High-Order Finite Volume Methods for Magnetohydrodynamics on Adaptive Cubed-Sphere Grids

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High-Order MHD on Adaptive Cubed-Sphere Grids
Main Application Driver: 3D Space-Physics Flows
Compressible Magnetohydrodynamic Plasmas - Cubed-Sphere Discretization

Images courtesy of SOHO/EIT consortium and NASA

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1. Conservation Laws - Magnetohydrodynamics
Models Compressible Conducting Fluid (Extension: Resistive MHD)

**Flow Governed by 3D Compressible MHD Equations**

- single-species fluid, isotropic pressure, magnetized inviscid compressible perfect gas (i.e. \( p = \rho RT \))

\[
\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho \vec{V} \\ \rho e \\ \vec{B} \end{pmatrix} + \vec{\nabla} \cdot \begin{pmatrix} \rho \vec{V} \vec{V} + \left( p + \frac{\vec{B} \cdot \vec{B}}{2} \right) \vec{I} - \vec{B} \vec{B} \\ (\rho e + p + \frac{\vec{B} \cdot \vec{B}}{2}) \vec{V} - (\vec{V} \cdot \vec{B}) \vec{B} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \eta \vec{T} \\ \eta (\nabla \times \vec{B}) \times \vec{B} \end{pmatrix}
\]

Inviscid Flux

\[ T_{i,j} = B_{j,i} - B_{i,j} \]

\[
\frac{\partial \vec{U}}{\partial t} + \vec{\nabla} \cdot \vec{F}_H (\vec{U}) + \vec{\nabla} \cdot \vec{F}_E (\vec{U}, \vec{\nabla} \vec{U}) = S_{\text{num}} + S_{\text{phy}}, \quad \nabla \cdot \vec{B} = 0
\]
Hyperbolic Conservation Laws - Discontinuities

High-order numerical methods are susceptible to oscillations at discontinuities (Gibbs phenomenon).

2,621,440 cells
Topics of Today’s Talk - Our Main Project Papers

1. Ivan, De Sterck, Northrup, and Groth; “Multi-Dimensional Finite-Volume Scheme for Hyperbolic Conservation Laws on Three-Dimensional Solution-Adaptive Cubed-Sphere Grids”, *JCP 2013*
   - second-order finite-volume method for MHD flows on 3D adaptive cubed-sphere grids

2. Susanto, Ivan, De Sterck, and Groth; “High-Order Central ENO Finite-Volume Scheme with Divergence Cleaning Approach for the Ideal MHD Equations”, *JCP 2013*
   - fourth-order finite-volume method for MHD (2D)
   - how to deal with $\nabla \cdot \vec{B} = 0$ on adaptive grids with high-order accuracy

3. Ivan, De Sterck, Susanto, and Groth; “High-Order Central ENO Finite-Volume Scheme for Hyperbolic Conservation Laws on Three-Dimensional Cubed-Sphere Grids”, *JCP 2015*
   - fourth-order finite-volume method for MHD flows on cubed-sphere grids
2. Discretizations of Spherical Domains

Several Options in the Literature

- Latitude-longitude grid constructs
- Cubed sphere
- Cartesian cut-cell approach
- Geodesic grid (e.g. icosahedron)
We Consider Cubed-Sphere Grids

Sadourny, 1972; Ronchi *et. al.*, 1996

(these images: Akshay Kulkarni)
3D Cubed-Sphere Grids
3. Parallel Adaptive Mesh Refinement (AMR)
Mechanics of Block-Based AMR (Simple 2D Example)

- Berger (1984); Berger & Colella (1989); Quirk (1991); De Zeeuw & Powell (1993); Quirk & Hanebutte (1993); Berger & Saltzman (1994); Groth et al. (1999, 2000); Keppens et al. (2011)
3D Cubed-Sphere Grids with Block-Based AMR

Ivan et al., “Multi-Dimensional Finite-Volume Scheme for Hyperbolic Conservation Laws on Three-Dimensional Solution-Adaptive Cubed-Sphere Grids”, (JCP 2013)
multi-block approach, ‘all blocks are treated equally’

