNNs

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Abstract

During the operating phase of a deep geological repository for radioactive waste (i.e. Andra's Cigéo project), the comparison between real data acquired by a network of sensors from one side and virtual data from predictive models (i.e. numerical simulation) from the other side, is one of the tools supporting its monitoring. Considering this long term (secular) monitoring, the implementation of spatio-temporal (4D) interpolation techniques may prove essential to ensure the consistency of data over time, especially under dynamic conditions (i.e. when the structure of the sensor network changes over time: loss of sensors linked to aging, drifts, replacements, additions, etc.). Graph neural networks are an appealing approach for such tasks, as they accurately represent physical phenomena (such as thermal conduction where energy conservation operates on nodes and heat flow operates on edges) and can model geometrical and local dependencies.

In this work, we leverage the availability of the experimental data acquired in Andra's Underground Research Laboratory (URL). The selected experiment, named ALC1605 (i.e. a HLW cell demonstrator), is highly instrumented with both distributed sensors (i.e. fiber optics) along with thermo-coules or point sensors. The cell demonstrator includes heat sources to induce thermal and mechanical loading of the cell. To develop an appropriate strategy overcoming the local drift and completion of sensor data over long periods of time, while maintaining overall consistency, two graph neural networks are developed.

The first graph neural network needs to label sensors as healthy or faulty given the temperature fields. Thus, this model takes the field of temperature from the sensors (at the current and past time steps) as inputs and return the state of each sensor, healthy or faulty. The learning process is supervised, using numerical simulation data that are manually deteriorated as well as real in situ data from faulty sensors, after manual labelling. The models used to perform this task are simple graph neural networks constructed using message passing layers and local classifiers. The mathematical model used is a variant of GraphSAGE (W.L. Hamilton & al. 2017) (1), while including elements form the GN (graph networks) framework (P.W. Battaglia & al. 2018) (2) because of the size of the graph considered. These results are weighted against simpler methods such as thresholding. Simple Graph

^{*}Speaker

Neural Networks based on unidimensional data from highly distributed sensors (i.e. fiber optics) are trained many different times with various parameters (such as aggregation functions, Losses and number of GNN layers) and are found to depict predictions matching or outperforming thresholding in precision (with true positive and true negative rates reaching up to 99%).

The second graph neural network is used to interpolate the temperature fields where sensors are faulty. Therefore, these models take a graph of sensors, their state (faulty or healthy) as well as the temperature field of healthy sensors in the surrounding neighborhood. The graph neural network returns the estimated temperature field at the faulty sensors' location. The spatio-temporal (4D) interpolation technique used is IGNNK (Inductive Graph Neural Network Kriging) (Y. Wu & al. 2020) (3). These results are compared versus other interpolation methods such as kNN or Kriging.

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Structure-preserving identification and reduction of mechanical systems

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Abstract

Constructing mechanical models based on experimental or simulation data becomes more and more relevant in engineering practice. On the one hand, the mechanical models, identified from experimental measurements, can be used for analysis and simulation. On the other hand, the models used in modern simulation software often need further reduction and should be re-constructed from the simulation results, because the original system operators are very difficult or impossible to access. Moreover, the identified mechanical system should be able to represent the system behavior for a longer time period and different load cases, which means that the original system properties and structural characteristics should be preserved. Due to the specific second-order ODE structure of the governing system of equations, in many cases not all of the system matrices can be reconstructed. In our work, we propose a methodology for the identification and reduction of mechanical systems from data via solving an optimization problem using some ideas from machine learning. We are able to identify all the system operators and preserve their original mathematical properties by including a reasonable parametrization of the system operators in the optimization problem. For linear mechanical systems, this ensures stability and interpretability of the resulting surrogate model. Additionally, we study systems with nonlinear material behavior and the possibility of applying non-intrusive reduction methods to them. Numerical experiments are performed using simulation data from finite element software.
Super-Resolution of Fluid-Dynamics Problems by Thermodynamics-Informed Deep Learning

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Abstract

Fluid dynamics involves very complex phenomena, some of what remains unresolved until today. Computational Fluid Dynamics (CFD) tools provide the user with accurate simulations, allowing to resolve problems involving most of those phenomena. Their main drawback is the computational cost, specially when complex phenomena (e.g. turbulence) are modelled. For that reason, machine learning approaches have been taken, for example to estimate aerodynamics of a new vehicle design when compared with others previously analysed by CFD (1), leading to real-time results with little loss of accuracy.

A field that could benefit from these approaches is predictive digital twins. Usually, when the user wants to know the behaviour of the flow under real operation conditions to predict its dynamical evolution, sensors are used. However, although sensors provide accurate measurements of the fields they are designed for, they can be placed only in some points of the domain, which means that spatial measurements are sparse. Moreover, frequently those measurements are sampled every certain time interval, meaning that they are not only sparse in space but also in time.

In the current work, we propose a Deep Learning approach to obtain a high-resolution estimation of the flow around an object when only low-resolution measurements of the most relevant fields of the flow are available: the pressure (P) and the velocity (Ux and Uy). For this approach, a database of unsteady flows around a cylinder has been generated using OpenFoam, an open-source CFD software. To obtain the database in both low-resolution and high-resolution, a post processing step is applied. Our approach codifies the geometry using its level set. This codification makes use of a regular grid, allowing us to take advantage of the Convolutional Neural Networks (CNN) architectures.

The method is trained in two phases. First, an Autoencoder (AE) is used to learn a low dimensional codification of the pressure and velocity fields (P, Ux, Uy) from the low-resolution measurements, using an encoder-decoder scheme, where both the encoder and the decoder are built using a CNN. The decoder is trained to produce the pressure and velocity fields in low and high-resolution, meaning that it can recover the high-resolution information taking only the low-resolution information as input. In the second step, a Structure Preserving Neural Network (SPNN) (3) is trained to calculate and integrate the temporal evolution of

^{*}Speaker

the flow in the low dimensional space. The SPNN applies the GENERIC (General Equation for Non-Equilibrium Reversible-Irreversible Coupling) (2) formalism, ensuring that the result obtained is thermodynamically consistent. Finally, in order to obtain the flow evolution, the decoder of the autoencoder is used, generating the high-resolution fields.

