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Petascale atmospheric models for the Community Climate System Model: new developments and evaluation of scalable dynamical cores

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Abstract. We present results from the integration and evaluation of the spectral finite-element method into the atmospheric component of the Community Climate System Model (CCSM). This method overcomes the atmospheric scalability bottleneck by allowing the use of a true two-dimensional domain decomposition for the first time in the CCSM. Scalability is demonstrated out to 86,200 processors with an average grid spacing of 0.25° (25 km). We present initial evaluations results using a standardized test problem with the full suite of CCSM atmospheric model forcings and subgrid parametrizations but without the CCSM land, ice, or ocean models. For this realistic setting, the true solution is unknown. Even convergence under mesh refinement is not expected, so we cannot rely on high-resolution reference solutions. Instead we focus on intermodel comparisons and use the Williamson equivalent resolution methodology to evaluate the results.

1. Introduction
Climate change models have been a crucial tool in the development of our understanding of the Earth’s climate. This understanding is crucial to determining the response of the Earth’s climate to increasing concentrations of greenhouse gases in the atmosphere. Further improvement of these models is needed if they are to be used to guide policy makers in the determination of safe levels of atmospheric greenhouse gas concentrations or to be used to evaluate climate change mitigation and adaptation strategies. Clearly, such next-generation models will require petascale, if not exascale, computing resources. Not withstanding the recent advent of the world’s first petascale computer, effectively using machines with O(100,000) processors for climate modeling remains a challenge because of several scalability bottlenecks present in all modern climate models – the largest bottleneck being created by the numerical methods used in the atmospheric component.

These numerical methods are encapsulated in the dynamical core of each atmospheric model. The dynamical core is the component that solves the partial differential equations governing the fluid dynamical aspects of the atmosphere. In addition, atmospheric models contain a suite of subgrid parametrizations for the many physical processes unresolved in an atmospheric model but which drive the dynamics. The physics parametrization suite includes such effects as convection, precipitation, and radiative forcings. Currently, most dynamical cores use latitude-longitude-based grids. These grids create a logically Cartesian orthogonal mesh suitable for
a wide array of numerical methods including finite volumes and spectral transform methods. The grid lines cluster at the pole, creating a potentially severe CFL restriction on the time step. There are many successful techniques to handle this pole problem; however, most of them substantially degrade parallel scalability by effectively limiting the model to one-dimensional domain decomposition strategies.

Hence there is now a renewed interest in the development and evaluation of scalable dynamical cores that use quasi-uniform grids for the surface of the sphere and avoid the pole problem. This is evidenced by the recent colloquium [1] held at the National Center for Atmospheric Research (NCAR). Nine modeling groups, close to 40 students, and dozens of keynote speakers met for two weeks to discuss numerical methods, evaluate new and existing dynamical cores, initiate the process of developing idealized test cases to facilitate model intercomparison and to objectively measure the strengths and weaknesses of proposed numerical methods. Data and results from this colloquium are being collected as of this writing. When completed, they will be made available to the community on a special portal to the Earth System Grid [2]. This will represent an unprecedented database of results from many different models all running a suite of standardized test cases at a wide range of resolutions.

Here we describe results from our recent integration of one of these dynamical cores into the CCSM. In particular, we have integrated the High Order Multiscale Modeling Environment (HOMME) [3] into the Community Atmospheric Model (CAM), the atmospheric component of the CCSM. We are motivated by the fact that HOMME is one of the most scalable dynamical cores and by previous work in which the physics parametrizations from CAM were incorporated into a spectral element model [4]. We use an improved formulation of the spectral element method that locally conserves both mass and energy [5, 6] and replaces the local element filter with a more isotropic hyperviscosity term. In addition, we make use of two key features of CAM that allow the HOMME dynamical core to be integrated directly into the full CCSM. The first is the process split dynamics/physics interface from [7], and the second is the infrastructure work to allow for unstructured grids in the CCSM described in [8]. The process split interface allows us to compute the physics parametrizations with a much larger time step as compared to the dynamics time step.

