Andrew Yeckel

Multiphysics challenges for the modeling of melt crystal growth systems

Department of Chemical Engineering and Materials Science
University of Minnesota
421 Washington Ave SE
Minneapolis
MN 55406-0132
yecke003@umn.edu
Lisa Lun
Hui Xie
Yousef Saad
Jeffrey J. Derby

Melt crystal growth presents several major challenges in numerical analysis of continuum mechanics, particularly in three-dimensional formulations. Problem complexity presents a significant technical challenge, requiring the integration of a large-scale furnace model with a strongly-coupled multiphysics transport problem of the Stefan moving-boundary type. Problem nonlinearity can be severe, due to high-temperature radiation heat transfer effects and strong, richly structured laminar flows of a transitional nature. Robust computing of steady-state solutions under these conditions can be achieved by Newton-Raphson iteration, but its desirable quadratic convergence property relies on our ability to compute a sufficiently accurate approximation to the inverse of a Jacobian matrix of the global system of equations. In addition, problem scaling in three dimensions weighs heavily in favor of iterative over direct solvers for this task, but developing effective solution methods is faced with several distinct challenges, three of which will be discussed here. All relate to reductions of the global, linearized system that are either advantageous, or forced by circumstance, in high-performance computing situations.

Due to time constraints, the first two challenges will only briefly be discussed. The first is finding an effective preconditioner for the incompressible Navier-Stokes equations for a closed, buoyancy-driven flow at high Rayleigh number. In mathematical terms, the Jacobian is made strongly skew by the temperature coupling in the Boussinesq term in the flow equations, an effect that habitually causes the iterative solver to stall. In physical terms, it is difficult to design physics-based preconditioners for these flows, which lack any obvious geometric simplification due to their tendency towards flow separation and steep internal layers. A block Jacobi/ILU(0)-based approach is tested and found to be limited in use to Rayleigh numbers well below those encountered in crystal growth practice, forcing us to seek alternatives.

The next challenge is the effect of the implicit constraint between temperature and problem geometry at the moving boundary of the Stefan problem. This too causes severe stalling of the iterative solver. Here the problem coupling is isolated to a few equations that determine the position of the crystal-melt interface, and it is possible to take advantage of a Schur complement-based reduction of the problem to develop a sequential iteration between geometry and temperature that results in linear systems much easier to solve than the full system. Since this iteration formulation is based on the full system of equations, the robustness of a strongly coupled approach can be attained that improves upon a simple fixed-point iteration.

The third challenge, which will be the primary focus of this presentation, is the complexity of the global simulation problem, for which it is costly to develop monolithic software that simultaneously represents all chosen phenomena at all scales in a single model. From a practical standpoint, problems of this scope favor a partitioned approach, in which a few major subdomains of the problem are tackled independently by existing software best suited to the task. The most powerful techniques are those that can be applied when the equations are solved by black-box computer codes that allow no intervention in their algorithms. Such methods can be used to link together existing best-in-class tools to tackle complex multiphysics and multiscale problems, without requiring extraordinary programming effort.

Towards this end, we have developed an approximate block Newton method to couple arbitrary black-box nonlinear solvers. This ABN method preserves the quadratic approximation properties of exact Newton iteration. The notion of a solver is abstract, encompassing any interpolations or other transformations of data exchanged between solvers. It is shown that the method behaves like a Newton iteration preconditioned by an inexact Newton solver derived from subproblem Jacobians. The method is demonstrated on several conjugate heat transfer problems modeled after melt crystal growth processes. Whereas a typical block Gauss–Seidel iteration fails about half the time for the model problems, quadratic convergence is achieved by the ABN method under all conditions studied.

This work has been supported in part by a seed grant from the Minnesota Supercomputing Institute and by the Department of Energy, National Nuclear Security Administration, under Award Numbers DE-FG52-06NA27498 and DE-FG52-08NA28768, the content of which does not necessarily reflect the position or policy of the United States Government, and no official endorsement should be inferred.