Keywords: Super-resolution, Deep Learning, Thermodynamics, Structure Preserving Neural Network

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Variational three-field reduced order modeling for nearly incompressible materials

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Abstract

In this work, a novel approach is proposed for formulating a reduced order model (ROM) specifically designed for nearly incompressible materials. The formulation is based on a three-field variational formulation to accurately represent the behavior of the nearly incompressible material. To construct the reduced order model, the full-scale model is initially solved using the finite element method (FEM), and snapshots of the displacement field are recorded and stored in a snapshot matrix. Proper orthogonal decomposition (POD) is then applied to extract the dominant modes, resulting in a reduced basis for the ROM. Additionally, the pressure field, which is another unknown in the system, is efficiently clustered using the k-means algorithm. This enables the formulation of a reduced order model that incorporates the clustered pressure field. To evaluate the performance of the proposed reduced order model, a comparison is made between the ROM with pressure clustering, the ROM without pressure clustering, and the FEM solution. The results clearly demonstrate that the ROM with pressure clustering outperforms the ROM without pressure clustering when considering a limited number of modes, specifically less than 10 displacement modes. The superiority of the ROM with pressure clustering is validated through two standard examples: a block in compression and Cook's membrane. In both cases, significant speedup factors are achieved compared to the FEM solution. Specifically, the block in compression example demonstrates a speedup factor of 59.2, while Cook's membrane achieves a speedup factor of 62.1. These results highlight the effectiveness of the proposed ROM approach in accurately capturing the behavior of nearly incompressible materials while significantly reducing computational costs. Keywords: Incompressibility, k-means; Hyperelasticity; reduced-order modeling; proper orthogonal decomposition

^{*}Speaker

A flexible decoupled strategy to use model reduction in the context of multiphysics problems

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Abstract

The simulation of coupled multiphysics problems is of great interest in many engineering applications, which increasingly involve interactions between various physical phenomena. In this context, exploring the coupling of different model types (e.g., simplified/fine model, data-based/finite element model) (1) that may arise from various engineering teams could be advantageous. One can then imagine using a high-fidelity model only for the physics of great importance for the targeted application while utilizing a simplified model to solve the other physics, thus reducing computational costs.

For this purpose, we use the LATIN solver extended to the resolution of multiphysics problems (2). The method consists of iteratively solving, in parallel, the decoupled problems corresponding to each physics (possibly represented by different models) and a coupled problem to ensure the coupling. The originality of the method, in contrast to classical decoupled incremental approaches, is that a solution over the entire spatial and temporal domain is provided at each iteration. Therefore, it is possible to apply efficient numerical strategies, such as model reduction with the Proper Generalized Decomposition (PGD) (3), to solve each physics. Another noteworthy aspect of this method is the possibility of starting with an existing solution, such as a truncated reduced-order model or a simple analytical solution, and enriching it on the fly with PGD modes (4).

An illustration of the developed method is proposed in the context of strongly coupled 3D thermo-mechanics by combining a full-order model with a simplified one. The numerical examples show the great modularity of the approach. The accuracy improvement enabled by the enrichment with PGD modes is also highlighted.

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^{*}Speaker

A Graph Neural Network (GNN) application to model thin shell deformations

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Abstract

Many structural mechanics problems have accurate solutions using simulation methods such as the finite element method (FEM). Despite FEM's success and widespread use in the scientific domain, physically coherent real-time simulations involving complex geometries and/or physical phenomena, remain an actively researched subject. Several authors have proposed using reduced-order models to tackle such complexities. Noticeably, Quercus et al. (1) used the GENERIC framework (2) to reconstruct the full-order dynamics of a rolling tire, ensuring that energy dissipative (entropy) and conservative (Hamiltonian) phenomena were properly addressed. The same group refined their previous approach combining the GENERIC framework with graph neural networks (GNN) (3). to fluid and solid mechanics problems. The proposed thermodynamics-informed graph neural network (TIGNN) is a deep learning method capable of predicting the temporal evolution of dissipative dynamic systems, namely the Couette flow of an Oldroyd-B fluid, a Viscoelastic bending beam, and the flow past a cylinder.

The current work proposes an application of the TIGNN deep learning method to model the deformation of thin shells under perpendicular loading. The structure considered is a regular (square/rectangular) shallow and thin spherical shell clamped on the straight edges, and with free curved edges. Thin shell type structures, such as a car door or hood, when subject to loading/deformation within certain ranges, often undergo a snap-through buckling phenomenon. This rapid transition between different geometric configurations is a nonlinear problem that, despite its complexity is properly addressed by commercial finite element packages. However, physically accurate real-time simulation of complex geometric structures undergoing buckling phenomena constitute a challenge, specially felt for applications involving virtual and mixed reality, where a *quasi* real-time response is critical for effective sensory immersion.

To apply the TIGNN deep learning method to our problem, a FEM simulation database for training, test, and validation, was produced using ABAQUS software package. Each FEM simulation consists of imposing a displacement across different mesh nodes, with timesteps

^{*}Speaker

of 0.001 s. The training data includes nodal displacements, rotations, and stresses, per structure node, per time step. Finally, different geometries were considered to enable a geometry independent learning of the underlying phenomena.

Keywords: Deep learning, Graph Neural Network, Snap-through

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A non-intrusive multi-physics PGD-based reduced model for the prediction of power electronic module lifetime

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Abstract

Power electronic modules transform the electrical grid current with respect to the need of the motor, and are key components of numerous electrical systems. Power modules are made of an assembly of multiple materials with different constitutive properties. The selfheating of the chip by Joule's effect and the difference of thermal expansion coefficients generate thermal stresses leading to crack propagation. In return, the crack modifies the module behavior by increasing electrical and thermal resistances. Cracks ultimately lead to module failure. The accurate modeling of the electro-thermo- mechanical module behavior is of paramount importance to predicting the module lifetime. However, multiple uncertainty sources decrease the reliability of lifetime models. Uncertainty quantification studies need to evaluate the lifetime model a high number of times and thus require a reduced model. In this work, we developed a reduced-order model based on the Proper Generalized Decomposition (PGD) to obtain an explicit representation of the solution with respect to space, time, and design parameters. The considered types of design parameters are material properties and geometric parameters. The studied model is a realistic industrial model that requires commercial finite element software, ANSYS. PyAnsys python packages are used to work interactively with ANSYS and to develop a non-intrusive approach to build the reduced model. To solve the multi-physics problem, a specific method has been developed. First, a strongly coupled electro-thermal problem is solved using an iterative method in which the crack length is parametrized. Then, the mechanical problem is solved in which the temperature field is the input. The crack length evolution, modeled with a cohesive zone model, is then obtained from the mechanical solution.

^{*}Speaker

Additive manufacturing and Proper Generalized Decomposition : a novel expanded-piecewise strategy to manage evolving domains within PGD

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Abstract

Proper generalized decomposition has been proven effective in a wide range of problems with fixed geometry and fixed mesh (1). This reduction order modelling technique does not require any knowledge of past solutions. It allows to construct a solution by combining time modes with normalized space modes built on this fixed domain. By doing so, it significantly reduces the computational cost, particularly for large non-linear problems (2).

