A high order spectral deferred correction time integration method in CAM-HOMME

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Summary

The inclusion of new physics, chemistry, and grid refinement of the recently released Community Atmosphere Model (CAM5) creates new algorithmic challenges, including coupled nonlinear multiscale processes and enhanced scalability requirements. To maintain scalability and throughput, a number of climate models have been returning to first order accurate fully explicit methods developed several decades ago. However, finer model grids require a superlinear reduction in the time step size to account for the smaller spatial scale and increased multiscale interactions (Keyes et al., 2006). It has been shown that spectral deferred correction (SDC) methods provide more accurate and efficient solutions for several multiscale applications (Dutt et al., 2000). A hybrid version of SDC outlined below has been implemented into the shallow water version of the spectral element dycore of the spectral element version of CAM (CAM-HOMME). It works by subdividing one time-step with p grid points and iteratively improving the solution by a low-order method (Huang et al., 2006, Jia and Huang (2008)). With p Gauss-Legendre quadrature points and backward Euler's method, the resulting SDC is of order 2p and A-/L-stable. Presently, this is referred to as SDC, and with some extension, a Krylov deferred correction (KDC) method, and is based upon a either forward Euler (explicit) or backward Euler (fully implicit (FI)) solution method and is applied to the suite of shallow water test cases from Williamson et al. (1992). This method is summarized below, and results showing accuracy improvements are presented. Solutions of test cases using S/KDC applied to the shallow water equations (TC1 and TC6) highlight the ability to generate solutions with errors below the uncertainty of the benchmark solution. Eighth order accuracy is demonstrated, which allows very long simulations without accumulating error at the rate of current time discretization schemes. The current SDC solver implementation utilizes a Fortran interface package within the Trilinos project, which allows fully tested, optimized, and robust code with a suite of parameter options to be included a priori.

Hybrid Deferred Correction Method

Spectral and Krylov Method for high order time integration

The deferred correction (DC) technique provides a framework to facilitate the construction of stable and efficient high-order methods. It works by first subdividing one time-step using p points, forming and iteratively solving the error equation on these p points with a low-order method, such as Euler's. With the choice of p Gauss-Legendre quadrature points, the DC is spectrally accurate and of order $2p$. With the backward Euler's method, the DC is A- and L-stable. Large time steps can be stably taken using DC methods while maintaining accuracy; this is particularly advantageous when dealing with long-time simulations.

The shallow water equation can be written most compactly as

$$\frac{\partial \varphi}{\partial t} = F(\varphi),$$

or its equivalent modified Picard integral form

$$\frac{\partial \varphi}{\partial t} = F\left(\varphi_0 + \int_0^t \frac{\partial \varphi}{\partial t} dt\right).$$

To work with deferred correction, we define and regard $\psi = \frac{\partial \varphi}{\partial t}$ as the unknown, and rewrite this equation in error equation form

$$\delta = \int_0^t [F(\varphi^{[0]} + \delta) - \psi^{[0]}]dt,$$

where $\psi^{[0]}$ or $\varphi^{[0]} = \varphi_0 + \int_0^t \psi^{[0]} dt$ is a provisional approximate solution, and $\delta = \varphi - \varphi^{[0]}$ is defined as the error.

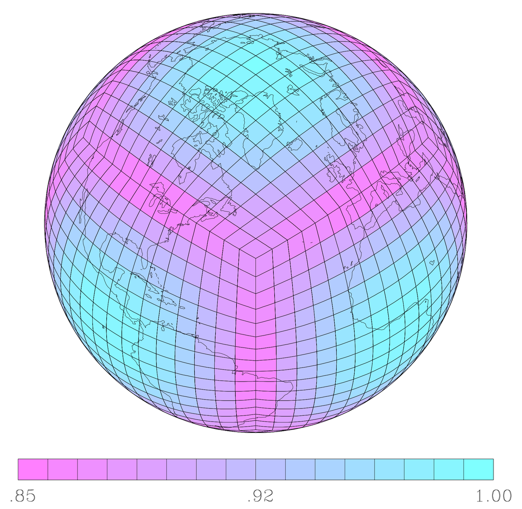
We subdivide one time-step into p steps according to the Gauss-Legendre quadrature. Within one time-step, we solve the above error equation on the intermediate p sub-time-steps, and accumulate the numerical solution to the provisional approximate solution $\psi^{[0]}$ and iterate this procedure until the prescribed tolerance for the error is reached and move on.

