Development of a Petascale Conservative Dynamical Core for Climate Simulation

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Overview

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- Summary
Motivation

- Why do we need a new climate model?
- Because, the existing models have serious limitations to satisfy all of the following properties:
  1. Local and global conservation
  2. High-order accuracy
  3. High parallel efficiency
  4. Geometric flexibility ("Local" method)
  5. Monotonic (non-oscillatory) advection
- **Discontinuous Galerkin Method (DGM)** based model has the potential to address all of the above issues
- Recently, the Spectral Element (SE) model in HOMME shown to efficiently scale $O(32,000)$ processors on IBM BG/L.
Discontinuous Galerkin Method (DGM) in 1D

- 1D scalar conservation law:

\[
\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0 \quad \text{in} \quad \Omega \times (0, T),
\]

\[
U_0(x) = U(x, t = 0), \quad \forall x \in \Omega
\]

- The domain \( \Omega \) (periodic) is partitioned into \( N_x \) non-overlapping elements (intervals) \( l_j = [x_{j-1/2}, x_{j+1/2}] \), \( j = 1, \ldots, N_x \), and \( \Delta x_j = (x_{j+1/2} - x_{j-1/2}) \)
A **weak formulation** of the problem for the approximate solution $U_h$ is obtained by multiplying the PDE by a *test function* $\varphi_h(x)$ and integrating over an element $l_j$:

\[
\int_{l_j} \left[ \frac{\partial U_h}{\partial t} + \frac{\partial F(U_h)}{\partial x} \right] \varphi_h(x) dx = 0, \quad U_h, \varphi_h \in V_h
\]

Integrating the second term by parts $\implies$

\[
\int_{l_j} \frac{\partial U_h(x, t)}{\partial t} \varphi_h(x) dx - \int_{l_j} F(U_h(x, t)) \frac{\partial \varphi_h}{\partial x} dx + \\
F(U_h(x_{j+1/2}, t)) \varphi_h(x_{j+1/2}^-) - F(U_h(x_{j-1/2}, t)) \varphi_h(x_{j-1/2}^+) = 0,
\]

where $\varphi(x^-)$ and $\varphi(x^+)$ denote "left" and "right" limits.
DGM-1D: Flux term ("Gluing" the discontinuous element edges)

- Flux function $F(U_h)$ is **discontinuous** at the interfaces $x_{j\pm1/2}$.
- $F(U_h)$ is replaced by a **numerical flux** function $\hat{F}(U_h)$, dependent on the left and right limits of the discontinuous function $U$. At the interface $x_{j+1/2}$,

$$\hat{F}(U_h)_{j+1/2}(t) = \hat{F}(U_h(x_{j+1/2}^-, t), U_h(x_{j+1/2}^+, t))$$

- Typical flux formulae (Approx. Reimann Solvers): Gudunov, Lax-Friedrichs, Roe, HLLC, etc.
Choose an orthogonal basis set $\mathcal{B}$ spanning the space $V_h^k$, s.t., approx. solution $U_h$ and $\varphi_h$ are in $V_h^k$.

Use a high-order Gaussian quadrature such as the Gauss-Lobatto-Legendre (GLL) quadrature rule

Map every element $I_j$ onto the reference element $[-1, +1]$ by introducing a local coordinate $\xi \in [-1, +1]$ s.t.,

$$\xi = \frac{2(x - x_j)}{\Delta x_j}, \quad x_j = (x_{j-1/2} + x_{j+1/2})/2 \implies \frac{\partial}{\partial x} = \frac{2}{\Delta x_j} \frac{\partial}{\partial \xi}.$$
The model basis set consists of Legendre polynomials, \( \mathcal{B} = \{ P_\ell(\xi), \ell = 0, 1, \ldots, k \} \)

\[
U_j(\xi, t) = \sum_{\ell=0}^{k} U_j^\ell(t) P_\ell(\xi) \quad \text{for} \quad -1 \leq \xi \leq 1, \quad \text{where}
\]

\[
U_j^\ell(t) = \frac{2\ell + 1}{2} \int_{-1}^{1} U_j(\xi, t) P_\ell(\xi) \, d\xi \quad \ell = 0, 1, \ldots, k.
\]

