Petascale Atmospheric General Circulation Models

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Abstract. The High-Order Method Modeling Environment (HOMME) is a framework to investigate using high-order element-based methods to build conservative and accurate atmospheric general circulation models. Currently, HOMME employs the discontinuous Galerkin and spectral element methods on a cubed-sphere tiled with quadrilateral elements to solve the primitive equations, and has been shown to scale to $\mathcal{O}(10K)$ processors of a Cray XT 3/4 and $\mathcal{O}(32K)$ processors of an IBM Blue Gene/L. Here we briefly describe the development of a baroclinic model using the discontinuous Galerkin option in the HOMME framework, present idealized test case results, and provide preliminary performance data.

1. Introduction
The future evolution of the Community Climate System Model (CCSM) into an Earth system model will require a highly scalable and accurate flux-form formulation of the dynamics of the atmosphere: flux form is required in order to conserve long-lived trace species in the stratosphere; accurate numerical schemes are essential to ensure high-fidelity simulations capable of capturing the convective dynamics in the atmosphere and their contribution to the global hydrological cycle; scalable performance is necessary to efficiently exploit the massively-parallel petascale systems that will dominate high-performance computing for the foreseeable future.

The High-Order Method Modeling Environment (HOMME) [5], developed by the Computational and Information Systems Laboratory at the National Center for Atmospheric Research (NCAR) in partnership with the Computational Science Center at the University of Colorado at Boulder (CU), is a framework to investigate using high-order element-based methods to build scalable, accurate, and conservative atmospheric general circulation models (AGCMs). The primary objective of the HOMME project is to provide the atmospheric science community a framework for building the next generation of AGCMs based on high-order numerical methods that efficiently scale to hundreds-of-thousands of processors, achieve scientifically useful integration rates, provide monotonic and mass conserving transport of multiple species, and can easily be coupled to community physics packages.

Currently, HOMME employs the discontinuous Galerkin (DG) and spectral element (SE) methods on a cubed-sphere tiled with quadrilateral elements to solve the primitive equations, and has been shown to scale to $\mathcal{O}(10K)$ processors of a Cray XT 3/4 and $\mathcal{O}(32K)$ processors of an IBM Blue Gene/L (BG/L) [12, 4]. The DG option in HOMME guarantees conservation while maintaining all the attractive computational features of the SE option. Here we briefly describe the development of a baroclinic model using the DG option in the HOMME framework [1], present idealized test case results, and provide preliminary performance data.
2. DG Baroclinic Model

2.1. Computational Domain

The globe (sphere) is decomposed into six identical regions by an equiangular central projection of the faces of an inscribed cube (see Fig. 1). This results in a nonorthogonal curvilinear $(x^1, x^2)$ coordinate system \((x^1, x^2) \in [-\pi/4, \pi/4]\). Each face of the cubed-sphere is partitioned into \(N_e \times N_e\) rectangular non-overlapping elements such that the total number of elements is \(6 \times N_e^2\). The transformation laws between cubed-sphere and regular sphere, and the associated metric tensors are in [10].

2.2. Hydrostatic Primitive Equations on the Cubed-Sphere

The hydrostatic primitive equations, consisting of the momentum, mass continuity, thermodynamic, and moisture transport equations, can be expressed as a conservative system in curvilinear coordinates. The prognostic variables are pressure thickness \(\delta p\), covariant wind vectors \((u_1, u_2)\), potential temperature \(\Theta\), and moisture variable \(q\).

\[
\begin{align*}
\frac{\partial u_1}{\partial t} + \nabla_c \cdot \vec{E}_1 &= \sqrt{G} u_2 (f + \zeta) - RT \frac{\partial}{\partial x^1} (\ln p), \\
\frac{\partial u_2}{\partial t} + \nabla_c \cdot \vec{E}_2 &= -\sqrt{G} u_1 (f + \zeta) - RT \frac{\partial}{\partial x^2} (\ln p), \\
\frac{\partial}{\partial t} (\Delta p) + \nabla_c \cdot (U^j \Delta p) &= 0, \\
\frac{\partial}{\partial t} (\Theta \Delta p) + \nabla_c \cdot (U^j \Theta \Delta p) &= 0, \\
\frac{\partial}{\partial t} (q \Delta p) + \nabla_c \cdot (U^j q \Delta p) &= 0,
\end{align*}
\]

where

\[
\begin{align*}
\nabla_c &= \left( \frac{\partial}{\partial x^1}, \frac{\partial}{\partial x^2} \right), \quad \vec{E}_1 = (E, 0), \quad \vec{E}_2 = (0, E), \quad E = \Phi + \frac{1}{2} (u_1 u_1 + u_2 u_2), \\
U^j &= (u^j_1, u^j_2), \quad \Delta p = \sqrt{G} \delta p, \quad \Theta = T \left( \frac{p_0}{p} \right), \quad \kappa = \frac{R}{C_p},
\end{align*}
\]

\(\sqrt{G}\) is the metric term, \(E\) is the energy term, \(\zeta\) is the relative vorticity, \(\Phi = gh\) is the geopotential height, and \(f\) is the Coriolis parameter (see [10] for details). Note that, because of the vertical Lagrangian coordinates, the vertical advection terms are absent from the above system.

2.3. Vertical Discretization

The vertical discretization is based on the 1-D vertical Lagrangian coordinates of [13, 8]. A terrain following Lagrangian vertical coordinate (see Fig. 2) can be constructed by treating any reference Eulerian coordinate as a material surface. Over time, the Lagrangian vertical surfaces deform and thus must be periodically remapped onto a reference coordinate. The hydrostatic atmosphere is vertically sub-divided into a finite number of pressure intervals or pressure thicknesses. The entire 3-D system can be viewed as a vertically stacked set of 2-D shallow water DG models coupled through the discretized hydrostatic relation.

