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Editorial: Data-driven modeling and optimization in fluid dynamics: From physics-based to machine learning approaches

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Editorial on the Research Topic
Data-driven modeling and optimization in fluid dynamics: From physics-based to machine learning approaches

Data-driven modeling has made a dramatic impact in computational science and engineering and, in particular, in computational fluid dynamics (CFD). One of the earliest uses of data in CFD is the proper orthogonal decomposition (POD), which was introduced by Lumley and his collaborators more than half a century ago. POD is based on a simple yet powerful idea: In the classical Galerkin framework (used in standard numerical methods, e.g., finite element or spectral methods), replace the general purpose basis functions with data-driven basis functions. This very simple idea has made a profound impact in CFD, reducing the computational cost of standard numerical methods by orders of magnitude and enabling challenging numerical simulations in shape optimization, flow control, and uncertainty quantification. Since Lumley's pioneering work, the field of data-driven modeling has witnessed a tremendous development. Probably the most exciting research area in this field is the use of machine learning. Over the last decade, the focus in data-driven modeling has shifted from physics-based strategies to machine learning approaches, in which instead of merely changing different components of classical methods (e.g., changing the basis in POD), one completely overhauls the entire framework (e.g., instead of using a Galerkin framework, one leverages machine learning algorithms to determine all the model operators).

At this point, one natural question is which strategy should be used in CFD? Should one use physics-based or machine learning models? We believe that, as is often the case when discussing numerical methods, the truth is somewhere in the middle. That is, we believe that data-driven models that combine the physical and mathematical insight with machine learning strategies can revolutionize CFD and break new barriers in shape optimization, flow control, and uncertainty quantification. This Research Topic, which consists of 10 articles written by leaders in the field, surveys recent developments in data-driven modeling in CFD, covering a spectrum of modeling strategies, from physics-based to machine learning modeling.

Kaneko and Fischer put forth an augmented-basis method (ABM) to stabilize reduced order models (ROMs) of turbulent incompressible flows. The new strategy augments the classical POD basis functions with divergence-free projections of a subset of the nonlinear interaction terms that constitute a significant fraction of the time-derivative of the solution. The numerical investigation shows that the ABM outperforms the standard ROM and the Leray regularized ROM. Huang et al. propose a component-based domain-decomposition framework for the modeling of large-scale systems that cannot be directly accessed using the high-fidelity simulations (e.g., rocket engines or wind farms). The new framework decomposes the full system into different components, each of which can flexibly adopt different modeling strategies (e.g., reduced order modeling or full order modeling), balancing physical complexity with accuracy requirements. The authors investigate the new framework in the numerical simulation of complex flows involving combustion dynamics. Tsai and Fischer propose a time-averaged error indicator for regularized ROMs of two-dimensional unsteady natural convection in a high-aspect ratio slot parameterized with the Prandtl number, Rayleigh number, and slot angle with respect to the gravity. The authors show that the Leray-regularized ROMs provide a robust strategy for this class of flows. Chan et al. show that, for variable density flows with under-resolved features, there are differences in robustness between entropy stable schemes which incorporate the entropy projection and those which do not. These differences in robustness are observed to depend on the density contrast and persist across a range of polynomial degrees, mesh resolutions, and types of discretization. Chacón Rebollo et al. propose a new low-rank tensorized decomposition (LRTD) to approximate the solution of parametric non-symmetric elliptic problems. Furthermore, they prove that the truncated LRTD expansion strongly converges to the parametric solution. Finally, the numerical investigation for convection-diffusion problems supports the theoretical developments and illustrates the computational efficiency of the new algorithm.

Schmekel et al. use data from a direct numerical simulation (DNS) of a turbulent channel flow to train a convolutional neural network (CNN) and predict the number and volume of the coherent structures in the channel over time. The numerical investigation shows that the proposed CNN accurately predicts the temporal evolution of the coherent structures and displays very good agreement with the reference data. Jacobsen and Duraisamy utilize variational autoencoders (VAEs) for nonlinear dimension reduction to disentangle the low-dimensional latent variables and identify independent physical parameters that generated the data. A disentangled decomposition is interpretable and can be transferred to, e.g., design optimization and probabilistic reduced order modeling. To characterize the training process of the VAEs and to study disentanglement, the authors use a porous media flow modeled by the two-dimensional steady-state Darcy equations. Popov and Sandu propose a significant improvement of the multifidelity ensemble Kalman filter (MFEnKF), which combines a full order physical model and a hierarchy of reduced order surrogate models to increase the computational efficiency of data assimilation. In this new strategy, the linear framework is generalized to leverage nonlinear projection and interpolation operators implemented using autoencoders. The new approach, named NL-MFEnKF, enables the use of a much more general class of surrogate models than MFEnKF. Heaney et al. combine nonintrusive reduced order modeling (NIROM) and domain decomposition to enable ROMs to make predictions for unseen scenarios. The authors successfully test the new strategy in the numerical simulation of chaotic time-dependent flow of air past buildings. Heiland et al. propose the use of CNNs and POD to construct very low-dimensional linear parameter varying (LPV) approximations to the incompressible Navier-Stokes equations (NSE). These LPV approximations could be leveraged in challenging NSE control applications. The authors illustrate their theoretical developments in the numerical simulation of a two-dimensional flow around a cylinder.

The 10 articles in this Research Topic survey recent developments in data-driven modeling in CFD, with a particular emphasis on turbulent flows. This is an exciting research area, with many open problems and grand challenges waiting to be addressed.

Author contributions

TI, MB, and LR contributed to this editorial.

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