Rigorous component-based coupling of first-principles and data-driven models

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This talk will describe several recent advancements in developing a rigorous mathematical framework for the domain decomposition-based coupling of arbitrary combinations of first-principles numerical methods with data-driven models under the flexible Heterogeneous Numerical Methods (fHNM) project at Sandia National Laboratories. After giving a high-level overview of this project and its research vision, we will take you on a deep dive into two of the coupling methods pursued under fHNM as they relate to the coupling of projection-based reduced order models (ROMs) with each other and with conventional full order models (FOMs): (1) alternating Schwarz-based coupling, and (2) coupling via generalized mortar methods (GMMs).

In the first part of the talk, we will discuss a recent extension of the Schwarz alternating method [1,2] that enables the creation of FOM-ROM and ROM-ROM couplings from nonlinear monolithic problems. This method works by performing an overlapping or non-overlapping domain decomposition (DD) of the physical domain, and solving a sequence of problems on these subdomains, with information propagating through carefully-constructed transmission conditions on the subdomain boundaries [3]. We will showcase recent results obtained by implementing this method in the open-source Pressio demo-apps library. Time-permitting, we will summarize our experience in applying the method to couple subdomain-local Physics-Informed Neural Networks (PINNs) with each other and with FOMs [4].

In the second part of the talk, we will present a new partitioned method that enables FOM-ROM and ROM-ROM coupling following a non-overlapping DD of the physical domain. At the crux of this method is a dual Schur complement system, which implicitly expresses a Lagrange multiplier, representing the interfacial flux, in terms of the state variables [5]. The solution of the Schur complement system and the application of an explicit time-stepping scheme allow for the subdomain equations to be decoupled and independently solved at each time step. Time-permitting, we will briefly mention some recent work that mitigates the cost of solving the required Schur complement problem by replacing it with a pre-trained Dynamic Mode Decomposition (DMD) or neural ODE (nODE) model.

We evaluate the new coupling methods on canonical test cases from several applications. Our results demonstrate that the proposed coupling methodologies are computationally efficient and capable of coupling disparate models without introducing numerical artifacts into the solution. Importantly, our results suggest that FOM-ROM and ROM-ROM couplings of the sort considered have the potential of improving the predictive viability of projection-based ROMs, by enabling the spatial localization of ROMs (via domain decomposition) and the online integration of high-fidelity information into these models (via FOM coupling). Sandia National Laboratories is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

References

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