The nodal basis set \( \mathcal{B} \) is constructed using Lagrange-Legendre polynomials \( h_j(\xi) \) with roots at Gauss-Lobatto quadrature points.

\[
U_j(\xi) = \sum_{j=0}^{k} U_j \, h_j(\xi) \quad \text{for} \quad -1 \leq \xi \leq 1,
\]

\[
h_j(\xi) = \frac{(\xi^2 - 1) P_k'(\xi)}{k(k + 1) P_k(\xi_j)(\xi - \xi_j)}.
\]

In any case, the mass matrix is diagonal.
Spatial Discretization

- **Gaussian Quadrature:**
  \[ \int_{-1}^{1} \omega(x)p(x)dx = \sum_{i=0}^{n} w_i p(x_i) \]
  GLL: \( \omega(x) = 1, \ x_0 = -1, \ x_n = 1 \)

- **Interpolation:** two options for basis functions

**Nodal expansion:** Lagrange basis

**Modal expansion:** Legendre basis
DGM: Explicit Time Integration

- Final Semi-discretized form \[ \frac{d}{dt} U_j = \mathcal{L}(U_j) \text{ in } (0, T) \]

- Strong Stability Preserving third-order Runge-Kutta (SSP-RK) scheme (Gottlieb et al., 2001)
  \[
  U^{(1)} = U^n + \Delta t \mathcal{L}(U^n) \\
  U^{(2)} = \frac{3}{4} U^n + \frac{1}{4} U^{(1)} + \frac{1}{4} \Delta t \mathcal{L}(U^{(1)}) \\
  U^{n+1} = \frac{1}{3} U^n + \frac{2}{3} U^{(2)} + \frac{2}{3} \Delta t \mathcal{L}(U^{(2)}).
  \]

  where the superscripts \( n \) and \( n + 1 \) denote time levels \( t \) and \( t + \Delta t \), respectively

- Note: The Courant number for the DG scheme is estimated to be \( 1/(2k + 1) \), where \( k \) is the degree of the polynomial, however, no theoretical proof exists when \( k > 1 \) (Cockburn and Shu, 1989).
DG-2D Spatial Discretization for an Element $\Omega$

2D Scalar conservation law

$$\frac{\partial U}{\partial t} + \nabla \cdot F(U) = S(U), \quad \text{in} \quad \Omega \times (0, T); \quad \forall (x^1, x^2) \in \Omega$$

where $U = U(x^1, x^2, t)$, $\nabla \equiv (\partial/\partial x^1, \partial/\partial x^2)$, $F = (F, G)$ is the flux function, and $S$ is the source term.

- **Weak Galerkin formulation**: Multiplication of the basic equation by a test function $\varphi_h \in V_h$ and integration over an element $\Omega$.

$$\frac{\partial}{\partial t} \int_{\Omega} U_h \varphi_h \, d\Omega - \int_{\Omega} F(U_h) \cdot \nabla \varphi_h \, d\Omega + \int_{\Gamma} F(U_h) \cdot \vec{n} \varphi_h \, d\Gamma = \int_{\Omega} S(U_h) \varphi_h \, d\Omega$$

where $U_h$ is an approximate solution in $V_h$.

- Can be extended to a system of equations
Along the boundaries (Γ) of an element the solution $U_h$ is discontinuous ($U_h^-$ and $U_h^+$ are the left and right limits).