We aim to extend this technique to evolving domains with a novel expanded-piecewise strategy. The space modes are calculated in an expanded space that comprises all the degrees of freedom throughout the simulation. To visualize the solution, the modes are then projected onto the current physical representation. The time modes are solved in a piecewise manner by dividing the time domain into intervals and initializing the time modes to zero after each interval. Each reset represents the addition of material into the domain, they are required to have proper initialization for these new material points. Interpolation operators can also be included for more complex initializations.

As an illustration, we chose the problem of additive manufacturing as it is a perfect example of evolving domain. Depending on various considerations such as technology, physics and viewpoint, there are numerous ways to simulate this manufacturing process (3). Our focus lies on a common macroscopic approach, often used with techniques like Direct Metal Deposition or Fused Filament Fabrication (4). This approach involves sequentially activating the hot boundary elements to simulate the addition of material. This aligns perfectly with the previously described PGD strategy as it involves an expanding boundary. We also discuss the impact of the number of points added during each activation and their initialization.

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A nonlinear reduced basis approximation of discrete contact problems in crowd motion

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Abstract

In this work we develop new model reduction approaches to predict the solutions of timedependent parametrized problems describing crowd motion in the presence of obstacles. The problem of interest is described by a discrete contact model (DCM) (Ref.(1)), which is formulated as a constrained least-squares optimization statement: the velocity field is seeked as the projection of the spontaneous velocities of each particle (which do not take into account the presence of other particles) into a feasibility set (which prevents the overlap between particles and between particles and obstacles).

The parametric variations in the problem are associated to the geometric configuration of the system (for example, the exit width) and to the initial positions of the particles. Parametric variations have a dramatic impact in the solution, both in terms of the particles positions and in the contact forces, which are represented by the Lagrange multipliers of the underling saddle-point problem.

We investigate new developments of the reduced-basis method and supervised machinelearning techniques to effectively find, in a decorrelated manner, primal and dual reduced spaces. Indeed, for the DCM of interest, linear approximation methods become ineffective, as outlined by the slow decay of the Kolmogorov n-width: the combination of a reduced basis technique with non-linear methods is promising to achieve a more satisfactory level of accuracy. As in (2), we perform a non-linear reconstruction (by Random Forest regression) from the first coordinates of a linear reduced basis approximation, in order to achieve a better performance than the linear reconstruction.

To assess the validity of the method, the nonlinear compressive strategy is then compared to more standard linear and nonlinear approximations. References

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Coupling of Deep Learning on Graphs and Model Order Reduction for Efficient Preliminary Sizing of Mechanical Structures in Aircraft Crash Simulations.

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Abstract

This abstract presents work focused on combining two disparate methodologies: deep learning on graphs and model order reduction. The former demonstrates promising generalization capabilities and efficient execution times, while the latter relies on physics-based resolution of the governing mechanical equations and has been gaining traction in industrial applications. In this work, conducted in collaboration with Safran Tech, the targeted application is the mechanical sizing of aircraft seats in airplane crash simulations.

The proposed methodology to unify the two approaches involves utilizing a graph-based deep learning model to initialize the solution of a corresponding reduced order model for the physical configuration. The key strength of the graph-based deep learning model lies in its training on a reasonably-sized database encompassing diverse seat geometries and topologies, demonstrating strong generalization capabilities towards other geometries/topologies (1). Maintaining a reasonable database size is crucial since industries do not possess databases as extensive as those used in other deep learning applications such as in image recognition. The neural graph network formalism allows one to consider highly-varied geometries and topologies within a single model in order to extract their behavior in relation to dynamic loading. The interest lies in being able to consider mechanical problems and seat designs that are not necessarily parameterizable. The adopted approach incorporates message-passing layers proposed in (1), as well as an autoregressive prediction layer similar to (2). Explorations into the usage of pooling layers and a Graph-Unet-like architecture (3) have also been considered here to further reduce the number of trainable parameters.

The subsequent reduced order model relies on the Proper Generalized Decomposition (PGD) approach (4) which exploits separability of spatial and temporal variables (5), and it has been implemented and adapted to our specific dynamic problem. The advantage of this approach is that it does not require databases or preliminary calculations, making it an *a priori* method. Consequently, it can be readily applied to various structural types, including aircraft seat design.

^{*}Speaker

Our proposed idea is to correct or enrich, if necessary, the solutions obtained from graphbased deep learning models using PGD modes calculated on-the-fly, such that a satisfactory residual is achieved for the governing partial differential equations. Such a coupled algorithm ensures fast simulation and robust "physical compliance" of the final solution by using both the real-time predictive speed of the artificial intelligence model as well as the error control of the reduced model. The long-term objective is to leverage these two methodologies to provide engineers with an efficient pre-sizing tool that surpasses the industry's current practices, thereby enhancing their innovation capacity and the strength of engineering design proposals (here in the context of aircraft seas).

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Data-Driven Reduced Order Model for Advection-Dominated problems using Neural-Network shifted-Proper Orthogonal Decomposition

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Abstract

Advection-dominated problems are commonly noticed in nature, in engineering systems, and in a wide range of industrial processes. For these problems, linear compression methods (proper orthogonal decomposition and reduced basis method) are not suitable, as the Kolmogorov N-width decay is slow, which leads to inefficient and inaccurate reduced order models. To accelerate the Kolmogorov N-width decay there are a few recent pre-processing techniques that can be used to transform the full-order solutions (3),(2),(1). Here, we use a neural-network based pre-processing technique (2) that automatically detects the optimal non-linear transformation of the full-order solutions by exploiting a deep-learning architecture. It consists of two neural networks, 1) ShiftNet, which finds the optimal shift for the full-order manifold, to accelerate the Kolmogorov N-width decay, and 2) InterpNet, which learns the reference configuration and able to reconstruct the shape of reference configuration for each shifted centroid distribution. In this work, we use this pre-processing technique to develop purely data-driven reduced order models for 1D traveling waves and a 2D two-phase flow simulation.

Keywords: shifted-POD (sPOD), Deep Neural Networks (DNNs), Reduced Order Model (ROM), Multi-phase simulation

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Enhanced LATIN-PGD in a multi-query framework

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Abstract

Assessing the risk of failure of a structure subjected to uncertain loadings requires multiple highly nonlinear computations. Indeed, numerous loadings scenarios must be taken into account, and for each scenario, the structure's nonlinear behaviour and dynamics response must be computed. To decrease the numerical cost of the study, a space-frequency Proper Generalised Decomposition (PGD) is employed to solve the dynamics equations of the problem (1).

In order to achieve further reduction in computational costs, a specific multi-query framework is introduced. This framework leverages the non-incremental nature of the LATIN solver (2) by exploiting similarities among the multiple solutions, as proposed in (3). The new simulation benefits from previous solutions to initialise the nonlinear iterative scheme and the associated reduced PGD basis. Looking for the master-guess simulation, i.e., the best case to accelerate the new computation, is particularly challenging for non-parametric loading scenarios. A physical-based strategy using the mechanical content of elastic dynamics responses is proposed to identify the best case among previous nonlinear simulations. In addition, an optimal order to perform the nonlinear simulations is designed by a genetic algorithm.