**Figure 1.** Tiling the surface of the sphere with quadrilaterals. An inscribed cube is projected to the surface of the sphere. The faces of the cubed-sphere are further subdivided to form a quadrilateral grid of the desired resolution. The Gnomonic equal angle projection is used, resulting in a quasi-uniform but nonorthogonal grid.

HOMME is used as a research tool to study several types of quadrilateral element-based dynamical cores. It can be run as a standalone model or as a component of CAM. Here we focus on HOMME’s spectral element dynamical core running within CAM, which we refer to
as CAM/HOMME. CAM/HOMME models the global circulation of the Earth’s atmosphere using the three-dimensional hydrostatic primitive equations. To eliminate the pole problem, CAM/HOMME uses an equal angle cubed-sphere grid [9, 10] to discretize the horizontal directions as shown in figure 1. In the radial direction, CAM/HOMME uses the hybrid $\eta$ pressure vertical coordinate system [11, 12]. CAM/HOMME uses the compatible spectral element formulation from [5, 6], where the compatibility property of the method is used to obtain local conservation of both mass and energy. CAM/HOMME is the first version of CAM that allows for full two-dimensional domain decomposition. It is also the first version of CAM that exactly conserves dry mass without the use of mass fixers, and conserves energy (exactly with exact time integration).

In what follows we first give an overview of the spectral element method and the form of the equations solved by CAM/HOMME. We then present results from aqua planet experiments. These simulations use the full suite of CAM forcings and subgrid physics parametrizations but without the CCSM land, ice, or ocean models. Because of the subgrid parametrizations, conventional mesh-refinement studies are not possible in this setting, so we rely on a resolution sensitivity and model inter-comparison methodology from [13, 14]. We present parallel scalability results that show the two-dimensional domain decomposition will be sufficient for CAM to achieve petascale performance levels at resolutions suitable for climate modeling.

2. Compatible spectral finite elements

The spectral finite element method is a variant of the traditional $h-p$ finite element method. This allows the method to easily handle the nonorthogonal irregular cubed-sphere grids generated by tiling the sphere with quadrilaterals. As with traditional $h-p$ methods, it relies on globally continuous polynomial basis functions. The equations of interest are solved in integral formulation. The unique feature of the spectral element method is that the elements are restricted to quadrilaterals so that the integrals can be approximated by highly accurate Gauss-Lobatto quadrature rules within each element. This allows the construction of compactly supported, globally continuous basis, and trial functions that are orthogonal, leading to a diagonal mass matrix. The diagonal mass matrix means that iterative methods are not needed to invert the mass matrix. Thus, time-dependent problems such as the atmospheric primitive equations can be solved with explicit or semi-implicit methods. It allows the method to remain efficient while retaining the geometric flexibility of unstructured finite elements grids. It also allows the method to run efficiently at very large values of $p$, which is why it is referred to as a spectral finite element method.

The method has proven accurate and effective for a wide variety of geophysical problems, including global atmospheric circulation modeling [10, 15, 16, 4] ocean modeling [17, 18, 19] and planetary scale seismology [20]. The method has unsurpassed parallel performance; it was used for earthquake modeling by the 2003 Gordon Bell Best Performance winner [20] and for climate modeling by a 2002 Gordon Bell Award honorable mention [21].

The compatible spectral element formulation used in CAM/HOMME locally conserves mass to within round-off error levels. In addition, the forcing terms (such as precipitation) that change the water content of the atmosphere are incorporated into the continuity equation so that CAM/HOMME exactly conserves the atmospheric dry mass, and thus no additional mass fixers such as those used in [12] are needed. The total energy conservation in CAM/HOMME is semi-discrete, meaning the conservation is exact (to within round-off error levels) with exact time stepping. With the leapfrog time-stepping scheme used in CAM/HOMME there is no dissipation introduced by the method for linear and quadratic terms such as mass, tracer mass, and internal energy. For cubic terms such as kinetic energy, dissipation is introduced by the time-stepping scheme that is proportional to $\Delta t^2$, resulting in an error in the conservation of total energy proportional to $\Delta t^2$. 