Solving the above error equation using Backward Euler's method is simply

$$\delta_m = \delta_{m-1} + \Delta t_m \left(F(t_m, \varphi^{[0]}_{m+1} + \delta_m) - \psi^{[0]}_{m+1}\right), m = 1..p$$

Spectral deferred correction (SDC) was originally introduced by Dutt, Greengard and Rokhlin and the Krylov deferred correction (KDC) by Huang, Jia and Minion is an accelerated version which provides same accuracy with better stability and efficiency.

A new dycore option within the Community Earth System Model (CESM): High-Order Methods Modeling Environment (HOMME)



Spectral Element Spatial Discretization

1. Domain: 6 cube faces mapped to the sphere and tiled into lat-lon elements
2. Within each element, variables are approximated by polynomial expansions
3. Communication is only needed at the element edges
4. Mesh refinement: add elements or increase order of spectral degree

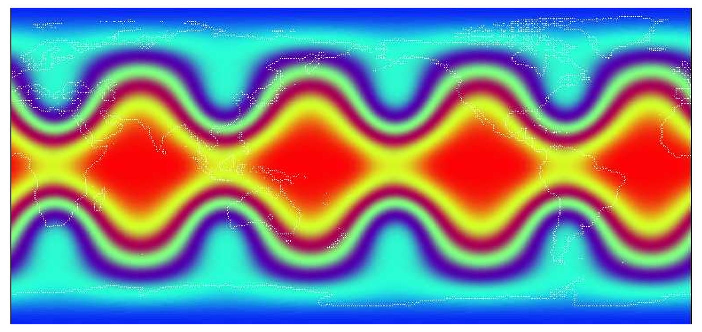
Combines favorable aspects of two discretizations onto a cubed sphere grid

Spectral Transform Methods	Finite Element Methods
High order accuracy	Geometric Flexibility
High convergence rate	Minimal Communication

*Developed at NCAR as part of DOE's Climate Chance Prediction Program (CCPP), HOMME has exhibited superior scalability and efficiency. The spectral element formulation as applied in HOMME locally conserves mass and energy (Taylor et. al, 2009).

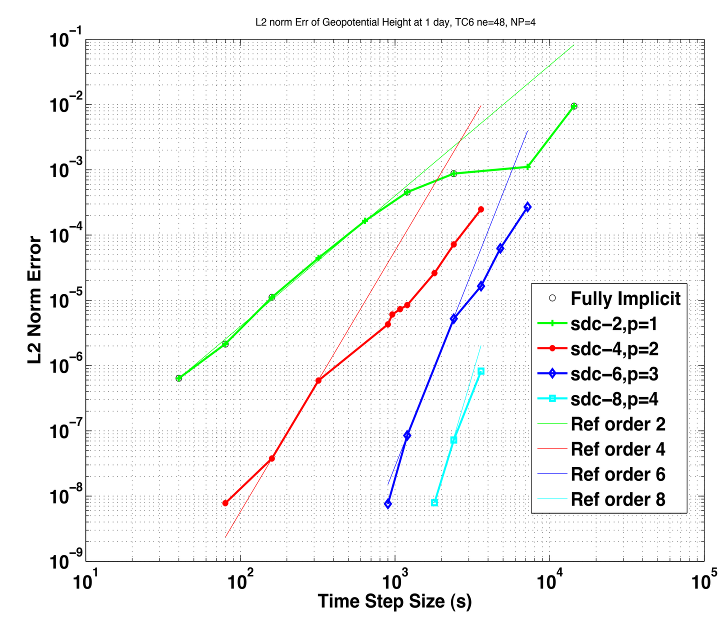
Shallow Water: Test Case 6

Nonlinear barotropic vorticity equations on the sphere



Test case 6 solves the barotropic vorticity problem on a sphere (left) and exercises the full nonlinear equations. The problem in SWTC6 uses a smaller scale separation between advection and gravity waves. Thus, an implicit and/or S/KDC based method, because they can utilize larger time step sizes, can provide a greater efficiency benefit as compared to advection CFL limited methods.