The proposed methodology offers a robust way to choose a path through the loading scenarios and a manner to exploit redundancy embedded in the different solutions of the multiple computations scenarios. The number of generated PGD modes and the total number of iterations are significantly lower than the cumulative cost of independently performing the different cases.

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^{*}Speaker

Investigation of PINNs and model reduction in structural dynamics for integration into an immersive device

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Abstract

This research project, conducted as part of the ANR JENII initiative, focuses on the development of digital twins for assembled mechanical structures that can be used within immersive and interactive devices (virtual reality) for educational purposes. These digital twins need to accurately reflect the physics of real systems, such as aerospace structures, in order to illustrate important mechanical design concepts to learners during practical exercises. The objective of this study is to provide credible simulated experimental results in real-time, including displacements, deformations and accelerations. This necessitates the efficient resolution of high-dimensional, potentially nonlinear mechanical problems for various loading configurations (intensity, location) and/or design parameter variations (geometry, boundary conditions). The developed method should be robust, particularly for problems involving dynamic loading scenarios (such as impact) that involve the transient regime of the studied system.

Parametric model reduction techniques (e.g., Proper Orthogonal Decomposition, High Order Singular Value Decomposition, Proper Generalized Decomposition), appear to be a promising approach to address this challenge, despite limitations in reconstructing the transient response of structures. The utilization of Deep Learning is also considered, employing the Physic-Informed Neural Network (PINN) paradigm, which combines advances in Machine Learning with the equations of mechanics. Furthermore, this framework offers the advantage of directly incorporating experimental data for model calibration and the inclusion of uncertainties in the trained model. However, scaling up the resolution of 3D dynamic problems and the development of a parametric model present scientific challenges.

This presentation provides a summary of the research conducted in these two fields through an academic example, leading to preliminary conclusions.

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Learning nonlinear constitutive laws with physics-augmented Neural Networks in the modified Constitutive Relation Error framework.

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Abstract

In the context of structural health monitoring (SHM), a novel approach is presented for learning constitutive laws using observable data. The proposed method utilizes a data-driven approach, employing a physics-augmented neural network to represent constitutive laws. The neural network takes strain as input and outputs free energy, ensuring thermodynamic consistency by considering the convexity of the free energy with respect to the Green-Lagrange tensor and stress derived from the free energy. Notably, this approach only requires partial strain or displacement measurements within the structure and boundary conditions, eliminating the need for strain-stress or strain-free energy pairs.

To train the neural networks, an unsupervised training process is employed using a modified Constitutive Relation Error (mCRE) as a training metric. The mCRE offers meaningful physical interpretation, serving as a prediction quality indicator during the inference phase of the neural network. The method builds upon prior work on the mCRE and introduces a new minimization procedure for nonlinear state laws.

As the proposed approach is intended for online training in SHM applications, it emphasizes the elimination of user-defined hyperparameters. Automatic and adaptive tuning of sensitive hyperparameters is proposed to ensure that the training results remain consistent. Additionally, the initialization process incorporates prior knowledge of the constitutive law being learned.

To validate the effectiveness of the proposed method, various test cases were evaluated. The results demonstrate remarkable performance in terms of the quality of the learned model, noise robustness, and low sensitivity to user-defined hyperparameters, as long as the training database includes a sufficient variety of loading cases.

A novel approach for the simulation of locally fluctuating viscoelastic materials

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Abstract

The realistic modelling of structures with inherent uncertainties, e.g. specifically uncertainties in the material properties, is fundamental for a precise assessment of its reliability. However, inelastic material behavior and local material fluctuations render simulations typically computationally expensive. This severly hinders the widespread use of stochastic information in engineering computations. The time-separated stochastic mechanics is a novel technique developed for the precise yet computationally efficient estimation of the stochastic characteristics of inelastic structures with random material properties. It is based on a separation of both the system equation, i.e. the balance of linear momentum, and the evolution equation for a visco-elastic material into stochastic and deterministic terms. Then, only a low number of deterministic FEM simulations and several fast matrix calculations are needed to approximate the stochastic behavior. In the poster, we present how the method can be adapted for local material fluctuations by combination with the Karhunen-Loeve expansion. In doing so, the number of FEM simulations required can be drastically reduced compared to the classic Monte Carlo method.

^{*}Speaker

Multi-Fidelity Model Order Reduction for Robust Design Optimization

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Abstract

Keywords: Robust Design Optimization, Multi-fidelity Techniques, Intrusive and Nonintrusive Model Order Reduction, Composite Wing Structures For optimization studies, the iterative procedures impose high computational expenses, especially for complex and industrial-scale designs. Within this contribution, the focus lies on robust design optimization (RDO) considering uncertain design parameters to ensure an insensitive optimum. While the consideration of the uncertainties is important with regard to safety and performance of structural designs, the high expenses require fast analysis schemes.

Therefore, a novel multi-fidelity technique exploiting simultaneously two different levels of projection-based model order reduction for efficient RDO is proposed (1, 2). In a first step, a classical snapshot-based scheme utilizes full-order simulations to identify a subspace via Proper Orthogonal Decomposition (POD). Then, a first reduced order model (ROM) is constructed via Galerkin projection and hyper-reduction as an intermediate-fidelity model. The second, i.e. the final low-fidelity model is obtained by an additional non-intrusive, data-driven reduction via regression models, which are trained in the identified subspace (3). The intermediate- (intrusive) and the low-fidelity (non-intrusive) models are then combined within a double-loop algorithm for RDO.

An optimization scheme based on Differential Evolution is implemented, which considers the robustness of a design, and is applied to structural optimization of an aircraft wing. Quantification of the robustness via a variance-based robustness measure allows its consideration as an additional objective. For efficient evaluation of the objectives, ROMs are created via intrusive and non-intrusive techniques. Within the iterative procedure, the intrusive ROM evaluates the objective function, whereas the non-intrusive ROM computes the robustness measure with little additional costs.

In order to test the multi-fidelity RDO scheme, two objective functions are evaluated. These are the tip displacement and tip twisting angle of the aircraft wing, under the variation of changing fiber orientation of the fiber-reinforced composite (4). A weighted sum approach combines the objective function and the robustness measure into one objective function. Applying the scheme to these optimization tasks successfully identifies optima with higher robustness compared to the optimum obtained by a standard optimization procedure. Significant computational speedup factors of 470 are achievable by utilizing the multi-fidelity ROMs, such that the computational cost of the training stages is fully compensated.