SciDAC 2008 IOP Publishing
doi:10.1088/1742-6596/125/1/012023

SciDAC 2008 IOP Publishing
doi:10.1088/1742-6596/125/1/012023
For realistic simulations some kinetic energy dissipation is needed in order to obtain a reasonable enstrophy cascade. This is especially true in a scheme such as CAM/HOMME, where the advection operator does not dissipate any kinetic or internal energy. Without additional terms, the only dissipation in the model is a trace amount introduced by the Robert filter in the leapfrog time-stepping scheme. To introduce additional dissipation, we use a $\nabla^4$ hyper-viscosity term modeled after that used in [12] but adapted for the spectral element method.

In [6] the energy balance was examined in detail, using a quasi-realistic baroclinic instability test. With average grid spacing of $1^\circ$ and an explicit time step for the dynamical core of 90 seconds, the dissipation of internal and potential energy was at the round-off error levels as expected. The dissipation of kinetic energy due to the Robert filtered leapfrog time-stepping scheme was on the order of $2 \times 10^{-6}$ W/m$^2$, while the kinetic energy dissipation explicitly introduced by the hyper-viscosity operator is much larger, on the order of 0.02 W/m$^2$. These values should be compared to the typical atmospheric forcing in a full climate model of around 2 W/m$^2$.

The spectral element method is capable of refinement in both $h$ (element size) and $p$ (polynomial degree within each element). For the runs presented here, we fix $p = 4$ and adjust the resolution by the choice of the number of quadrilateral elements used to tile the sphere.

3. The hydrostatic primitive equations

In CAM/HOMME, we solve the hydrostatic primitive equations using the hybrid $\eta$ pressure vertical coordinate system from [11, 12]. The equations, neglecting dissipation and forcing terms are given by

$$\frac{\partial \mathbf{u}}{\partial t} + (\zeta + f) \mathbf{k} \times \mathbf{u} + \nabla \left( \frac{1}{2} \mathbf{u}^2 + \Phi \right) + \frac{RT}{p} \nabla p + \frac{\partial \mathbf{u}}{\partial \eta} = 0 \tag{1}$$

$$\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T + \frac{\partial T}{\partial \eta} = 0 \tag{2}$$

$$\frac{\partial}{\partial t} \left( \frac{\partial p}{\partial \eta} \right) + \nabla \cdot \left( \frac{\partial p}{\partial \eta} \mathbf{u} \right) = 0 \tag{3}$$

$$\frac{\partial}{\partial t} \left( \frac{\partial q}{\partial \eta} \right) + \nabla \cdot \left( \frac{\partial q}{\partial \eta} \mathbf{u} \right) = 0 \tag{4}$$

There are prognostic equations for the horizontal velocity vector (tangent to the surface of the sphere) $\mathbf{u}$, the temperature $T$, the quantity $\frac{\partial p}{\partial \eta}$, and specific humidity $q$. The equations are written with $\mathbf{u}$ and $T$ as the prognostic variables to minimize the number of cubic nonlinearities that appear. The resulting system is not written in conservation form, nor is there a prognostic equation for total energy, as this is not required to obtained energy conservation when using a compatible numerical method. CAM/HOMME also advects two additional tracers, cloud liquid and cloud ice, using equations identical to equation 4.

In the $\eta$ coordinate model, $\frac{\partial p}{\partial \eta}$ can be thought of as a mass density. The prognostic variables are functions of $\eta$ and coordinates describing the surface of the sphere. The divergence, gradient and curl operators shown are the standard two-dimensional operators acting on the surface spherical coordinates only. The vorticity is denoted by $\zeta = \nabla \times \mathbf{u}$, $f$ is a Coriolis term, $R, R_v, c_p, c_{pv}$ are constants and

$$T_v = \left[ 1 + \left( \frac{R_v}{R} - 1 \right) q \right] T \quad c_p^q = \left[ 1 + \left( \frac{c_{pv}}{c_p} - 1 \right) q \right] c_p.$$ 

There are two additional prognostic equations for the geopotential height field $\Phi$ and the pressure vertical velocity $\omega$.

$$\Phi = \Phi_s + \int_{\eta}^{1} T_v \frac{\partial p}{\partial \eta} d\eta \quad \omega = \mathbf{u} \cdot \nabla p - \int_{\eta_{top}}^{\eta} \nabla \cdot \left( \frac{\partial \mathbf{u}}{\partial \eta} \right) d\eta$$

