Singletrack Dynamical Core Roadmap

This document outlines the development and testing necessary to evaluate and fulfill Singletrack dynamical core requirements. Based on the section 2 and 3 from the *SingleTrack Dynamical Core Requirements Report*, dynamical core evaluation and development will require some combination of the following:

1. (1) Testing for conservation where conservation is not exact.
2. (2) Testing to measure efficiency of dynamical core components.
3. (3) Testing of transport characteristics (some SE, FV3 and MPAS results in the literature).
4. (4) Development of capabilities not yet existing in the dynamical cores.
5. (5) Tests measuring the efficiency and scaling of the core (both transport and dynamics).

Requirements and evaluations that require atmospheric physics are not included in the dynamical core roadmap presented here; these tests and evaluations will need to be accomplished in collaboration with physics subgroup.

MPAS roadmap

The latest release version of the MPAS dynamical core (MPAS Version 6.1) contains most of the major developments and optimizations except for the regional capability that exists in a development branch. The version of MPAS that exists in CAM (i.e. CIME) is from MPAS Version 4, and it does not contain many of the optimizations of MPAS-V6.1 and it does not have all the latest algorithmic upgrades. Given that Singletrack will use CIME and some version of the CESM/CAM/CIME infrastructure, engineering a build of MPAS/CAM pulling MPAS from its development or its release repository is a very high priority, but it is not listed here. Fortunately, many (perhaps all) of the dynamical core requirements considered by the Singletrack dynamical core subgroup can be evaluated using the standalone MPAS V6.1 because there should not be significant degradation of MPAS dynamical core performance with its build in CAM.

The following developments and testing needs are those identified in Table 2 in the *SingleTrack Dynamical Core Requirements Report*.

Ongoing and future MPAS dynamical core developments and testing:

1. (1) Testing for conservation of energy and angular momentum (requirement 4): We have preliminary results from MPAS V4. We need to repeat with V6.1 in CAM that would include further tuning for the CAM/climate configuration.
2. (2) Efficiency of components and overall dycore efficiency (requirements 1, 2, 19 and 20): Transport, dry dycore - testing can be done in standalone version - need to determine

tests or pull results from previous testing? These tests could be part of more general benchmarking for throughput and scaling. e.g. requirements 1, 19 and 20.

(3) Regional capability: The initial phase of regional MPAS testing is almost complete. The MPAS developers will be doing a code clean-up along with a cleanup of necessary utilities before a public release. The question of how CIME/CESM/CAM will accommodate regional applications needs to be addressed in other subgroups and the Singletrack group.

    Progress concerning the development of a regional version of MPAS, that we expect will be released sometime early in 2019, is given in the presentation available at http://www2.mmm.ucar.edu/wrf/users/workshops/WS2018/oral_presentations/2.4.pdf

Geospace applications needs

(4) Geospace configuration (requirement 18): High-top thermodynamics - need to evaluate the use of coupled potential temperature (density * potential temperature) as a prognostic variable in MPAS for high-top applications. Also need to evaluate the height coordinate and upper boundary conditions, etc for these applications. Will any major changes be needed to MPAS to accommodate high-top thermodynamics?

(5) Geospace configuration (requirement 17): Deep atmosphere capability - need to implement 3D-variable gravity, complete Coriolis term (already available in MPAS) and geometry. This should be a straightforward task given the height coordinate used in MPAS.

    Technical details concerning a deep atmosphere equations implementation of MPAS is given in the document available at http://www2.mmm.ucar.edu/people/skamarock/Presentations/MPAS_and_NWP.pdf

(6) Geospace configuration (requirement 16): Species dependent mean molecular mass and specific heats - need to evaluate the inclusion of this generalization into the MPAS nonhydrostatic compressible solver. If feasible then implement.

(7) Evaluate height coordinate and upper boundary conditions, etc for these applications.

(8) Geospace configuration (requirement 15): Efficient 2 way 3D inline grid coupling - need to evaluate with the infrastructure group, consider implementation if feasible.