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Nonlinear model order reduction with mesh adaptation for hyperbolic systems

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Abstract

Numerical approximation of hyperbolic systems has many applications. We are sometimes led to look for multiple numerical solutions for a given range of parameters. Thus, it is useful to rely on the dependence of the solutions to the associated parameters in order to reduce the marginal cost of the high-fidelity (HF) simulations. In order to do so, we use model order reduction techniques (MOR).

The main challenge of studying nonlinear advection dominated partial differential equations in the framework of parametric MOR is the parameter-dependent discontinuities. This deteriorates the speed of decay of the Kolmogorov n-width which is a fundamental hypothesis for linear model reduction (8). Moreover, the discretization of hyperbolic PDEs often leads to a stiff system of equations which makes the HF solver expensive. Mesh adaptation is an efficient approach to reduce the computational cost of simulations whilst increasing the accuracy of computations (2)(4). However, MOR techniques typically rely on a single HF discretization which is incompatible with adapting the mesh for different values of the parameters.

We propose to construct a reduced order model (ROM) using reduced basis (RB) technique coupled with anisotropic mesh adaptation and a registration method (9). The aim is to extend mesh adaptation techniques to build a mesh that is accurate for a range of parameters. Mathematically, anisotropic mesh adaptation process is formulated as finding the optimal mesh elements' sizes and orientations that minimize some error model, under a constraint on the number of mesh vertices. A nonlinear process is used to ensure the convergence towards the optimal mesh/solution couple with respect to a hessian-based a posteriori error estimator (6). In this work, the mesh adaptation is parameter dependent in order to successfully track the solution features for the range of parameters of interest. We rely on linear subspace projection-based MOR to construct the ROM (5). Registration tracks the features of the solution field and allows us to discretize the parametric PDE with a single HF discretization, which allows the use of mesh adaptation process in the framework of MOR.

We first apply the algorithm to a 1D nozzle flow. We use Discontinuous Galerkin finite element method for the discretization of Euler equations to which we add local artificial viscosity to thicken the width of the shock regions. Registration is then used to track the

^{*}Speaker

solution features to a reference configuration. Mesh adaptation in this 1D reference configuration consists in the distribution of nodal points for which we resort to Boor's algorithm. The RB is then constructed using a greedy algorithm based on a residual-based error model (10).

The second application is a 2D transonic flow past a bump. In this case we use anisotropic mesh adaptation based on the continuous mesh model (7). More precisely, we adapt the mesh based on the hessian of the Mach number. We use MMG software (1)(3) to build the adapted mesh. The steps of discretization and construction of RB follow the same ideas as the 1D case.

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On a non-intrusive version of the LATIN-PGD method for non-linear transient thermal problems

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Abstract

Reduced-order methods have emerged in Mechanical engineering communities as powerful strategies for achieving efficient numerical simulations. Approaches such as Proper Orthogonal Decomposition (POD), Reduced Basis (RB) or Proper Generalized Decomposition (PGD) (1) have demonstrated their effectiveness in significantly reducing CPU time. Despite a high degree of maturity and a wide range of applications, the development of these methods in the industrial world is hindered by the difficulties of integrating them into finite element codes. Indeed, these methods are often regarded as intrusive, requiring operations that are atypical for industrial finite element codes. Recently, Siemens has made progress by implementing model reduction solutions natively in its Simcenter Samcef non-linear structural solver. Using a weakly-intrusive reformulation of the method, the LATIN-PGD algorithm (2-3) was implemented as close as possible to the source code, leading to a significant reduction in the computation time associated with quasi-static non-linear mechanical problems typically encountered in industrial environments (4).

This work addresses a current restrictive limitation by extending the weakly-intrusive formulation of the LATIN-PGD method to encompass transient behavior, with a focus on thermal problems. Different strategies have been studied and compared, focusing on ease of implementation and code integration. The implementation is carried out in Samcef source code to capitalize on past developments and include all the non-linearities, element types and tools available in the software. Such an approach should substantially speed up computation time for all the non-linear transient thermal problems that Samcef can handle. In this context, additive manufacturing is an interesting case study, as it often involves excessive computation times of the printed part thermal history. The speedup of thermal simulations would be a first step towards the simulation of building process for very large parts. However, to reach this scope of application, the challenge of dealing with an evolving spatial domain using reduced-order methods has yet to be met. In the meantime, other applications could be targeted to showcase the promising potential of the method.

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Removing Inconsistencies of Reduced Bases in Parametric Model Order Reduction by Matrix Interpolation

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Abstract

Simulations of complex dynamical systems using the Finite Element Method (FEM) can become computationally very expensive since large systems of equations have to be solved for multiple instances in time or frequency. Projection-based model order reduction (MOR) methods are a state of the art technique to reduce the numerical effort for solving dynamical systems. Here, the system is projected onto a lower dimensional subspace which is suited to approximate the desired solution and where the system is much easier to evaluate. In applications such as optimization or uncertainty quantification, one is interested in having a reduced model that can be evaluated with little computational effort and provides sufficiently accurate results for a wide range of parameters. Parametric Model Order Reduction (pMOR) methods are able to retain these parametric dependencies in the reduced-order model. Many of those methods require an affine representation of the parametric dependency, which is difficult to realize for e.g. geometric parameters. (2)

Parametric MOR strategies based on matrix interpolation do not require such affine parametric dependency (3). In these methods, local reduced models are first computed for a set of samples in the parameter space. Afterwards, a generalized coordinate system is constructed from the collected reduced bases, into which all local reduced systems are transformed. In case all local reduced-order models are described in the same or a similar coordinate system after the transformation, a meaningful interpolation of the reduced operators can be performed to obtain the solution for queried parameter points with little computational effort. However, it is not guaranteed that a transformation to the generalized coordinate system is possible for all local reduced-order models as the reduced bases for different samples might span different subspaces. This can, for example, happen due to mode switching and truncation of some of those modes in the reduction. This introduces inconsistencies in the training data for the matrix interpolation as the reduced operators are described in different coordinate systems. Consequently, the predicted reduced-order models are not sufficiently accurate. In an existing approach to remove the inconsistencies, the local reduced bases are further truncated by removing the parts of the subspace that are not consistent with the generalized coordinate system. Whether an inconsistency occurs, is determined by measuring the angles between the subspaces. (1)

In this work, we propose an extension of this method for cases when the truncation of

^{*}Speaker

switched modes occurs several times in the parameter space. Furthermore, a second approach for removing inconsistencies in the reduced basis is proposed in which the parameter space is partitioned into regions, such that in each region all sampled reduced-order models are consistent. Both methods allow to use pMOR by matrix interpolation robustly for wide parameter ranges. The results obtained for a cantilever beam reduced with Modal Truncation show that both proposed approaches lead to significant improvements of the relative error of the predicted output.

