Accelerating mod/sim workflows through hybrid domain decomposition-based models and the Schwarz alternating method

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Multi-scale methods are essential for the understanding and prediction of the behavior of engineering systems when a small-scale event will eventually determine the performance of the entire system. In this talk, I will discuss a novel recently-proposed [1,2] approach that enables concurrent multi-scale coupling in finite deformation quasistatic and dynamic solid mechanics by leveraging the domain decomposition-based Schwarz alternating method. The approach is based on the simple idea that, if the solution to a partial differential equation (PDE) is known in two or more regularly shaped domains comprising a more complex domain, these local solutions can be used to iteratively build a solution for the more complex domain. The proposed methodology has a number of advantages over competing multiscale coupling methods, most notably its concurrent nature, its ability to couple non-conformal meshes with different element topologies and different time integrators with different time steps for dynamic problems all without introducing non-physical artifacts into the solution, and its non-intrusive implementation into existing codes.

In the first part of the talk, I will describe the formulation and theoretical properties of the Schwarz alternating method as a means for concurrent multiscale coupling of conventional high-fidelity finite element models in quasistatic and dynamic solid mechanics. I will show several large-scale numerical examples demonstrating the method's numerical properties and convergence based on its implementation in two massively-parallel HPC codes: Albany/LCM and Sierra/Solid Mechanics. I will demonstrate the method's power in accelerating mod/sim workflows and enabling multi-query analysis by simplifying greatly the task of meshing complex multi-scale geometries.

The Schwarz alternating method has the advantage that it can couple not only different discretizations but also different solvers/model types. In the second part of the talk, I will discuss a recent extension of the Schwarz alternating method to enable coupling of conventional full order models (FOMs) with projection-based reduced order models (ROMs), and projection-based ROMs with each other [3], towards enabling the "plug-and-play" integration of data-driven models into existing multi-scale and multi-physics coupling frameworks with minimal intrusion. The new approach is based on the following ingredients: (i) a decomposition of the physical domain of interest into two or more overlapping or non-overlapping subdomains, (ii) the construction of either a FOM or a projection-based ROM in each of the subdomains, (iii) the definition of appropriate transmission boundary conditions (BCs) which will propagate information between the overlapping subdomains, and (iv) the introduction of a Schwarz iteration process in which the ROM and FOM solutions on each subdomain are successively updated (to convergence) in an iterative manner. I will demonstrate on some numerical examples that the proposed methodology has 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). I will additionally demonstrate that cost savings are possible by introducing additional parallelism into the algorithm through concurrent subdomain solves, i.e., additive Schwarz.

References

[1] A. Mota, I. Tezaur, C. Alleman. “The alternating Schwarz method for concurrent multi-scale coupling”, Comput. Meth. Appl. Mech. Engng. 319 (2017) 19-51.

[2] A. Mota, I. Tezaur, G. Phlipot. “The Schwarz alternating method for dynamic solid mechanics”, Int. Meth. Numer. Meth. Engng. 121 (21) (2022) 5036-5071.

[3] J. Barnett, I. Tezaur, A. Mota. "The Schwarz alternating method for the seamless coupling of nonlinear reduced order models and full order models", in Computer Science Research Institute Summer Proceedings 2022, S.K. Seritan and J.D. Smith, eds., Technical Report SAND2022-10280R, Sandia National Laboratories, 2022, pp. 31-55. https://arxiv.org/abs/2210.1255