Selection optimization for solvers of simulations

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Many important application problems are modeled mathematically by partial differential equations (PDEs), i.e., equations describing the interaction and evolution of quantities and their derivatives. In general, no solution formulae exist for PDEs. Hence, numerical schemes must be employed to express the problem at hand in computer-tractable form and to compute (approximate) solutions. Different applications typically lead to different requirements, e.g., maximizing accuracy in safety-critical scenarios, or minimizing runtime in weather prediction.

The process of solving a partial differential equation starts with discretization, and solving the resulting linear equation system. To solve a linear equation system you have to choose a solver scheme, including an iterative solver and a performance enhancing preconditioner. In our work we focus on the solver class of Krylov subspace methods (e.g. Conjugate Gradient [1], Generalized minimal residual method [3]) with suitable preconditioners (e.g. dual threshold incomplete LU factorization [4]). Some of these solver schemes even require a problem dependent adaption through parameter selection.

The choice of which scheme to use and how to set its parameters depends on the requirements and goals of the application at hand. Furthermore a selection can only be slightly justified a priori and therefore needs extensive data collection [2] or is done in a manner of try and error. This means that a good selection does not ensure an optimal selection and depends on the experience of the researcher. We present a new approach to automate and optimize the selection that gives us the opportunity to reuse data as requirements and optimization goals change.

References

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