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Structural optimization of cruise ships with non-intrusive ROMs

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Abstract

The shipbuilding industry is facing a radical change toward solutions with a smaller environmental impact. To this end, the early design process of passenger cruise ships can be seen as an optimization problem with the objective of reducing the usage of raw steel, operational costs, and thus the impact on the environment.

We present a structural optimization pipeline (1) able to tackle large-scale problems, exploiting non-intrusive reduced order modeling, parameter space reduction, and machine learning to build efficient surrogates of commercial finite element analysis solvers. The optimization of mass, cost, and deformation at a given point is carried out in single and multi-objective fashion, through Bayesian optimization and genetic algorithms. The stability constraints, affected by regulatory certifications and manufacturing processes, are fully integrated into the optimization loop without any external intervention.

The framework has been tested on commercial passenger ship hulls, in collaboration (2) with Fincantieri SpA, with increasingly complex parameterizations of up to 76 design parameters. Our methods are able to provide new and interesting solutions, in a fraction of the time needed following the classical design methods. Interactive tools for the interrogation of the reduced order models and optimization results streamline the integration in the existing industrial computational framework and design process.

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Thermodynamics-informed Graph Neural Networks for Lagrangian fluid simulation

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Abstract

Key Words: CFD, Geometric Deep Learning, Learned simulators, Thermodynamics In the context of modern industry, augmented reality (AR) has emerged as a promising technology that combines the physical world with virtual elements to enhance productivity and efficiency. One significant area of interest within the realm of physical scenario simulations is fluid dynamics.

Currently, Computational Fluid Dynamics (CFD) tools offer users accurate simulations, enabling companies to save substantial resources compared to traditional methods such as wind tunnel experiments. However, a major drawback of this approach is the extensive CPU time required to run a single simulation. The computational cost increases significantly due to the complex physics underlying these models and the large mesh size necessary for analyzing the geometry. In an effort to reduce this high processing time, Deep Learning (DL) is being employed to address the issue, resulting in real-time results with minimal loss of accuracy.

We present a DL approach for estimating fluid sloshing in a glass (1). We propose utilizing both geometric and thermodynamic information to enhance the accuracy and generalization of the resulting integration scheme. To leverage the information provided by the Lagrangian description of movement, we will apply graph neural networks (GNNs) (2). The use of geometric deep learning reduces data consumption due to the symmetries present in the problem.

The architecture is designed to learn the GENERIC (General Equation for Non-Equilibrium Reversible-Irreversible Coupling) (3) structure of the problem, which is an extension of the Hamiltonian formalism used to model more general non-conservative dynamics.

The employed architecture is based on Thermodynamics-Informed graph neural networks (4). A database is constructed using a CFD tool and utilized to train the graph-based architecture. The network is tested on various geometries, encompassing different filling volumes and vessel shapes containing the fluids.

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Interpretable reduced order modeling using neural autoencoders

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Abstract

Solving simulation problems such as turbulent flows for industrial applications requires the discretization of partial differential equations on extremely high dimensional meshes. These high-dimensional discretizations yield complex systems of equations that often require access to supercomputers to be solved. This creates a significant limitation to the use of numerical simulation methods in the industrial context. At the same time, most systems evolve on relatively low dimensional manifolds, meaning that the high dimensional representations used by methods such as Finite Elements are not optimal for the simulation of physical systems. This suggests that computational gain can be achieved by identifying better representation spaces for the solutions of simulation problems.

This issue is directly related to the field of dimensionality reduction, which proposes methods to identify the low dimensional manifolds on which most datasets lie to simplify their analysis. Using linear dimensionality reduction methods such as the Proper Orthogonal Decomposition (POD) method, reduced order models have been constructed to summarise the state of dynamical systems using a small number of features ((1)). These methods rely on data to construct a basis of linear modes that optimally represent the system at hand. They have for example been used in combination with regression methods to construct fully data-driven reduced order models ((2)). Linear reduction methods also have the advantage of being interpretable and can be used in combination with existing physical equations to construct hybrid models combining both equations derived from first principles and datadriven components ((3,4)).

Unfortunately, these linear reduction methods have also been shown to be limited for the reduction of dynamical systems ((5)). Indeed, while the intrinsic dimension of most systems is relatively low, the manifolds on which they evolve can be strongly nonlinear. Meaning that such low dimensional manifolds are not accurately approximated as linear subspaces, as is the case with linear reduction methods. To address this issue, a wide range of non-linear reduction methods have been applied to dynamical systems. Most notably, neural autoencoders have shown impressive performance for the reduction (and reconstruction) of a system's state ((6)).

^{*}Speaker

At the same time, the use of nonlinear reduction methods limits the possibility of constructing theoretically grounded and interpretable models that leverage previously known physical models. Thus, they often require the use of fully data-driven dynamical models such as recurrent neural networks for the approximation of the dynamics of the chosen reduced representation. To address this issue, we propose an approach to learn an interpretable and theoretically grounded dynamical model that evolves the latent representation of a dynamical system in time. The dynamics are learned from data as a time-continuous model constructed around a linear term, completed by a non-Markovian nonlinear closure.

We show in our work that the form of our model can be justified using the theory of partially observed systems through the Mori-Zwanzig formalism ((6)). Moreover, we show that for certain systems, the framework is able to transform a high-dimensional partial differential equation into a quasi-linear ordinary differential equation yielding an interpretable, low-dimensional system that can be simulated efficiently and is easily interpreted.

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Extended Quasicontinuum Method for Modeling Lattice Systems with Heterogeneities

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Abstract

Lattice networks are indispensable to study heterogeneous materials such as concrete or rock as well as textiles and woven fabrics. Due to the discrete character of lattices, they quickly result in a large amount of degrees of freedom. The Quasicontinuum Method (QC) is resolving this challenge by interpolating the displacement of the underlying lattice with a finite element mesh. In this study the QC Method is expanded with enrichment strategies from the eXtended Finite Element Method (XFEM) to include material interfaces using nonconforming meshes and improve the computational efficiency of the method. Different enrichment strategies have been compared in their accuracy and convergence behavior. These Heaviside enrichment is thereby the most accurate and the most straightforward to implement. In addition, a first order interaction based summation rule is applied and adapted for the extended QC for elements intersected by a material interface and complements the Heaviside enrichment uniquely. Three different numerical examples haven been studied using the standard and extended QC and compared to the Direct Numerical Simulation. The extended QC predicts the results below a 5% error threshold with almost one order of magnitude fewer degrees of freedom than the standard QC.