Therefore, the analytic flux $\mathbf{F}(U_h) \cdot \mathbf{n}$ must be replaced by a numerical flux such as the Lax-Friedrichs Flux:

$$\mathbf{F}(U_h) \cdot \mathbf{n} = \frac{1}{2} \left[ (\mathbf{F}(U_h^-) + \mathbf{F}(U_h^+)) \cdot \mathbf{n} - \alpha (U_h^+ - U_h^-) \right].$$

For the SW system, $\alpha$ is the upper bound on the absolute value of eigenvalues of the flux Jacobian $\mathbf{F}'(U)$; (Nair et al., 2005)

$$\alpha^1 = \max \left( |u^1| + \sqrt{\Phi G^{11}} \right), \quad \alpha^2 = \max \left( |u^2| + \sqrt{\Phi G^{22}} \right)$$
DGM is a hybrid approach \((\text{DG} \iff \text{SE} + \text{FV})\)

- The domain \(D\) is partitioned into non-overlapping elements \(\Omega_{ij}\) such that the element boundaries are discontinuous.
- Based on conservation laws but exploits the spectral expansion of SE method and treats the element boundaries using FV “tricks.”
DG-2D: Spatial Discretization

High-order nodal basis set

The nodal basis set is constructed using a tensor-product of Lagrange-Legendre polynomials \( h_i(\xi) \) with roots at Gauss-Lobatto quadrature points.

\[
h_i(\xi) = \frac{(\xi^2 - 1) P'_N(\xi)}{N(N+1) P_N(\xi_i)(\xi - \xi_i)}; \quad \int_{-1}^{1} h_i(\xi) h_j(\xi) = w_i \delta_{ij}.
\]

where \( P_N(\xi) \) is the \( N^{th} \) order Legendre polynomial, and \( w_i \) weights associated with the Gauss quadrature.

- The approximate solution \( (U_h) \) and test function \( (\varphi_h) \) are represented in terms of nodal basis set.

\[
U_{ij}(\xi, \eta) = \sum_{i=0}^{N} \sum_{j=0}^{N} U_{ij} h_i(\xi) h_j(\eta) \quad \text{for} \quad -1 \leq \xi, \eta \leq 1,
\]

- The nodal version was shown to be more computationally efficient than the modal in (Dennis et al., 2006).
Final form for the nodal discretization leads to the ODE:
\[
\frac{d}{dt} U_{ij}(t) = \frac{4}{\Delta x_i \Delta x_j w_i w_j} \left[ I_{\text{Grad}} + I_{\text{Flux}} + I_{\text{Source}} \right],
\]

For a system of conservation laws, solve the ODE system:
\[
\frac{d}{dt} U = L(U) \quad \text{in} \quad (0, T) \times \Omega
\]

Time integration: Explicit third-order Runge-Kutta (SSP) scheme \((Gottlieb et al., 2001)\)

Options for explicit diffusion \((\nabla^2 \text{ or } \nabla^4)\).

Boyd-Vandeevan spatial Filter

Optional Monotonic Limiter (for scalar fields)
DG-2D Gaussian Hill Advection (Levy, Nair & Tufo, 2007)

Scaling Plots

**Strong scaling** is measured by increasing the number of processes running while keeping the problem size constant.

**Weak scaling** is measured by scaling the problem along with the number of processes, so that work per process is constant.
The **Discontinuous Galerkin (DG)** model is the conservative option in the HOMME framework.

**HOMME Grid:** The sphere is decomposed into 6 identical regions, using the equiangular projection (Sadourny, 1972)

- Local coordinate systems are free of singularities
- Creates a non-orthogonal curvilinear coordinate system

**Cubed Sphere Geometry:**

Logical cube-face orientation
HOMME Grid System

Metric Tensor $G_{ij}$, [Cubed-Sphere ⇔ Sphere] Transform

Central angles $x^1, x^2 \in [-\pi/4, \pi/4]$ are the independent variables.

$$G_{ij} = \frac{R^2}{\rho^4 \cos^2 x^1 \cos^2 x^2} \begin{bmatrix} 1 + \tan^2 x^1 & -\tan x^1 \tan x^2 \\ -\tan x^1 \tan x^2 & 1 + \tan^2 x^2 \end{bmatrix}$$

where $\rho^2 = 1 + \tan^2 x^1 + \tan^2 x^2$, $i, j \in \{1, 2\}$

- Metric tensor in terms of longitude-latitude ($\lambda, \theta$):

$$G_{ij} = A^T A; \quad A = \begin{bmatrix} R \cos \theta \partial \lambda / \partial x^1 & R \cos \theta \partial \lambda / \partial x^2 \\ R \partial \theta / \partial x^1 & R \partial \theta / \partial x^2 \end{bmatrix}$$

