Robust Quasi-Newton Methods for the Coupling of Partitioned Multi-Physics Simulations within the Parallel Coupling Software preCICE.

Klaudius Scheufele*, **Miriam Mehl*** **and Florian Lindner***

* Institute of Parallel and Distributed Systems (IPVS)
University of Stuttgart
Universitätstraße 38, 70569 Stuttgart, Germany
e-mail: klaudius.scheufele@ipvs.uni-stuttgart.de,

ABSTRACT

While allowing for higher accuracy and more realistic results, multi-physics simulations induce challenges such as multi-scale effects, instabilities, and moving geometries. By breaking up multi-physics simulations into single-physics problems, we gain full flexibility in adding or exchanging model parts and reusing existing solvers. preCICE is a library for flexible numerical coupling of single-physics solvers. It uses a partitioned black-box coupling approach, thus requiring only minimal access to existing solvers, which fosters quick and effortless coupling. Inter-solver parallelism and parallel communication techniques help to exploit the massively parallel capabilities of current and future HPC machines. Communication between coupling participants is done in a decentralized fashion by a peer to peer approach thus minimizing blocking barriers in the process. Data mapping between non-conformal meshes is done via radial-basis-function interpolation. The actual coupling is realized in an implicit way (i.e., retrieving the monolithic solution) using fixed-point equation solvers at the coupling surface in every time step. preCICE offers different schemes and fixed-point acceleration methods to cope with inherent instabilities and strong interactions. Quasi-Newton methods that only use input/output relations from the solvers turned out to be particularly suited. We compare two types of quasi-Newton methods with respect to convergence speed, robustness and parallel performance. The first type is known as IQN-ILS [1] and is a matrix-free method. Explicit incorporation of passed information into the secant equation can in some cases greatly improve the performance. This introduces a further degree of freedom that is highly problem dependent. Re-using too much passed information may lead to a highly ill-conditioned system and numerical breakdown. We use efficient filtering methods to eliminate 'bad' information. This leads to a more robust and almost parameter-free method if we re-use an (infinitely) large number of passed information together with the said powerful filter. The second type is a generalized Broyden method [2] that incorporates previous information implicitly in the approximation process without additional tuning of parameters. Yet, this comes at the price of explicitly storing an explicit the Jacobian matrix which induces quadratic complexity. To solve this issue, we present an efficient restart alternative based on a low rank approximation of the Jacobian [3]. This yields a robust and parameter free linear complexity algorithm and good parallel efficiency. Both quasi-Newton methods are judged against a true Newton solver in terms of robustness and convergence properties for a simple one-dimensional flexible tube scenario.

REFERENCES

[1] J. Degroote, K.-J. Bathe, and J. Vierendeels. Performance of a new partitioned procedure versus a monolithic procedure in fluid-structure interaction. C & S, 87(11-12):793801, 2009

[2] A.E.J. Bogaers, S. Kok, B.D. Reddy, and T. Franz. Quasi-Newton methods for implicit black-box FSI coupling. Comput Methods Appl Mech Eng, 279:113132, September 2014.

[3] K. Scheufele and M. Mehl. Robust Multi-Secant Quasi-Newton Variants For Parallel Fluid-Structure Simulations – And Other Multi-Physics Applications. SIAM SISC SI 2016, sub.