SE roadmap

Current status of SE:

A new version of the SE dynamical core has been committed to the CAM trunk. This version is a reformulation of the spectral-element dynamical core in dry-mass vertical coordinates with comprehensive treatment of condensates and energy (see Lauritzen et al., 2018; submitted; for details). It also contains the option of performing tracer transport with CSLAM (only uniform resolution grids are supported at this point).

Current development of SE:

- Testing of CAM-SE and WACCM-SE with CAM6 physics (including using CSLAM for tracer transport) – some "tweaking" of viscosity and/or changes in topography smoothing is being investigated; this work is scheduled to be part of the CESM2.1 release.

  This work is primarily done by Lauritzen (CGD) with some software engineering support.

- Implementation of the existing SE dycore in WACCM-X, including mapping capability needed to couple with the ionosphere dynamics module (the coupling is funded by HAO). Include major species transport (variable M, R and C_p) in the SE dycore, providing the current WACCM-X capability with SE instead of FV.

  This work is primarily done by Liu (HAO) and Lauritzen (CGD) with some software engineering support.

Possible future development of SE (non-hydrostatic and deep atmosphere version):

For high horizontal resolution applications (~<10km) a non-hydrostatic version of SE is necessary. For high-top applications a deep atmosphere formulation is highly desirable. Such a formulation is much simpler in a 'z'-based vertical coordinate system than hybrid-sigma (Yessad and Wedi; ECMWF, 2011). Hence it is recommended to implement a non-hydrostatic shallow-atmosphere version of SE based on a terrain-following height coordinate first.

More specifically, CISL's Ram Nair wrote a roadmap for the non-hydrostatic version of SE (see Appendix). The following are the main design considerations as laid out by Nair:

- Use CAM-SE framework as much as possible and exploit the present parallel software infrastructure of the hydrostatic code. The horizontal aspects of the SE discretization will remain the same, this includes cubed-sphere grid system, local mesh refinement, tracer transport and hyperviscosity (biharmonic) operations.
- Fully compressible 3D Euler system of equations suitable for spherical curvilinear grids and deep atmospheric domain. Momentum equations in the vector invariant form, flux-form equations for the continuity and transport equations.
- Terrain following height-based vertical z-coordinates with staggered FD/FV discretization. This is a major change to the present CAM-SE design.
- Time integration will be based on classical split-explicit Runge-Kutta formulation combined with an implicit treatment of acoustic terms in the vertical direction. This will

alleviate the stringent CFL stability requirement resulting from tiny grid spacing in the vertical, while being parallel efficient.

The details of the deep extension of CAM-SE are given by Ram Nair's roadmap (see Appendix). A significant advantage of the gnomonic cubed-sphere approach in SE is that the metric terms for the deep atmosphere extension are exact; hence gradient, curl and divergence operators easily extend to deep atmosphere metrics. This may not be true for other dynamical cores.

In Nair's roadmap, Liu and Lauritzen have recommended to change the prognostic variable from potential temperature (theta) to temperature to accommodate high-top thermodynamics, as theta becomes ill-defined above the homopause (~110km). Nair responded that such a change could be accommodated.

It is important to realize that the development of a deep non-hydrostatic dynamical core with consistent thermodynamics is a basic research topic and therefore has a longer time-scale.

Expertise and staffing considerations

With the termination of CISL's Ram Nair position, the expertise in non-hydrostatic deep atmosphere modeling with the SE dycore is no longer available internally at NCAR. So either NCAR would have to form partnerships with external institutions or build up the expertise in-house.

DOE has independently developed a non-hydrostatic version of SE based on the 'Laprise' formulation i.e. using a pressure coordinate (Mark Taylor; personal communication). The DOE non-hydrostatic SE core is planned to replace the hydrostatic SE code after version 1 release of E3SM after which it would be publicly available (planned this summer; Mark Taylor personal communication). As mentioned above however, a pressure-based coordinate is not recommended for deep atmosphere extension.