4
where $\Phi_s$ is the prescribed surface geopotential height (given at $\eta = 1$) and $\eta_{top}$ is the $\eta$-surface at the top of the model. We note that in the $\eta$ coordinate system, the pressure is given by

$$p(\eta) = A(\eta)p_0 + B(\eta)p_s$$

for a constant reference pressure $p_0$. The functions $A$ and $B$ are prescribed to control the spacing of the $\eta$-surfaces and $\eta = A(\eta) + B(\eta)$. These functions are chosen to allow the coordinate system to transition from a pure pressure coordinate system near the top of the atmosphere to a terrain following coordinate system near the surface. With this relation, equation 3 can be rewritten as a prognostic equation for surface pressure $p_s$ and a diagnostic equation for $\dot{\eta} \frac{\partial p}{\partial \eta}$,

$$\frac{\partial}{\partial t} p_s + \int_{\eta_{top}}^{1} \nabla \cdot \left( \frac{\partial p}{\partial \eta} \mathbf{u} \right) d\eta = 0$$

$$\dot{\eta} \frac{\partial p}{\partial \eta} = -\frac{\partial p}{\partial t} - \int_{\eta_{top}}^{\eta} \nabla \cdot \left( \frac{\partial p}{\partial \eta} \mathbf{u} \right) d\eta,$$

where $\frac{\partial p}{\partial t} = B(\eta)\frac{\partial p_s}{\partial t}$. The remaining equations are discretized in the form shown in equations 1, 2 and 4.

4. Aqua planet experiments

When using three-dimensional dynamical cores to simulate idealized configurations without subgrid-scale physics, both short time integrations and climate statistics are observed to converge under mesh refinement [22, 23]. However, physics parametrizations represent subgrid-scale processes and thus generate a significant amount of grid-scale forcings. Under mesh refinement, these forcings will remain at the grid scale, resulting in a term that can be considered as never fully resolved. Thus it is not expected that full atmospheric models will converge under mesh refinement [13]. In order to study the effects of these parametrizations in the simplest possible setting, a suite of aqua planet experiments was proposed in [24]. In these experiments, the model is run with the full physics parametrizations, but the surface boundary conditions are greatly simplified by prescribing a planet covered with water and with a fixed sea surface temperature (SST).

We follow the methodology outlined in [13, 14]. In that work, aqua planet simulations are performed with two dynamical cores in CAM: an Eulerian core based on spherical harmonics (CAM/EUL) and a finite volume core on a latitude/longitude grid (CAM/FV). Williamson shows that some of the sensitivity of the solutions to resolution is in fact due to the large physics time step and can be avoided by using a physics time step of 5 min. In order to further reduce the sensitivity, all simulations are made using the CAM Eulerian dynamical core T85 physics parametrizations tunings. The simulations are started from a previously generated aqua planet state and run for 14 months. The time-averaged statistics presented here are taken from the past 12 months. In this regime, many large scale features are observed to converge under mesh refinement, but many other quantities still show a strong dependence on resolution.

In Table 1 we summarize several global mean quantities related to precipitation, one of the most heavily parametrized processes in CAM. The CAM/EUL data was taken from [13]. First note the large monotonic signal in all the quantities as a function of grid resolution. Compared to these differences, the agreement between CAM/EUL and CAM/HOMME when grouped as shown in the table is remarkable. This initial pairing and the choice of hyperviscosity coefficient were based on the equivalence established between CAM/FV and CAM/EUL in [14]. This suggests that CAM/HOMME at 1.0°, 0.5° and 0.25° resolutions is comparable to CAM/EUL at T42, T85, and T170 resolutions, respectively. However, the table also shows that further tuning of the viscosity coefficients in CAM/HOMME at 1.0° can produce results somewhere between the T85 and T170 CAM/EUL results if the viscosity is reduced. A similar conclusion holds for CAM/HOMME at 0.5°.
Table 1. Global mean quantities as a function of resolution. CAM/HOMME results are presented with an average grid spacing of 1.9, 1 and 0.5 degrees. CAM/EUL results are presented with a spectral truncation of T42, T85, T170 and T340. Both models were run with the CAM standard 26 vertical levels.