Capturing small scale effects in problems with microstructure via mesh-informed neural networks

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Abstract

Many applications in computational physics are characterized by the presence of microstructures, complex formations that can give rise to intricated patterns at multiple scales, such as, soil fractures in porous media or vascular networks in biological tissues. When it comes to many-query applications, such as those typical of optimal control or uncertainty quantification, capturing the fine details originating from the small scales becomes extremely challenging because of the elevated computational cost entailed by classical PDE solvers. On top of this, even for second-order elliptic PDEs commonly found in engineering applications, traditional projection-based reduced order models (ROMs) fail to resolve these issues, as their approximations typically suffer from oversmoothing, which makes it extremely hard to recover the local effects happening at the small scales. To address this, we propose an alternative nonintrusive strategy that combines classical proper orthogonal decomposition (POD) with a suitable neural network (NN) model to account for the small scales. Specifically, we employ sparse mesh-informed neural networks (MINNs) (1), which can handle both spatial dependencies in the solutions and in the model parameters simultaneously. We evaluate the performance of the proposed approach through a couple of benchmark experiments, and later apply it to the case of oxygen microcirculation in biological tissues (2).

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Hyper-reduced modeling of damage and plasticity: Robustness and accuracy using path-following methods

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Abstract

Simulations incorporating damage and plasticity are computationally expensive. Especially in the context of uncertainty quantification and optimization where numerous simulations have to be conducted, reduced order models (ROM) are being employed. In this contribution, the snapshot-based proper orthogonal decomposition (POD) is used to reduce the system of equations that needs to be solved repeatedly. Due to the nonlinearities of the investigated problem, the quantities that need to be recomputed in the full space in every iteration are further reduced by means of the discrete empirical interpolation method (DEIM) (1). In general, the POD-based DEIM approach leads to a hyper-reduced order model (HROM) that significantly reduces the simulation time while maintaining a certain degree of accuracy (2).

As structures with damage and plastic material behavior show phenomena such as softening and snapback, the arc-length method is utilized. The reduced form of the arc-length method leads to reduced stability of the simulation (3). Measures to counteract the complications are presented and the resulting HROM is thoroughly investigated for its robustness, efficiency and accuracy. To show the performance of the presented methodology, an application to a structural example with uncertain material parameters is presented.

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An Integrated Time-domain Approach for Gearbox Motion and Noise Prediction using Krylov Subspace MOR

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Abstract

Recent research has led to major advances in applications of Krylov subspace model order reduction (MOR) techniques for vibroacoustic simulations. A time-domain stable formulation has been derived both for bounded and unbounded domains (1,2). Further efforts to make such time-domain models more efficient have enabled their application to digital twin development of large-scale models (3,4). This paper exploits such techniques to propose a novel framework for unified motion and vibro-acoustics modeling of complex mechanical systems. In particular, the primary application tackled in this work is the simulation of sound radiated by gearboxes.

Gearbox noise prediction requires integrating multibody dynamic and vibroacoustic simulations. State-of-the-art approaches solve these physics separately, performing motion simulations in the time domain followed by frequency domain vibroacoustic analysis (5). This approach is cumbersome and computationally inefficient for several reasons. Firstly, it requires the user to switch multiple times between a motion and a vibroacoustic solver. Secondly, it requires a fast Fourier transform (FFT) to convert time-domain data to frequency domain, and an inverse FFT if time-domain acoustic results are needed (e.g. for auralization). Thirdly, the accurate simulation of inherently transient phenomena, such as ramp-up scenarios, is particularly challenging.

To address these issues, a procedure is proposed to concurrently solve motion and acoustics in the time domain using a coupled model. The approach relies on a floating frame of reference (FFR) formulation (6), inspired by flexible multibody dynamic simulations, to simultaneously capture gear motions and sound radiation. This method doesn't take into account any direct coupling between rigid body motion and acoustics. This is a good assumption in the case of a gearbox, where the vibrations of the fixed housing are considered as the only source of noise. The fine spatio-temporal resolution needed to achieve accurate results poses a key challenge. This work overcomes such computational barriers by leveraging Krylov MOR, which reduces acoustics degrees of freedom by several orders of magnitude while retaining accuracy and stability. This enables, for the first time, integrating motion simulations with high-fidelity vibro-acoustics in a single solver.

^{*}Speaker

The unified approach is demonstrated on a real-life gearbox model. Our method is validated through comparison with results obtained using separate motion and vibro-acoustic full order models in the time domain. We then demonstrate, with several numerical experiments, that the new integrated approach is both computationally more efficient and enables a simplified workflow compared to current state-of-the-art techniques for gearbox noise prediction. Other possible applications include the analysis of electric motors' noise emissions.

The proposed strategy has significant implications for multiphysics analysis, setting the stage for optimization and design exploration of low-noise systems. This could unlock numerous applications requiring integrated transient modeling of complex structural-acoustic systems, such as Executable Digital Twins.

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A Methodology for the Design of Modular Structures Based on Model Order Reduction by POD

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Abstract

Finite element analysis of complex structural systems, which can be put together from independent modules, is computationally expensive. To increase computational efficiency, we have developed a new model order reduction technique that exploits the idea of reducing substructures independently of each other (1). This means that the reduction of the degrees of freedom of the global system of equations is performed at the substructure level, i.e. modules (substructures) are reduced separately before being assembled. The dominant mechanical behavior of each individual module is represented by the POD modes, which form the projection matrix. The prediction quality of this model order reduction technique strongly depends on the selection of the sampled data. Therefore, we introduce and investigate new sampling strategies that are more suitable for the proposed method. The performance of these strategies is evaluated and measured by their ability to achieve the required model accuracy. The proposed model order reduction method is coupled with the tied contact algorithm (2) to allow for a more flexible connection of substructures. A handful of numerical examples are shown to demonstrate the suitability of the presented methodology for the design of complex modular structures.

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Projection-based model order reduction for a representative structural volume of a nuclear containment building

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Abstract

Numerical simulations play a pivotal role in aiding engineering decisions within industrial projects. This work stems from the critical need to perform extensive simulations in assessing the structural integrity of aging containment structures in nuclear power plants, focusing on large prestressed concrete structures. Recent research efforts have concentrated on realistic modeling of the thermo-hydro-mechanical (THM (1)) behavior of concrete in such structures, considering the complex thermo-activated phenomena governing the behavior of heterogeneous and porous concrete. To address this challenge, we have adopted a weak THM coupling approach, tailored to represent the delayed material deformations experienced by large structures, a valid assumption under normal operating conditions of containment buildings. As detailled above, engineers often need to repeat simulations for slightly varied configurations, introducing prohibitive costs, especially in optimization procedures relying on high-fidelity (HF) solvers for such mechanical behaviors. This works aims to devise an intrusive proper model order reduction (pMOR) procedure for mechanical simulations of double-walled power plant containment buildings, with an application to a representative structural volume of a nuclear containment building.

