

QN and RBF -- Two Universal Coupling Components and their Efficient Implementation

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ABSTRACT

QN and RBF, in the long form quasi-Newton and radial basis functions, are classes of methods that allow to tackle two issues in multi-physics simulations: QN can be used to set up fast converging outer iterative schemes in a multi-physics simulation involving separate pieces of software for each of the ‘physics’. RBFs can provide a discretization-independent mapping method at non-matching interfaces. If they are combined in a smart way, implemented using sophisticated algorithms, and enhanced with an efficient MPI- or socket-based inter-code point-to-point communication, they allow to establish multi-physics simulation environments in a very easy, flexible, and efficient way on high performance computing architectures. This can even be done based on black-box solvers. Thus, one can fully exploit the efficiency and functionality of existing solvers without any re-implementation or new implementation of the single-physics solvers. We’ve implemented different variants of QN and RBF in the coupling library preCICE (www.precice.org), which has been developed over the last years collaboratively in the groups in Stuttgart and Munich.

Although the potential of QN has been recognized and exploited very early, the commonly used variants still had several drawbacks: they did not allow for inter-solver parallelism and required the tuning of unknown parameters in a costly try-and-error manner. Radial basis function mappings suffered from the global support of the basis functions resulting in a linear system with dense system matrix and either poor approximation accuracy or very high condition numbers of the interpolation system. We present optimized and modified versions of both methods along with parallel and scalable algorithms for all numerical components and their implementation in the coupling tool preCICE. preCICE fully exploits parallelism within the solvers, within the coupling numerics, and between the solvers. Numerical results show the efficiency and robustness of the coupling for various applications.

REFERENCES

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