At every time step \(\delta p\) is predicted at model levels and used to determine pressure at Lagrangian surfaces by summing the pressure thickness from top \((p_{\text{top}})\) to bottom \((p_\ell)\) such that \(p_\ell = p_{\text{top}} + \sum_{k=1}^{\ell} \delta p_k\). The geopotential height at interfaces is obtained by using the hydrostatic relation, i.e., \(\Delta \Phi = -C_p \Theta \Delta \Pi\) where \(\Pi = \left( \frac{p}{p_0} \right)^\kappa\), and summing the geopotential height from bottom \((\Phi_\ell)\) to top, \(\Phi_\ell = \Phi_s + \sum_{k=1}^{\ell} \Delta \Phi_k\). For the baroclinic model, the velocity fields \((u_1, u_2)\),
Figure 1. The cubed-sphere is tiled with non-overlapping elements ($\Omega_k$) spanning the entire surface of the globe. Each element is further mapped onto a reference GLL grid for high-order integration.

Figure 2. Schematic of the vertical 1-D Lagrangian coordinates. The Lagrangian coordinates are conservatively remapped onto a reference Eulerian coordinates at regular intervals of time.

The moisture $q$, and total energy ($\Gamma_E$) are remapped onto the reference Eulerian coordinates using the 1-D conservative cell integrated semi-Lagrangian (CISL) method developed in [9]. The temperature field $\Theta$ is retrieved from the remapped total energy $\Gamma_E$.

2.4. Spatial DG Discretization

The flux form of Eq.(1-5) can be generalized such that

$$\frac{\partial}{\partial t} U + \nabla_c \cdot \vec{F}(U) = S(U),$$

(7)

where $U = [u_1, u_2, \Delta p, \Delta p \Theta, \Delta p q]^T$ denotes prognostic variables, $\vec{F}(U)$ is flux function, and $S(U)$ is the source term. For each element $\Omega_k$ of the computational domain (globe), the weak Galerkin formulation [2] of the DG baroclinic system (7) can be written as

$$\frac{\partial}{\partial t} \int_{\Omega_k} U_h \cdot \varphi_h d\Omega_k - \int_{\Omega_k} \vec{F}(U_h) \cdot \nabla_c \varphi_h d\Omega_k + \oint_{\partial \Omega_k} \vec{F}(U_h) \cdot \vec{n} \varphi_h ds = \int_{\Omega_k} S(U_h) \cdot \varphi_h d\Omega_k,$$

(8)

where $U_h$ is an approximate solution and $\varphi_h$ is the test function, and both belong to the finite dimensional space $V_h(\Omega)$ of orthogonal polynomials. The discontinuities at the element boundaries ($\partial \Omega_k$) are resolved by solving an approximate Riemann problem with the Lax-Friedrichs numerical flux formula as described in [10]. $U_h$ is expanded in terms of a tensor-product of Lagrange basis functions ($h_i$) of order $N_v$ defined at the Gauss-Lobatto-Legendre (GLL) points such that $U_h = \sum_{i=1}^{N_v} \sum_{j=1}^{N_v} U_{ij} h_i h_j$. The weak formulation (8) is further simplified by evaluating the integrals with a high-order accurate GLL quadrature formula. The resulting DG discretization leads to following system of ordinary differential equations,

$$\frac{dU_h}{dt} = L(U_h), \quad U_h \in (0,T) \times \Omega_k,$$

(9)

and is solved by a third-order Runge-Kutta method as described in [3, 10].

3. Numerical Experiments with Idealized Tests

To validate the DG baroclinic model, we have performed idealized tests such as the Jablonowski-Williamson baroclinic instability test [7] and Held-Suarez tests [6]. The baroclinic instability
test is used to assess the evolution of baroclinic waves in the northern hemisphere using quasi-realistic initial conditions. Figures (3) and (4) show simulated fields after 8 and 11 days, and provide a comparison to reference results obtained from the global spectral and finite-volume models available in the CCSM framework [7]. DG HOMME performance is shown in Fig. (5).

**Figure 3.** The left panel shows the temperature field at 850 hPa for the baroclinic instability test after 8 days with DG HOMME. The central panel shows the corresponding surface pressure. The right panel shows the reference surface pressure from the NCAR global spectral model (T85). Both use 26 vertical levels and an approximate horizontal resolution of 1.4°.

**Figure 4.** Surface pressure evolution after 11 days for the baroclinic instability test. The left panel shows results from DG HOMME ($N_e = 26$, $N_v = 6$). The central panel is a reference simulation from the NCAR global spectral model (T170). Both use 26 vertical levels and an approximate horizontal resolution of 0.7°. The right panel shows a 16-day time trace of minimum surface pressure for the DG, T170, and finite-volume ($0.5° \times 0.625°$) models (see [7] for details).

4. **Summary**
A high-order DG conservative baroclinic model has been developed in the HOMME framework. Idealized tests show that the new model is accurate, free from ‘spectral ringing’ (see Fig. 3), and has parallel performance comparable to that of the SE baroclinic model in HOMME. However, the DG baroclinic model employs explicit Runge-Kutta time integration with moderate time step size resulting in a lower integration rate. Improved time integration schemes, monotonic limiters, and integration with CAM physics are ongoing research projects.
Figure 5. Performance on a 2048 processor IBM BG/L system. The left panel shows results from the baroclinic instability test and the right panel shows results from the Held-Suarez test [6].

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