Component-based coupling of first-principles and data-driven models

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This poster describes several recent advancements in developing a rigorous mathematical framework for the domain decomposition- (DD-)based coupling of arbitrary combinations of first-principles numerical methods with projection-based reduced order models (ROMs). Three coupling frameworks are detailed: (1) alternating Schwarz-based coupling, (2) optimization-based coupling, and (3) coupling via generalized mortar methods (GMMs). The first two methods are iterative in nature, whereas the third method is monolithic.

The first approach, the Schwarz alternating method, works by performing an overlapping or non-overlapping 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. The second approach, optimization-based coupling, performs a non-overlapping DD of the physical domain and minimizes the difference between the solutions on the subdomain interfaces subject to the governing partial differential equations (PDEs) as constraints. The final approach, also based on a non-overlapping DD, imposes solution and flux continuity along subdomain interfaces weakly using Lagrange multipliers, and solves a Schur complement system for the Lagrange multiplier update at each time-step. We demonstrate that the subdomain equations can be decoupled through the application of an explicit time-stepping scheme, and that the cost of solving the Schur interface problem can be mitigated using Dynamic Mode Decomposition (DMD) or neural ODE (nODE) interface flux surrogates.

We evaluate the new coupling methods on several challenging test cases. Our results demonstrate that the proposed coupling methodologies are computationally efficient and capable of coupling disparate models without introducing numerical artifacts into the solution.