We propose a projection-based model order reduction approach for assessing the aging of large prestressed concrete structures. These simulations entail a multi-modeling approach, incorporating a three-dimensional nonlinear thermo-hydro-activated rheological model for concrete and a one-dimensional linear thermo-elastic model for prestressing cables. A kinematic linkage connects concrete and steel nodes, assuming coincident displacements at corresponding points. We introduce an adaptive algorithm leveraging Proper Orthogonal Decomposition (POD) and Greedy strategy (2) to construct a reduced order model (ROM). The nonlinearity of the operator entails that the computational cost of the ROM assembly scales with the size of the HF model. To mitigate this bottleneck, we present a hyper-reduction strategy based on empirical quadrature (EQ (3)), involving the construction of a reduced mesh to speed up online assembly costs of the ROM. We provide numerical results utilizing

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a widely-used industrial-grade finite element solver for structural mechanics (code_aster (4)) on a standard section of a double-walled containment building.

First, we validate our approach by reproducing HF simulation results for the same parameters without considering parametric variability. Subsequently, we extend our methodology to address parametric variations. Our numerical findings indicate the efficiency of the implemented model reduction and hyper-reduction procedures, resulting in notable speedups even with relatively coarse mesh resolutions, while maintaining satisfactory approximation accuracy for critical variables of interest, such as prestress loss in cables and sensor-measured deformations.

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EXPLORING THE POTENTIAL OF MACHINE LEARNING FOR MULTISCALE TOPOLOGY OPTIMIZATION IN STRUCTURAL DESIGN

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Abstract

In recent times, the application of artificial intelligence techniques in topology optimization methods has emerged as a vibrant area of investigation (1). These models, based on machine learning, have primarily focused on generating optimized designs directly or expediting the optimization procedures. Enhancing the resolution of structural problems at multiple scales poses a significant challenge in this domain.

This study introduces a novel approach for accelerating the fine scale topology optimization process using machine learning techniques. The multiscale topology optimization involves solving a global optimization problem for material distribution. Subsequently, the macro problem is subdivided into cells or regions where the resolution is enhanced through fine scale topology optimization in each cell. Given the potential significant number of cells, the computational cost associated with such an algorithm is substantial. To address this, we exploit the repetitive nature of cell structures and build a surrogate model that allows us to obtain the finite element solution of each cell (required for the iterative optimisation process) at a considerably reduced computational expense.

In this presentation, we present the algorithm employed for the fine scale topology optimization process, considering its limitations and performance across selected problems. Additionally, we will showcase preliminary results obtained from this methodology, along with potential application areas such as topology-optimized infill designs applicable to prosthesis or lightweight mechanical structures.

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Numerical solution of Poisson partial differential equations in high dimension using deep neural networks

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Abstract

The aim of this article is to analyze numerical schemes using two-layer neural networks with infinite width for the resolution of the high-dimensional Poisson-Neumann partial differential equations (PDEs) with Neumann boundary conditions. Using Barron's representation of the solution with a measure of probability, the energy is minimized thanks to a gradient curve dynamic on the \$2\$ Wasserstein space of parameters defining the neural network. Inspired by a work from Bach and Chizat, we prove that if the gradient curve converges, then the represented function is the solution of the elliptic equation considered. In contrast to the works of Bach and Chizat, the activation function we use here is not assumed to be homogeneous to obtain global convergence of the flow. Numerical experiments are given to show the potential of the method.

^{*}Speaker

Model reduction for non-linear structural problems with multiple contact interfaces: application to the modeling of mooring lines for floating offshore wind turbines

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Abstract

Keywords: Model reduction, PGD, frictional contact, LATIN method, DDM, wire ropes.

The context of this work concerns the simulation of the loading on a part of a mooring line of a floating offshore wind turbine in order to accurately predict its fatigue life. Mooring lines are often assembly of different material segments including spiral strand wire ropes. These ropes consist in a complex assembly of steel wires wrapped together in a twisted helical assembly of different wire layers around a single core wire. Due to their peculiar architecture, tension and bending loadings induce complex frictional phenomena between the wires that may induce fretting fatigue damage. A direct finite element analysis of the wire mechanics in order to predict fatigue life is computationally costly, since such kind of problem involves simulating the complex evolution of contact and friction conditions between the wires of the wire rope (1, 2). In order to overcome these difficulties, we will focus on model reduction methods but also on domain decomposition methods in order to efficiently deal with the multiscale content of a non-linear problem with multiple contact interfaces.

The main challenges of the problem derive from the large number of frictional contact interactions in such application. Indeed, a reduced-order model may not efficiently capture and represent singular and propagating phenomena at the contact interfaces, such as long frictional cracks, macro sliding, sliding fronts and contact detachment between the wires.

In literature one can cite a posteriori approaches with reduced basis enrichment such as the non-negative matrix factorization method (3) or the cone-projected greedy algorithm (4). A priori methods, which build the reduced basis on the fly throughout the computation, rely on the Proper Generalized Decomposition (PGD) (5) in the framework of the LATIN non-incremental nonlinear solver (6). In this work, the proposed strategy aims at solving

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the frictional contact between the spiral strand wires in a robust and efficient way. It combines the following techniques : 1) Domain Decomposition Methods (DDM), in particular the mixed DDM based on the LATIN method (2), 2) a priori model reduction based on the PGD. This approach will be investigated in order to reduce the computational cost of the analyses.

In this context, the first step is to investigate the potential reducibility of the addressed problem. An a posteriori SVD analysis has been performed on the solution of a tension and bending calculation on a metric cable section developed in (1, 2) subjected to small-amplitude oscillating loads around a pre-loaded state. A general good potential for reducibility for the different contact quantities (normal contact forces, frictional forces, inter-wire slip) is observed, due to the small variations in contact conditions induced by the particular loading. The outermost layers result to be the most critical especially for frictional forces, where bending effects are more pronounced and the contact conditions are more variable. Space modes depict a multi-scale behaviour with first global structural modes and subsequent localized modes around the sliding zones. This suggests that a multiscale computational strategy may be beneficial.

Thereafter academic examples which are representative of the physical problem at hand have been investigated with the proposed approach. A one-dimensional benchmark model of a wire of the wire rope, subjected to traction and pressure and in contact with a frictional interface, has been analyzed to highlight how the introduction of domain decomposition, allowing for the separation of sticking and sliding zones, allows for more efficient creation of local reduced bases in order to be more accurate in areas where it is needed. The analysis also shows that domains with similar contact conditions present similar modes, which suggests the idea of sharing reduced bases in order to improve efficiency. The introduction of a proper coarse-scale problem for the DDM strategy allows to improve performances.

Finally, the LATIN-based multiscale mixed DDM with PGD (7, 8) is applied to two-dimensional benchmark contact problems, representative of a layer of wires of the wire. It is shown to what extent the DDM coarse-scale problem and the introduction of the PGD, which builds reduced basis per subdomain, can be efficient in the case of multiple contact interfaces.

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