Advancing parabolic operators in thermodynamic MHD models: Explicit super time-stepping versus implicit schemes with Krylov solvers

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ABSTRACT

We explore the performance/scaling of using explicit super time-stepping (STS) algorithms versus implicit schemes with Krylov solvers for integrating parabolic operators in thermodynamic MHD models of the solar corona. Specifically, we compare the second-order Runge-Kutta Legendre (RKL2) STS method with implicit backward Euler computed using the preconditioned conjugate gradient (PCG) solver with both a point-Jacobi and a non-overlapping domain decomposition ILU0 preconditioner. The algorithms are used to integrate a scalar operator (anisotropic Spitzer thermal conduction) and a vector operator (artificial kinematic viscosity) at time-steps much larger than the explicit Euler limit. A key component of the comparison is the use of a real-world simulation on large HPC systems, with special attention placed on the parallel scaling of the algorithms. It is shown that, for the specific problem and model used, the RKL2 method generally surpasses the implicit method with PCG solvers in performance and scaling, but suffers from accuracy limitations in some localized regions of the grid.

Keywords

Algorithm scaling, Super time-stepping, Iterative solvers, Magnetohydrodynamics, Solar corona

1. INTRODUCTION

When simulating complex physical systems, very often there are processes that act on widely different time-scales which can make integrating the system computationally unfeasible. For simulating the Solar corona with a magnetohydrodynamic (MHD) model, many varied time-scales exists including the plasma flow speed, slow and fast magnetosonic wave speeds, the Alfvén wave speed, resistivity, kinematic viscosity, and thermal conduction. In addition to the physical time-scales involved, there also exists numerical time-step restrictions which must be adhered to for stability of explicit finite difference algorithms (such as the Euler method) and are a function of grid cell size.

There exists a number of methodologies which allow for the violation of some or all of the explicit numerical time-step restraints when integrating the MHD equations. For the highly restrictive parabolic operators, they are first isolated through operator-splitting so they can be treated separately as

$$\frac{\partial \mathbf{u}}{\partial t} = F(\mathbf{u}), \qquad (1)$$

where F is the parabolic operator acting on the variable $\mathbf{u}$. This poster explores the efficiency of two methods for integrating the most time-consuming parabolic operators: thermal conduction $[1/\rho\,\nabla\cdot(\kappa_0\,T^{5/2}\,\hat{\mathbf{b}}\hat{\mathbf{b}}\cdot\nabla T)]$ and viscosity $[1/\rho\,\nabla\cdot(\nu\rho\nabla\mathbf{v})]$. These are (1) an implicit scheme with Krylov solvers and (2) a super time-stepping scheme. We describe both methods, and (after a simple validation of results) show performance and scaling results for a real-world Solar coronal simulation on two HPC systems (SDSC's Comet and TACC's Stampede).

2. IMPLICIT BACKWARD EULER SOLVED WITH PRECONDITIONED CONJUGATE GRADIENT

One of the easiest-to-implement L-stable implicit methods for integrating Eq. (1) is the backward Euler scheme that, when applied, leads to a large sparse system of equations that must be solved:

$$\frac{\mathbf{u^{n+1}} - \mathbf{u^{n}}}{\Delta t} = F(\mathbf{u^{n+1}}) \rightarrow \mathbf{M}\,\mathbf{u^{n+1}} = \mathbf{u^{n}}.$$

For the operators discussed here, F is linear (sometimes through linearization) and positive definite ($\mathbf{M}$ is symmetric).

SC '16 November 13–18, 2016, Salt Lake City, UT, USA
ACM ISBN 978-1-4503-2138-9.
DOI: 10.1145/1235

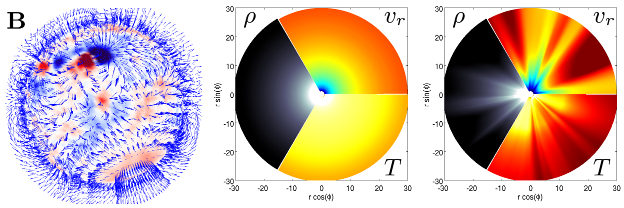

Figure 1: Initial conditions (left,middle) and simulation results (right) for the test case used.