- The matrix $A$ is used for transforming spherical velocity ($u, v$) to the covariant ($u_1, u_2$) and contravariant ($u^1, u^2$) vectors.
Hydrostatic Prognostic Equations in Flux Form (Curvilinear coordinates)

\[
\frac{\partial u_1}{\partial t} + \nabla_c \cdot E_1 + \dot{\eta} \frac{\partial u_1}{\partial \eta} = \sqrt{G} u^2 (f + \zeta) - R T \frac{\partial}{\partial x_1} (\ln p)
\]

\[
\frac{\partial u_2}{\partial t} + \nabla_c \cdot E_2 + \dot{\eta} \frac{\partial u_2}{\partial \eta} = -\sqrt{G} u^1 (f + \zeta) - R T \frac{\partial}{\partial x_2} (\ln p)
\]

\[
\frac{\partial}{\partial t} (m) + \nabla_c \cdot (U^i m) + \frac{\partial (m \dot{\eta})}{\partial \eta} = 0
\]

\[
\frac{\partial}{\partial t} (m \Theta) + \nabla_c \cdot (U^i \Theta m) + \frac{\partial (m \dot{\eta} \Theta)}{\partial \eta} = 0
\]

\[
\frac{\partial}{\partial t} (mq) + \nabla_c \cdot (U^i q m) + \frac{\partial (m \dot{\eta} q)}{\partial \eta} = 0
\]

\[
m \equiv \sqrt{G} \frac{\partial p}{\partial \eta}, \nabla_c \equiv \left( \frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2} \right), \eta = \eta(p, p_s), G = \det(G_{ij}), \frac{\partial \Phi}{\partial \eta} = -\frac{R T}{p} \frac{\partial p}{\partial \eta}.
\]

Where \( m \) is the mass function, \( \Theta \) is the potential temperature and \( q \) is the moisture variable. \( U^i = (u^1, u^2), E_1 = (E, 0), E_2 = (0, E) \); \( E = \Phi + \frac{1}{2} (u_1 u^1 + u_2 u^2) \) is the energy term. \( \Phi \) is the geopotential, \( \zeta \) is the relative vorticity, and \( f \) is the Coriolis term.
A “vanishing trick” for vertical advection terms!

- Terrain-following Eulerian surfaces are treated as material surfaces.
- The resulting Lagrangian surfaces are free to move up or down direction.
3D Prognostic Equations with Vertical Lagrangian Coordinates

- Lagrangian treatment of the Vertical coordinates results in $\dot{\eta} = 0$ and the mass function $m = \sqrt{G}\delta p = \Delta p$ (pressure thickness).

- Contravariant formulation preserves the familiar “vector invariant” form for the momentum equations.

**Momentum Equations:** No explicit vertical advection terms

\[
\begin{align*}
\frac{\partial u_1}{\partial t} + \nabla_c \cdot E_1 &= \sqrt{G}u^2 (f + \zeta) - RT \frac{\partial}{\partial x^1}(\ln p) \\
\frac{\partial u_2}{\partial t} + \nabla_c \cdot E_2 &= -\sqrt{G}u^1 (f + \zeta) - RT \frac{\partial}{\partial x^2}(\ln p)
\end{align*}
\]

\[
\nabla_c \equiv \left( \frac{\partial}{\partial x^1}, \frac{\partial}{\partial x^2} \right), \quad E_1 = (E, 0), \quad E_2 = (0, E),
\]

\[
E = \Phi + \frac{1}{2} \left( u_1 u^1 + u_2 u^2 \right)
\]
3D Prognostic Equations: Flux-Form Continuity Equations

Temperature field is advected with the mass variable $\Delta p$

\[
\frac{\partial}{\partial t} (\Delta p) + \nabla_c \cdot (U^i \Delta p) = 0
\]
\[
\frac{\partial}{\partial t} (\Theta \Delta p) + \nabla_c \cdot (U^i \Theta \Delta p) = 0
\]
\[
\frac{\partial}{\partial t} (q \Delta p) + \nabla_c \cdot (U^i q \Delta p) = 0
\]

where $U^i = (u^1, u^2)$, $\Delta p = \sqrt{G}\delta p$, $\delta p$ is the pressure thickness, and $\Theta$ is the potential temperature.

