Other - Colloquium on Artificial Intelligence Research and Optimization

Physics-constrained data-driven physical simulations, using machine learning

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March 02, 2022 - 03:00 pm

Abstract:

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A data-driven model can be built to accurately accelerate computationally expensive physical simulations, which is essential in multi-query problems, such as inverse problem, uncertainty quantification, design optimization, and optimal control. In this talk, two types of data-driven model order reduction techniques will be discussed, i.e., the black-box approach that incorporates only data and the physics-constrained approach that incorporates the first principle as well as data. The advantages and disadvantages of each method will be discussed. Several recent developments of generalizable and robust data-driven physics-constrained reduced order models will be demonstrated for various physical simulations as well. For example, a hyper-reduced time-windowing reduced order model overcomes the difficulty of advection-dominated shock propagation phenomenon, achieving a speed-up of O(20~100) with a relative error much less than 1% for Lagrangian hydrodynamics problems, such as 3D Sedov blast problem, 3D triple point problem, 3D Taylor–Green vortex problem, 2D Gresho vortex problem, and 2D Rayleigh–Taylor instability problem. The nonlinear manifold reduced order model also overcomes the challenges posed by the problems with Kolmogorov's width decaying slowly by representing the solution field with a compact neural network decoder, i.e., nonlinear manifold. The space–time reduced order model accelerates a large-scale particle Boltzmann transport simulation by a factor of 2,700 with a relative error less than 1%. Furthermore, successful application of a physics-constrained data-driven method for meta-material lattice–structure design optimization problems will be presented. Finally, the library for reduced order models, i.e., libROM (https://www.librom.net), and its webpage and several YouTube tutorial videos will be introduced. They are useful for education as well as research purpose.

Speaker's Bio:

Youngsoo is a computational math scientist in CASC under Computing directorate at LLNL. He is currently leading data-driven reduced order model development team for various physical simulations, with whom he developed the open source codes, libROM (https://www.librom.net) and LaghosROM (https://github.com/CEED/Laghos/tree/rom/rom). libROM is a library for reduced order models and LaghosROM implements reduced order models for Lagrangian hydrodynamics (https://authors.elsevier.com/c/1e3CuAQEIviQh). He has earned his undergraduate degree for Civil and Environmental Engineering from Cornell University with applied mathematics as minor and his PhD degree for Computational and Mathematical Engineering from Stanford University. He was a postdoc in Sandia National Laboratory and Stanford University prior to joining LLNL in 2017.

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