Optimizing the computational Rubik's cube: Balancing numerics, performance, and abstractions in multimodel solvers

Vijay S. Mahadevan* **and Lois Curfman McInnes†**

*,† Mathematics and Computational Science Division
Argonne National Laboratory (ANL)
9700 S. Cass Avenue
Lemont, IL, 60439, USA.
e-mail: mahadevan@anl.gov, curfman@mcs.anl.gov

ABSTRACT

The computational needs of coupled multiphysics and multiscale solvers are complex and may sometimes require sacrificing algorithmic performance for enhancing numerical accuracy or stability, especially when bringing together implementations that are not necessarily written within a common software infrastructure. For instance, in nuclear engineering and climate science problems, because of the sheer number of physical model definitions and their nonlinear field interactions, well-designed software abstractions are essential in order to integrate single-physics model implementations into a cohesive multiphysics solver for HPC machines. In such cases, research scientists need to make informed decisions about optimal algorithmic options that work in conjunction with the right physical and numerical approximations [1] in order to maximize efficacy (computational time to solution vs numerical accuracy).

General multiphysics solvers need to encompass and expose options for analyzing, testing, and comparing different coupling schemes with varying numerical stability and accuracy traits within a unified platform. However, design of such software can become complicated when the infrastructures for vectors, matrices, Krylov solvers, and unstructured meshes are not shared between the physics components. Flexible abstractions or adaptors are hence required to translate between these fundamental linear algebra or topological representations in order to alleviate concerns about data layout and movement between models in a consistent fashion, without affecting the ability to concurrently execute various coupling schemes.

Expressing the global coupled spatiotemporal problem as a blocked system of nonlinear algebraic equations (at least conceptually), regardless of the individual subsystem implementation, can allow for using balanced approximations that can seamlessly tackle problems spanning different physical regimes. We use these ideas to present potential variations in coupling (explicit, semi-implicit or fully implicit) schemes that can be implemented, by building on a flexible multimesh projection and hierarchical nonlinear solver framework, made possible through carefully designed software kernels and interfaces [2]. We also investigate whether one can deliver sustained and portable performance on various architectures without sacrificing discretization and solver accuracy, if the appropriate coupling kernel abstractions are chosen to maximize concurrency. Building on such flexible designs can help shield scientific software from variations in problem settings, new physics needs, heterogeneous hardware environments, and so forth, thereby boosting overall research productivity of computational scientists.

REFERENCES

[1] Keyes, D. E., et al. Multiphysics simulations: Challenges and opportunities. *Int. J. High. Perf. Comp. Appln.* (2013) **27**(*1*): 4–83.

[2] Larson, J. W. Ten organising principles for coupling in multiphysics and multiscale models. *ANZIAM Journal*, (2009) **48**:1090-1111.