Vertical layers are coupled with the hydrostatic relations:

\[
\Delta \Phi = -C_p \Theta \Delta \Pi, \quad \Delta \Phi = -RT \Delta \ln p
\]

where $\Pi = \left(\frac{p}{p_0}\right)^\kappa$ and $T$ Denotes the layer mean temperature.
The Remapping of Lagrangian Variables

**Vertically moving Lagrangian Surfaces**

- Over time, Lagrangian surfaces deform and thus must be remapped.
- The velocity fields \((u_1, u_2)\), and total energy \((\Gamma_E)\) are remapped onto the reference coordinates using the 1-D conservative cell-integrated semi-Lagrangian (CISL) method \((Nair & Machenhauer, 2002)\)

\[
\Delta P = \text{Pressure thickness}
\]

\[
\Delta P \quad \text{Lagrangian Surface}
\]

Terrain-following Lagrangian control–volume coordinates
The prognostic variables $u_1, u_2, \delta p, \Theta$ and $q$ are staggered w.r.t $p$ and $\phi$.

The remapping frequency is $O(10) \times \Delta t$

Potential temperature $\Theta$ is retrieved from the remapped total energy

$$\Gamma_E = c_p T + \frac{\delta(p\phi)}{\delta p} + K_E$$
The Vertical Lagrangian Dynamics

The hydrostatic pressure at Lagrangian surface, *Lin (MWR, 2004)*

\[ p_\ell = p_{\text{top}} + \sum_{k=1}^{\ell} \delta p_k, \quad \ell = 1, 2, 3, ..., N \]

where \( p_{\text{top}} \) represents the pressure at the model top, \( p_\ell \) denotes the pressure at each Lagrangian surface. There are total \( N + 1 \) Lagrangian surfaces span \( N \) layers.

The geopotential height at Lagrangian surface:

\[ \Phi_\ell = \Phi_s + \sum_{k=N}^{\ell} \Delta \Phi_k, \quad \ell = N, N - 1, ..., 1 \]

where \( \Phi_s \) represents the surface geopotential height at the model bottom and \( \Phi_\ell \) denotes the geopotential height at each Lagrangian surface.
Flux-form SW equations (Vector invariant form)

Nair et al. (MWR, 2005)

\[
\begin{align*}
\frac{\partial u_1}{\partial t} + \frac{\partial}{\partial x_1} E &= \sqrt{G} u^2 (f + \zeta) \\
\frac{\partial u_2}{\partial t} + \frac{\partial}{\partial x_2} E &= -\sqrt{G} u^1 (f + \zeta) \\
\frac{\partial}{\partial t} (\sqrt{G} h) + \frac{\partial}{\partial x_1} (\sqrt{G} u^1 h) + \frac{\partial}{\partial x_2} (\sqrt{G} u^2 h) &= 0
\end{align*}
\]

where \( G = \det(G_{ij}) \), \( h \) is the height, \( f \) Coriolis term; energy term and vorticity are defined as

\[
E = \Phi + \frac{1}{2} (u_1 u^1 + u_2 u^2), \quad \zeta = \frac{1}{\sqrt{G}} \left[ \frac{\partial u_2}{\partial x_1} - \frac{\partial u_1}{\partial x_2} \right].
\]
DG-3D Model: Computational Domain

Flux is the only “communicator” at the element edges

- Each face of the cubed-sphere is partitioned into $N_e \times N_e$ rectangular non-overlapping elements (i.e., total $6 \times N_e^2$).
- Each element is mapped onto the Gauss-Lobatto-Legendre (GLL) grid defined by $-1 \leq \xi, \eta \leq 1$, for integration.
Horizontal Advection: Moving Vortices on the Sphere

Deformational Flow Test: Nair & Jablonowski (MWR, 2007)

- The vortices are located at diametrically opposite sides of the sphere, the vortices deform as they move along a prescribed trajectory.