A time step convergence analysis was performed for SWTC6 for a suite of p Gauss-Legendre quadrature points, similar to a previous analysis of the FI method implemented in HOMME (Evans et al. 2010). Spectral order p=1,2,3,4 are presented and as predicted, demonstrate 2*p order accuracy. Eighth order accuracy is a new result for a spectrally discretized temporal integration scheme. Like SWTC1, the short time integration of the test cases do not produce significant differences in the temporal schemes. However over long time integrations, especially in circumstances where the model is not strongly forced, it is expected that errors due to low order schemes are reduced using higher order S/KDC schemes.



Citations:

A. Dutt, L. Greengard, V. Rokhlin, Spectral deferred correction methods for ordinary differential equations, BIT 40 (2) (2000) 241–266.
K. Evans , M. Taylor and J. Drake (2010). Accuracy Analysis of a spectral element atmospheric model using a fully implicit solution framework, Mon. Wea. Rev.**138**:3333-3341.
J. Huang , J. Jia and M. Minion (2006). Accelerating the Convergence of Spectral Deferred Correction Methods , J. Comp. Phys., **21:** 633-656.
J. Jia and J. Huang (2008). Krylov Deferred Correction Accelerated Method of Lines Transpose, J. of Comp. Phys., **227**: 1739-1753.
R. Jakob-Chien, J.J. Hack, and D.L.Williamson (1995). "Spectral Transform Solutions to the Shallow Water Test Set." J. Comp. Phys. **119**: 164-187.
Keyes, D.E., Reynolds, D.R., and C. Woodward, (2006). "Implicit solvers for large scale nonlinear problems." J. Phys. Conf. Series **46**: 433-442.
Williamson, D.L., and J. B. Drake, J. J. Hack, R. Jakob, and P.L. Swarztrauber, (1992). "A Standard Test Set for Numerical Approximations to the Shallow Water Equations in Spherical Geometry." J. Comp. Phys. **102**: 211-224.

Acknowledgements:

LDRD

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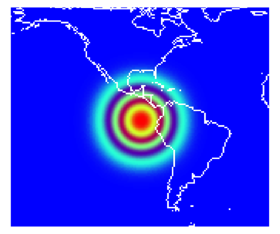
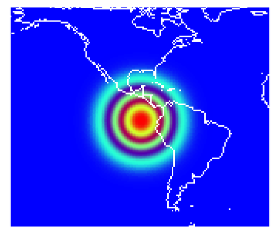
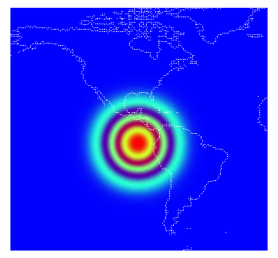
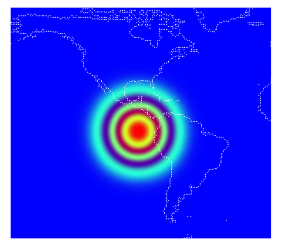
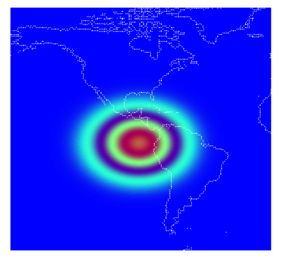
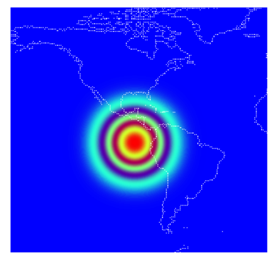
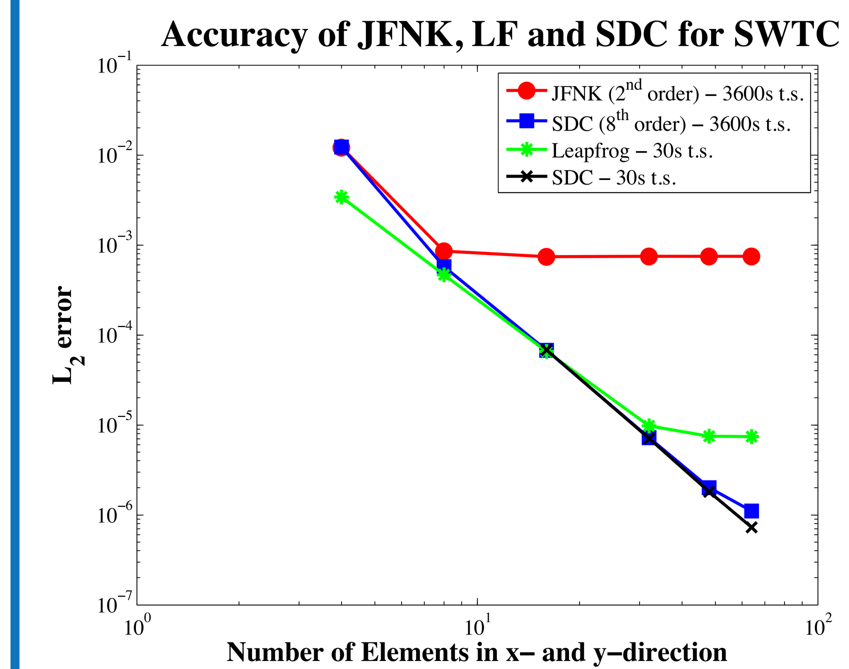
Shallow Water: Test Case 1

