



Numerical Analysis Seminar

Physics-guided interpretable data-driven simulations

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Abstract

A computationally expensive physical simulation is a huge bottleneck to advance in science and technology. Fortunately, many data-driven approaches have emerged to accelerate those simulations, thanks to the recent advancements in machine learning (ML) and artificial intelligence. For example, a well-trained 2D convolutional deep neural network can predict the solution of the complex Richtmyer–Meshkov instability problem with a speed-up of 100,000x [1]. However, the traditional black-box ML models do not incorporate existing governing equations, which embed underlying physics, such as conservation of mass, momentum, and energy. Therefore, the black-box ML models often violate important physics laws, which greatly concern physicists, and require big data to compensate for the missing physics information. Additionally, it comes with other disadvantages, such as non-structure-preserving, computationally expensive training phase, non-interpretability, and vulnerability in extrapolation. To resolve these issues, we can bring physics into the data-driven framework. Physics can be incorporated into different stages of data-driven modeling, i.e., the sampling stage and model-building stage. Physics-informed greedy sampling procedure minimizes the number of required training data for a target accuracy [2]. Physics-guided data-driven model better preserves the physical structure and is more robust in extrapolation than traditional black-box ML models. Numerical results, e.g., hydrodynamics [3,4], particle transport [5], plasma physics, and 3D printing, will be shown to demonstrate the performance of the data-driven approaches. The benefits of the data-driven approaches will also be illustrated in multi-query decision-making applications, such as design optimization [6,7].

Reference

- [1] Jekel, Charles F., Dane M. Sterbentz, Sylvie Aubry, Youngsoo Choi, Daniel A. White, and Jonathan L. Belof. "Using Conservation Laws to Infer Deep Learning Model Accuracy of Richtmyer-meshkov Instabilities." arXiv preprint arXiv:2208.11477 (2022).
- [2] He, Xiaolong, Youngsoo Choi, William D. Fries, Jon Belof, and Jiun-Shyan Chen. "gLaSDI: Parametric Physics-informed Greedy Latent Space Dynamics Identification." arXiv preprint arXiv:2204.12005 (2022).
- [3] Copeland, Dylan Matthew, Siu Wun Cheung, Kevin Huynh, and Youngsoo Choi. "Reduced order models for Lagrangian hydrodynamics." *Computer Methods in Applied Mechanics and Engineering* 388 (2022): 114259.
- [4] Kim, Youngkyu, Youngsoo Choi, David Widemann, and Tarek Zohdi. "A fast and accurate physics-informed neural network reduced order model with shallow masked autoencoder." *Journal of Computational Physics* 451 (2022): 110841.
- [5] Choi, Youngsoo, Peter Brown, William Arrighi, Robert Anderson, and Kevin Huynh. "Space-time reduced order model for large-scale linear dynamical systems with application to Boltzmann transport problems." *Journal of Computational Physics* 424 (2021): 109845.
- [6] McBane, Sean, and Youngsoo Choi. "Component-wise reduced order model lattice-type structure design." *Computer methods in applied mechanics and engineering* 381 (2021): 113813.
- [7] Choi, Youngsoo, Gabriele Boncoraglio, Spenser Anderson, David Amsallem, and Charbel Farhat. "Gradient-based constrained optimization using a database of linear reduced-order models." *Journal of Computational Physics* 423 (2020): 109787.

Date:	Sept 14, 2023 (Thursday)
Time:	11:00am - 12:00noon
Venue:	ZOOM: https://hku.zoom.us/j/ Meeting ID: 913 6532 3891 Password: 310656

All are welcome