A very common method of solving such systems are Krylov subspace iterative solvers, and in the case of symmetric operators, the Conjugate Gradient (CG) method. In order to allow the CG method to converge to the solution efficiently, the system is preconditioned with an approximate inverse of the matrix, leading to the preconditioned-CG method (PCG). See Ref. [3] for a detailed overview of these solvers.

One difficulty with using the PCG method is selecting and computing an inexpensive yet efficient preconditioner (PC). Here, we use two relatively simple communication-free PCs: 1) Point-Jacobi/diagonal scaling (PC1), which uses the inverse of the diagonal as the PC. This is very inexpensive to formulate and apply, but is limited in effectiveness. 2) Non-overlapping domain decomposition with zero-fill incomplete LU factorization (PC2), which is much more expensive to formulate and apply, but is also much more effective. One drawback of PC2 is that, due to the non-overlapping implementation, the PC becomes less effective as the number of processors increase.

3. EXPLICIT RUNGE-KUTTA LEGENDRE SUPER TIME-STEPPING SCHEME

A relatively recent class of schemes for integrating parabolic operators without numerical restriction on the time-step size are called 'super time-stepping'/'extended stability' (STS) methods. The main idea behind them is to use a Runge-Kutta multi-stage scheme with stages added for stability rather than accuracy. For a given desired time-step, a number of stages (s) and specialized coefficients for each stage are found for which the advance is stable. For our problem, the number of stages is $\propto 1/\Delta x$; much less than what would be needed if integrating at the explicit Euler limit ($\propto 1/\Delta x^2$).

The STS methods can easily handle non-linear operators, do not require global communications, and, due to their explicit nature, are very easy to implement. The STS method we use is the 2nd-order Runge-Kutta Legendre (RKL2) method [2] as it displays favorable stability properties in cases of nonlinear and/or non-continuous diffusion coefficients.

4. REAL-WORLD TEST CASE

In order to make a fair (and useful) comparison of the methods, we use a production run of the MAS Solar coronal model [1]. The simulation uses observed surface magnetic fields as an inner boundary condition, and integrates the MHD equations to a quasi-steady-state solar wind coronal solution. The initial conditions and final relaxation solution are shown in Fig. 1.

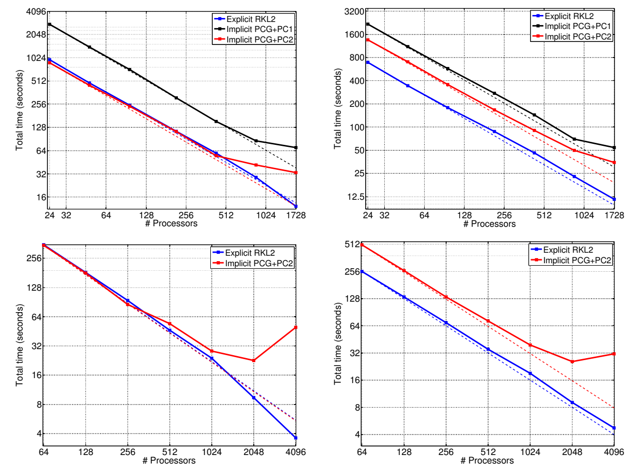

Figure 2: Scaling result for integrating thermal conduction (left) and viscosity (right) on Comet (top) and Stampede (bottom).

5. RESULTS AND CONCLUSIONS

We show several timing results for running the simulation using each algorithm run on a range of processor numbers up to the maximum allowed processors for our allocation. The runs are performed on both the Stampede system at TACC and the Comet system at SDSC. Timing results are shown in Fig. 2. We find that the use of the RKL2 method outperforms the implicit PCG method for the chosen test problem and implementation. Notably, the scaling of the RKL2 method is much better for the given problem size, allowing the code to scale to much higher processors numbers than the implicit solvers.

The RKL2 results, while globally accurate, did not properly damp out grid-level oscillations in velocity caused by under-resolved structures in some areas near the transition region. Future work will include mitigation of this problem, as well as developing OpenACC implementations of the algorithms.

For a detailed report of this study, see our recently submitted publication [4].

6. ACKNOWLEDGMENTS

This work is supported by AFOSR, NASA, and NSF. HPC resources provided by XSEDE.

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