<table>
<thead>
<tr>
<th>Model/Resolution</th>
<th>Physics</th>
<th>Hyperviscosity Coefficient</th>
<th>Convective Precipitation (mm/day)</th>
<th>Large-scale Precipitation (mm/day)</th>
<th>Cloud Fraction</th>
<th>Precipitable Water (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>EUL T42</td>
<td>5</td>
<td>$1 \times 10^{16}$</td>
<td>1.71</td>
<td>1.11</td>
<td>0.65</td>
<td>20.21</td>
</tr>
<tr>
<td>HOMME 1.9</td>
<td>5</td>
<td>$1 \times 10^{16}$</td>
<td>1.76</td>
<td>1.14</td>
<td>0.66</td>
<td>20.09</td>
</tr>
<tr>
<td>EUL T85</td>
<td>5</td>
<td>$1 \times 10^{15}$</td>
<td>1.59</td>
<td>1.38</td>
<td>0.60</td>
<td>19.63</td>
</tr>
<tr>
<td>HOMME 1.0</td>
<td>5.5</td>
<td>$1 \times 10^{15}$</td>
<td>1.59</td>
<td>1.43</td>
<td>0.61</td>
<td>19.67</td>
</tr>
<tr>
<td>HOMME 1.0</td>
<td>5.5</td>
<td>$3 \times 10^{14}$</td>
<td>1.45</td>
<td>1.58</td>
<td>0.59</td>
<td>19.71</td>
</tr>
<tr>
<td>EUL T170</td>
<td>5</td>
<td>$1.5 \times 10^{14}$</td>
<td>1.44</td>
<td>1.62</td>
<td>0.55</td>
<td>19.13</td>
</tr>
<tr>
<td>HOMME 0.5</td>
<td>5</td>
<td>$1.5 \times 10^{14}$</td>
<td>1.48</td>
<td>1.62</td>
<td>0.55</td>
<td>19.36</td>
</tr>
<tr>
<td>HOMME 0.5</td>
<td>5</td>
<td>$5.0 \times 10^{13}$</td>
<td>1.39</td>
<td>1.70</td>
<td>0.53</td>
<td>19.18</td>
</tr>
<tr>
<td>EUL T340</td>
<td>5</td>
<td>$1.5 \times 10^{13}$</td>
<td>1.36</td>
<td>1.75</td>
<td>0.50</td>
<td>18.75</td>
</tr>
</tbody>
</table>

Figure 2. Time-averaged, zonally averaged surface pressure for CAM/HOMME at 1.9°, 1.0°, and 0.5° resolutions plotted respectively in orange, red, and blue.

We now turn to time-averaged, zonally averaged data. We start with the surface pressure, plotted for three different resolutions in figure 2. This should be compared with figure 3 in [13]. As with the global means, there is a strong signal with resolution, but relative to these differences there is good agreement between the CAM/HOMME and CAM/EUL results. When the equivalent resolutions are paired, the pairing is similar to what was found with the global means, except that the 0.5° result as actually quite close to the T340 result.

The time-averaged, zonally averaged total cloud fraction is plotted in figure 3. This should be compared with figure 4 in [13] and figure 2 in [14]. Here again there is a strong signal with resolution, but now the agreement between CAM/HOMME and CAM/EUL is not as clear cut. The decrease in cloud fraction with resolution is quite similar, but CAM/HOMME has consistently fewer clouds at $-15°$ latitude. CAM/HOMME 0.5° does obtain good agreement for the rest of the domain as compared to the T170 and CAM/FV 0.5° results.
The time-averaged, zonally averaged total precipitation is plotted in figure 4. This plot should be compared with figure 2 in [13]. The data is consistent with the conclusions drawn in that paper: the larger scales in the equatorial region have converged and the variation in the global averages comes from the remainder of the domain.