References

Lauritzen, P.H. and co-authors, 2017: NCAR CESM2.0 release of CAM-SE: A reformulation of the spectral-element dynamical core in dry-mass vertical coordinates with comprehensive treatment of condensates and energy: *J. Adv. Model. Earth Syst.*, submitted (December 8, 2017)

Lauritzen, P.H. M.A. Taylor, J. Overfelt, P.A. Ullrich, R.D. Nair, S. Goldhaber and R. Kelly, 2016: CAM-SE-CSLAM: Consistent finite-volume transport with spectral-element dynamics.: *Mon. Wea. Rev.*. DOI:10.1175/MWR-D-16-0258.1

Yessad, K. and N.P. Wedi, 2011: The hydrostatic and non-hydrostatic global model IFS/ARPEGE: deep-layer model formulation and testing, ECMWF Technical Memorandum No. 65

Appendix: Roadmap written by R. Nair (CISL)

Extension of the CAM-SE Dynamical-Core to a Non-hydrostatic Model and Beyond: Project Overview

(R. D. Nair, CISL, October 15th 2017)

Introduction

The High-Order Method Modeling Environment (HOMME) is a modeling framework developed at the CISL/NCAR to foster the state-of-the-art numerical methods for atmospheric modeling. The spectral-element (SE) version of HOMME is used as the default dynamical core for the CAM framework, known as the CAM-SE, and is a petascale model with local mesh refinement capability. However, a major drawback of the CAM-SE model is that the governing equations are based on the hydrostatic approximation, which limits the horizontal resolution about 25 km. As spatial resolutions become finer, the use of the hydrostatic approximation becomes inappropriate at the smallest resolved scales. The CAM-SE employs pressure (mass) based vertical coordinates with a 'shallow' atmosphere approximation (with constant radius of earth and simplified Coriolis term), this limits the top of the atmosphere to be at about 30 km height. In order to address these limitations, and prepare the CAM-SE framework for future high-resolution climate modeling applications, require a major design change. Extending the CAM-SE framework to a non-hydrostatic (NH) model with ability to handle deep atmospheric simulations is of great interest at the NCAR divisions including CGD, ACD and HAO.

Project Goals

New generation climate models are based on NH dynamics following compressible Euler or Navier-Stokes system of equations, which are capable of high-resolution cloud resolving global simulations with horizontal resolution of a few km or finer. The 'deep' atmosphere is typically of O(100) km in the vertical where the radius of earth and gravity varies radially, and allows accurate representation of the Coriolis force terms. The ultimate goal of this project is to extend CAM-SE dynamical core to a NH model with an option for deep atmosphere simulation. Following are the main design considerations.

- Use the CAM-SE framework as much as possible and exploit the present parallel software infrastructure of the hydrostatic code. Horizontal aspects of the SE discretization will remain the same, this includes cubed-sphere grid system, local mesh refinement, tracer transport and hyperviscosity (biharmonic) operations.
- Fully compressible 3D Euler system of equations suitable for spherical curvilinear grids and deep atmospheric domain. Momentum equations in the vector invariant form, flux-form equations for the continuity and transport equations.
- Terrain following height-based vertical z-coordinates with staggered FD/FV discretization. This will be a major change for the present CAM-SE design, z-coordinates are more suitable for deep atmosphere modeling and free of time (pressure) dependent metric terms.
- Time integration will be based on classical split-explicit Runge-Kutta formulation combined with an implicit treatment of acoustic terms in the vertical direction. This will alleviate the stringent CFL stability requirement resulting from tiny grid spacing in the vertical, while being parallel efficient.

Deep-Atmosphere Formulation

Consider the 3D flux-form of the compressible Euler equations on a rotating sphere (earths's atmosphere) then the prognostic equations for fluid motion can be written in terms of 3D wind vector (fluid velocity) $\mathbf{V}$, density ρ, potential temperature θ and moisture variables q_k. Upon splitting of the density and pressure as $\rho = \overline{\rho} + \rho'$ and $p = \overline{p} + p'$, where the mean values $\overline{\rho}$ and $\overline{p}$ are in hydrostatic balance $\partial\overline{p}/\partial z = -\overline{\rho}g$, we have the flux-from governing equations in the following general form (without specifying a particular horizontal coordinate system):