- Analytical solution is known and the trajectory is chosen to be a great circle along the NE direction ($\alpha = \pi/4$).
SW Test-2: Geostrophic Flow \((Nair et al., MWR 2005)\)

- High-order accuracy and spectral convergence

Steady state geostrophic flow \((\alpha = \pi/4)\). Max height error is \(\mathcal{O}(10^{-6})\) m.

\[\text{(a) DG 150x8x8: Geostrophic Flow (Day-5)}\]

\[\text{(b) Height Difference (Num - Exact)}\]

\[\text{DGM: SW Test-2, Convergence}\]

\[\text{Normalized Errors}\]

\[\text{Degree of the Legendre Polynomial}\]

\[\text{Normalized Errors vs Degree of the Legendre Polynomial}\]

\[\text{Normalized Errors vs Degree of the Legendre Polynomial}\]
No “spectral ringing” for the height fields

Flow over a mountain ($\approx 0.5^\circ$). Initial height field (left) and after 15 days of integration (right).
DG-3D: Baroclinic Instability Test

(JW-Test) Jablonowski & Williamson (QJRMS, 2006)

- To assess the evolution of an idealized baroclinic wave in the Northern Hemisphere.
- The initial conditions are quasi-realistic and defined by analytic expressions. Analytic solutions do not exist.
JW-Test: Evolution of Surface Pressure over the NH

- Baroclinic waves are triggered by perturbing the velocity field at (20°E, 40°N)
- This test case recommends up to 30 days of model simulation
- Ne = Nv = 8 (approx. 1.6°) with 26 vertical levels and \( \Delta t = 30 \) Sec.
DG-3D Model Vs. NCAR Spectral Model

- The HOMME-DG dynamical core successfully simulates baroclinic instability.

Simulated temperature (K) and surface pressure (hPa) at day 8 for a baroclinic instability test with the HOMME-DG model and the NCAR global spectral model (right). The horizontal resolution is approximately 1.4°.

Note that the DG solution is free of “spectral ringing”.
Jablonski-Williamson Baroclinic Test (Convergence)

Ps: Ne=3, Nv=10, Ni=18, Day 9

Ps: Ne=4, Nv=10, Ni=18, Day 9

Ps: Ne=6, Nv=10, Ni=18, Day 9

T@850mb: Ne=3, Nv=10, Day 9

T@850mb: Ne=4, Nv=10, Day 9

T@850mb: Ne=6, Nv=10, Day 9
Simulated surface pressure at day 11 for a baroclinic instability test with DG model, and NCAR global spectral model and a FV model. The models use 26 vertical levels and with approximate horizontal resolution of 0.7°.
DG-3D parallel performance: Sustained Mflops on IBM BG/L (1024 DP nodes, 700 MHz PPC 440s): Approx. 9% peak

Held-Suarez (preliminary) test: 800 days idealized climate simulation (1° resolution, 26 vertical levels, $\Delta t = 10$ Sec)
Summary

- The DG-3D model successfully simulates the Baroclinic instability test and the results are comparable with that of the NCAR global spectral model.

- The preliminary scaling results are impressive and comparable to the SE version in HOMME.

- The explicit R-K time integration scheme is robust for the DG-3D model, but very time-step restrictive.

- More efficient time integration schemes are required for practical climate simulations. Possible approaches: Semi-implicit, IMEX-RK, Rosenbrock with optimized Schwarz, etc..

- Future Work: Coupling of the CAM/CCSM physics for the real climate simulations in HOMME. Targeting for large-scale parallelism with $O(100K)$ processors.