In Fig. 5, we plot precipitation probability density functions. This plot should be compared with Fig. 5 in [14]. As with all the other metrics we have examined, there is a strong dependence on resolution, but by choosing different resolution pairs the models can be seen to agree well. The pairings between CAM/HOMME and CAM/EUL continue to hold, except the 1.0° result with a 10 mm bin size appears much closer to the T340 than T170 result.

Grid imprinting is of special concern for methods on non-latitude/longitude grids, as any such grid will have some anisotropy and must contain a few special points. For the cubed-sphere grid, the main concern is anomalous forcing of an \( m = 4 \) mode caused by the 8 special points at the cube corners that appear in the mid-latitudes. To examine this issue, we plot the time averaged pressure vertical velocity (\( \omega \)) field from both CAM/HOMME and CAM/EUL in figure 6. This field is very sensitive to grid-scale noise and is susceptible to grid imprinting. The noise in \( \omega \)
Figure 5. CAM/HOMME probability density function of 6-hour mean precipitation in the equatorial band between ±10 latitude, for 1.9, 1.0 and 0.5 degree resolutions. The left figure uses a bin size of 1 mm, while the right figure uses a bin size of 10 mm.

Figure 6. Time-averaged pressure vertical velocity ($\omega$) on an $\eta$-surface near the model top for CAM/EUL at T85 and CAM/HOMME at 1.0°. is not significantly different from that found in the near perfectly isotropic CAM/EUL model. We attribute this to the fact that CAM/HOMME is using relatively high-order (fourth-order) numerics and is an $h-p$ type finite-element method that has a long history of dealing with grids far more unstructured and anisotropic than the cubed sphere.

5. Scalability results
The parallel scalability of CAM/HOMME is demonstrated in Fig. 7. We present benchmark results from the IBM BG/L system installed at Lawrence Livermore National Laboratory (106,496 nodes in a torus interconnect, each with two 700 MHz processors) and Tbird, an Intel/Infiniband-based Linux cluster (4480 nodes, each with dual 3.6 GHz Intel EM64T processors) installed at Sandia National Laboratories. The figure shows the integration rate
Figure 7. Integration rate measured in simulated years per day is plotted as a function of the number of processors, for several different resolutions. Because of memory constraints, the BG/L results were obtained using only one processor per node, except for the largest run on 86,200 processors that used both processors on each node.

(simulated years per day) obtained as a function of number of processors at several resolutions. Each curve represents a fixed resolution, so that the total amount of work was kept constant while the processor count was increased. Data from the BG/L runs at 1.4, 0.5 and 0.25 degree resolutions used up to 1536, 21600, and 86400 processors, respectively. These processor counts result in parallel decompositions as fine as one element per processor, the limit of our domain decomposition approach. The thin black line represents perfect parallel scalability. As can be seen in the figure, at moderate processor counts CAM/HOMME obtains close to perfect scalability. Reasonable scalability is obtained even at the limit of one element per processors.

6. Conclusions
The highly scalable dynamical core HOMME has been integrated into CAM, the atmospheric component of the CCSM. Initial results from aqua planet simulations using the full physics subgrid parametrization suite suggest that CAM/HOMME produces results in agreement with other dynamical cores in CAM. In particular, for many quantities, CAM/HOMME at 1° resolution is comparable to CAM/EUL at a resolution between T85 and T170, while CAM/HOMME at 0.5° resolution is comparable to CAM/EUL at a resolution between T170 and T340. The CAM/HOMME sensitivity of all quantities examined to mesh refinement is also similar to CAM/EUL and CAM/FV.

CAM/HOMME is the first non-latitude/longitude dynamical core integrated into CAM, demonstrating the CAM physics/dynamics interface is capable of handling unstructured grids. The parallel scalability of HOMME is maintained within this interface. At 0.25°, CAM/HOMME scales effectively to 86,200 processors, or 1 element per processor. This research suggests that at slightly higher resolutions CAM/HOMME will easily scale to the processor counts expected for upcoming petascale computers. At resolutions of 0.5° and 0.25°, the LLNL BG/L computer is capable of running CAM/HOMME at integration rates of at least 5 simulated years per day, the conventional target for climate integrations.

Acknowledgments
This work supported in part by the DOE/BER SciDAC Project, Modeling the Earth System.
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