$$\begin{aligned}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{V}) &= 0 \qquad (1)\\
\frac{\partial \rho \mathbf{V}}{\partial t} + \nabla \cdot (\rho \mathbf{V} \otimes \mathbf{V}) &= -\nabla p' - \rho' g \hat{\mathbf{k}} - 2\rho \mathbf{\Omega} \times \mathbf{V} + \mathbf{F}_M \qquad (2)\\
\frac{\partial \rho \theta}{\partial t} + \nabla \cdot (\rho \theta\, \mathbf{V}) &= 0 \qquad (3)\\
\frac{\partial \rho q_k}{\partial t} + \nabla \cdot (\rho\, q_k \mathbf{V}) &= 0 \qquad (4)
\end{aligned}$$

where $(2\rho\mathbf{\Omega} \times \mathbf{V})$ is the Coriolis force term, $\mathbf{F}_M$ is the forcing term including the diffusive fluxes, $\mathbf{\Omega}$ is earth's angular velocity and $\hat{\mathbf{k}}$ is the radial unit vector. The gravity term in general $g = g(r)$ is dependent on the radial distance r from the earth's center.

In order to formulate the deep atmosphere model, it is convenient introduce the following height ratio in terms earth's mean radius a,

$$r_a = \frac{r}{a}. \qquad (5)$$

Many practical models including the CAM-SE use 2D + 1D decomposition for 3D discretization, where the 1D coordinates represents the vertical coordinate system. We consider the height based z-coordinate which use the height above mean surface level z such that $r = a + z$. Thus the basic mathematical 3D operators such as the gradient and divergence for an arbitrary scalar (ψ) or vector ($\mathbf{V}$) can be written as

$$\begin{aligned}
\nabla \psi &= \nabla_h \psi + \hat{\mathbf{k}} \frac{\partial \psi}{\partial z} \qquad (6)\\
\nabla \cdot \mathbf{V} &= \nabla_h \cdot \mathbf{v} + \frac{1}{r^2} \frac{\partial r^2\, w}{\partial z}, \qquad (7)
\end{aligned}$$

where ∇_h is horizontal (2D) gradient operator, $\mathbf{v} = \mathbf{V}_h$ and $w = \mathbf{V} \cdot \hat{\mathbf{k}}$ are the horizontal and vertical components, respectively. Using the ratio r_a we can redefine the operators as follows:

$$\begin{aligned}
r_a^2\, \nabla \psi &= \nabla_h (r_a \psi) + \hat{\mathbf{k}}\, r_a^2 \frac{\partial \psi}{\partial z} \qquad (8)\\
r_a^2 \nabla \cdot \mathbf{V} &= \nabla_h \cdot (r_a \mathbf{v}) + \frac{\partial r_a^2\, w}{\partial z}, \qquad (9)
\end{aligned}$$

For the cubed-sphere geometry ∇_h is the curvilinear (tensor form) gradient and $\nabla_h \cdot$ divergence operators which are defined at the surface level (shallow atmosphere), as currently approximated in the CAM-SE model. We can use the same operators at any discrete vertical level z, by multiplying the ratio r_a relevant to that particular level. Similarly 'curl' and diffusion operators as well as the the Jacobian of gnomonic mapping ($\sqrt{G} = |AA^T|$) and cube-to-sphere transformation matrices A, A^T can be redefined as a function of the discrete vertical z.

The vertical discretization is based on height-based terrain-following ξ-coordinates such that

$$\xi = \frac{z_{top}(z - z_s)}{z_{top} - z_s} \qquad (10)$$

where z_{top} is top of the model level, typically $O(100)$ km for the deep atmosphere, and $z_s = z_s(x^1, x^2)$ is the prescribed surface topography in cubed-sphere (x^1, x^2) coordinates.

A simplified shallow-atmosphre model for initial testing

The proposed model development goes through different phases, first we consider a simplified version of compressible Euler equations, which are close to the current CAM-SE formulation, but with the height-based vertical coordinates (similar to that used in ICON). Simplified form of 3D equations on the sphere , in vector-invariant form in orthogonal (x^1, x^2, z)-coordinate system:

$$
\begin{aligned}
\frac{\partial u}{\partial t} + \frac{\partial K_h}{\partial x^1} + w\frac{\partial u}{\partial z} - (\zeta + f)v &= -\theta\,\frac{\partial P}{\partial x^1} \qquad (11)\\
\frac{\partial v}{\partial t} + \frac{\partial K_h}{\partial x^2} + w\frac{\partial v}{\partial z} + (\zeta + f)u &= -\theta\,\frac{\partial P}{\partial x^2} \qquad (12)\\
\frac{\partial w}{\partial t} + u\frac{\partial w}{\partial x^1} + v\frac{\partial v}{\partial x^2} + w\frac{\partial w}{\partial z} &= -\theta\,\frac{\partial P}{\partial z} - g \qquad (13)\\
\frac{\partial \rho}{\partial t} + \nabla\cdot(\mathbf{V}\rho) &= 0 \qquad (14)\\
\frac{\partial \rho\,\theta}{\partial t} + \nabla\cdot(\mathbf{V}\rho\,\theta) &= 0 \qquad (15)
\end{aligned}
$$

where $\mathbf{V} = (u, v, w)$, ζ relative vorticity, f Coriolis term, K_h horizontal kinetic energy term, and

$$
P = c_p\left(\frac{R_d}{p_0}\rho\,\theta\right)^{(R_d/c_v)}. \tag{16}
$$

The above system is closed by the equation of state, where pressure $p = C_0(\rho\theta)^\gamma$, and $C_0 = R_d^\gamma p_0^{-R_d/c_v}$. The reference surface pressure $p_0 = 10^5$ Pa, and the other thermodynamic constants are given by $\gamma = c_p/c_v$, R_d =287 J kg^{-1} K^{-1}, $c_p = 1004$ J kg^{-1} K^{-1}, $c_v = 717$ J kg^{-1} K^{-1}.

Project Timelines

A major research focus for the past year has been preparation for CAM-SE to achieve this goal. To this end a prototype 2D NH model with SE discretization in the horizontal and FV/FD discretization in the vertical has been developed. The split-explicit time integration and vertical boundary conditions associated with z-coordinates have been successfully tested for the 2D model. A prototype 3D NH model based on discontinuous Galerkin (DG) method known as HOMAM (high-order multiscale atmospheric model) is already existing in the HOMME framework. The DCMIP benchmark test-cases used for HOMAM can be ported into the CAM-SE framework for initial development and the validation and verification of the new NH code. The development of the new NH model in the CAM-SE framework will have three major stages. Following are the details of the stages and the expected timelines.

- Stage-1, [*January – June 2018*]: Create a new branch in the latest CAM-SE trunk exclusively for the NH development, with help for CGD staff and software experts. This stage is mostly for establishing the software infrastructure.
    - Implement vertical height based z-coordinates, without orographic metrics.
    - Use simplified Euler system without orography and fully explicit time-stepping.
    - Validate the code with simple DCMIP tests such as inertia-gravity wave propagation.
- Stage-2, [*July – Dec 2018*]: This stage is for the shallow atmosphere NH simulations.
    - Introduction of orography, use more complete form of Euler equations. Validate with the DCMIP test for mountain-induced wave propagations.

  - Implementation of split-explicit time stepping. Checking the accuracy parallel efficiency
  - Validate with the baroclinic instability tests, idealized climate test such as the Held-Suarez tests. Energy and angular momentum conservation study.

- Stage-3, [*January – Dec, 2019*]: This stage is for deep atmospheric model extension.
  - Generalize the prognostic equations for deep-atmospheric equation terms including general Coriolis term, modify cubed-sphere specific transformation metric/Jacobians. Validate with the deep-atmospheric benchmark tests.
  - Test energy angular momentum conservation etc.
  - Include the tracer transport schemes already working CAM-SE
  - Aqua-planet and AMIP-class simulations with the deep atmosphere. Parallel scalability studies.
  - Experiment with variable resolution global grid (static AMR).

FV3 roadmap

FV3 is being implemented into the CESM through a NOAA funded project. The code is pulled from a common repository shared with NOAA. Since FV3 it being implemented in the CESM framework, it will require little effort to run the test case suite and evaluate the performance of FV3 (once the tests are implemented for CAM-SE under the CESM simpler models “umbrella”).

FV3 publications and documentation:

https://www.gfdl.noaa.gov/fv3/fv3-documentation-and-references/

More information being gathered.