On Scalable Multiphysics Solvers

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ABSTRACT

The largest runs up-to-now are usually performed for simple symmetric positive definite systems. It is a reasonable approach when measuring the overall scalability of an algorithm/implementation. However, in order to have an impact in science and industry, we must extend scalability to the most challenging applications, since these are the ones that really require extreme scale simulation tools, e.g., multiscale, multiphysics, nonlinear, and transient problems. In this talk, we will discuss some of our experiences in the development of FEMPAR, an in-house finite element multiphysics and massively parallel simulator.

On one hand, we will talk about how to deal in a parallel element-based environment with multiphysics simulations that involve interface coupling, e.g., fluid-structure interaction. Our approach is based on the partition of topological meshes, and ghost element information, in order to define locally the degrees of freedom and the unknowns that must be communicated among processors.

On the other hand, we will discuss how we deal with the resulting multiphysics (non)linear systems. We have two different approaches to the problem: block preconditioning and monolithic solvers. Block preconditioning techniques are interesting in the sense that they allow us to decouple complex multiphysics problems into simpler (probably) one physics simulations. However, in order for block preconditioners to be effective, we must define effective approximation of Schur complement systems, which can be a complicated (and very heuristic) task. We will show how we have implemented complex (recursive) block preconditioning strategies in FEMPAR using abstract definitions of operators, and how this framework has been applied to different multiphysics solvers.

We will also discuss how we can reach sustained scalability up to large core-counts (about 400,000 cores in a BG/Q). Our in-house numerical linear algebra solvers are based on multilevel domain decomposition techniques, and their very efficient practical implementations based on overlapped and asynchronous techniques. We will consider two different approaches, the first one being a combination of block-preconditioning and multilevel domain decomposition, whereas the second one will be a truly monolithic domain decomposition approach.

Many multiphysics simulations are also multiscale, and the use of adaptively refined meshes can reduce even orders of magnitude the computational cost of simulations with respect to uniformly refined meshes. The possibility to reach extremely scalable adaptive multiphysics solvers would open the door to unprecedented simulations of challenging problems that are out of reach nowadays. In this sense, we will show how we are dealing with scalable adaptive solvers in FEMPAR, via a combination of the p4est library for parallel mesh refinement and dynamic load balancing in our element-based framework. Further, we will show how we modify our solvers to deal with nonconforming meshes through interfaces, and the effect of cheap space-filling curve partitions on solver robustness.