Specified velocities advect a height anomaly around the sphere

Test case 1 is a simple test case of a Gaussian hump anomaly advected around a sphere using prescribed velocities. To assess error, SWTC1 provides an analytic solution from which to compare. We have used spatial discretizations of 96 elements with np=8 and 48 elements with np=4, both of which are fine enough to minimize spatial error and produce similar results. In the regional plots of the height field below, the top left and right pictures show the anomaly prescribed at the start of the simulation. After 12 days (1 rotation around the globe), the anomalies are displayed just below the initial condition for both integration methods and show that the explicit and KDC are able to reproduce the height anomaly quite well. This is the typical length of the SWTC1 simulation to assess the ability of the numerical method to maintain the anomaly for a reasonable period of time. In the plots below the 12 day integration, same the anomaly has been advected around the globe for 912 days, or about 2.5 years. Although the KDC method is able to maintain the anomaly very closely, the explicit scheme is diffused in magnitude and location. Below these regional plots, the relative error of the methods is presented.

Explicit		KDC
	Initial cosine bell anomaly	
	Anomaly after 12 days using explicit (left) and KDC (right)	
	Anomaly after 912 days using explicit (left) and KDC (right)	



One way to view the utility of high order time integration is relative to spatial error. The plot to the left presents the L2 norm of error for simulations using JFNK and SDC with large time step sizes and leapfrog and SDC with small time step sizes over a range of resolutions. When the temporal error is relatively small, the 4th order slope of the spatial error used in HOMME is evident. For a given time integration scheme, the temporal error will remain relatively constant with varying resolution. 8th order SDC with a 30 second time step produces temporal error below the spatial error down to fine scale simulations (221K points ~1/2 degree spacing). Even with a 3600s time step size, the SDC method produces error below the spatial error for most resolutions. Leapfrog with a 30s time step also produces low error levels with a 30 second time step, but not as low as SDC with an hour long time step size. Also, because leapfrog is limited to small time steps, efficiency for long integrations will be limited. JFNK with a 3600s time step shows that temporal error is dominant for most reeolutions. Implicit methods are not time step limited, but if low order accuracy is used, accuracy may be a trade-off for efficiency. The next step of this research is to develop scalable preconditioners for SDC and assess efficiency for large time step and fine scale spatial configurations of HOMME.

Summary

Recent work to implement a high order accurate time integration scheme in CAM-HOMME using a hybrid spectral deferred Krylov (SDC and KDC) method has demonstrated 2nd, 4th, 6th, and 8th order accuracy, depending on the value of temporal p refinement. It has been shown that simulations using the hybrid deferred correction method produce solutions that are more accurate than traditional methods even with much larger (~100x greater) time steps. These higher order schemes can prevent accumulating error terms that exist with lower order methods run for many time steps. Although short time integrations with low order accurate time integration schemes do not produce solutions that are visibly different than the results from simulations using hybrid SDC, it is shown that longer time integrations with first order accurate leapfrog, unlike hybrid SDC, diverge significantly from the true solution.