- multi-dimensional discretization (handle unequal stencil size)
- multi-block code with unstructured root block connectivity
- consistently keep track of \((i,j,k)\) orientation and ordering of adjacent blocks (we use ‘Computational Fluid Dynamics General Notation System’ (CGNS))

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4. High-Order CENO FV Formulation \( O(\Delta x^n), n \geq 2 \)

Ivan et al., “High-Order Central ENO Finite-Volume Scheme for Hyperbolic Conservation Laws on Three-Dimensional Cubed-Sphere Grids”, (JCP 2015)

**Semi-Discrete Integral Form for a Hexahedral Element**

\[
\frac{d\bar{U}_{ijk}}{dt} = -\frac{1}{V_{ijk}} \iint_{\partial V} \left( \bar{F}_H + \bar{F}_E \right) \cdot \bar{n} \, da + \frac{1}{V_{ijk}} \iiint_V S \, dv = \mathbf{R}_{ijk}(\bar{U})
\]

**Semi-Discrete Form for High-Order Residual \( \mathbf{R}_{ijk}(\bar{U}) \)**

\[
\frac{d\bar{U}_{ijk}}{dt} = -\frac{1}{V_{ijk}} \sum_{l=1}^{N_f} \sum_{m=1}^{N_G} \left( \omega \left( \bar{F}_H + \bar{F}_E \right) \cdot \bar{n} \, \Delta a \right)_{ijk,l,m} + \frac{1}{V_{ijk}} \sum_{v=1}^{N_V} \left( \omega S \right)_{ijk,v}
\]

**High-Order Solution Procedure**

- High-order solution reconstruction
- Riemann problems at interfaces
- Time integration procedure
Flow Governed by 3D Compressible MHD Equations

- single-species fluid, isotropic pressure, magnetized inviscid compressible perfect gas (i.e. \( p = \rho RT \))

\[
\begin{align*}
\frac{\partial}{\partial t} \begin{bmatrix} \rho & \rho \vec{V} & \rho e \end{bmatrix} + \vec{\nabla} \cdot \begin{bmatrix} \rho \vec{V} \vec{V} + \left( p + \frac{\vec{B} \cdot \vec{B}}{2} \right) \vec{I} - \vec{B} \vec{B} \\ \left( \rho e + p + \frac{\vec{B} \cdot \vec{B}}{2} \right) \vec{V} - (\vec{V} \cdot \vec{B}) \vec{B} \end{bmatrix} &= S \\
\vec{\nabla} \cdot \\ \begin{bmatrix} 0 \\ 0 \\ \eta \vec{T} \\ \eta (\vec{\nabla} \times \vec{B}) \times \vec{B} \end{bmatrix} & = S
\end{align*}
\]

Inviscid Flux

\[ T_{i,j} = B_{j,i} - B_{i,j} \]

\[
\frac{\partial \vec{U}}{\partial t} + \vec{\nabla} \cdot \vec{F}_H (\vec{U}) + \vec{\nabla} \cdot \vec{F}_E \left( \vec{U}, \vec{\nabla} \vec{U} \right) = S_{\text{num}} + S_{\text{phy}}, \quad \vec{\nabla} \cdot \vec{B} = 0
\]
Potential Benefits of High-Order AMR Approaches

Linear reconstruction on uniform mesh

- $E_1 = 5.04E-05$
- $E_2 = 0.00024$
- $E_3 = 0.0072$
- Cells: 4,000,000

Cubic reconstruction with AMR

- $E_1 = 8.22E-05$
- $E_2 = 0.00069$
- $E_3 = 0.00624$
- Cells: 43,300

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High-Order MHD on Adaptive Cubed-Sphere Grids
Overview of Central Essentially Non-Oscillatory (CENO) Reconstruction

- Use high-order CENO approach (Ivan & Groth, 2007, 2011, 2014)

\[
    u^K_{ijk}(\vec{r}) = \sum_{p_1=0}^{K} \sum_{p_2=0}^{K} \sum_{p_3=0}^{K} \sum_{p_1+p_2+p_3 \leq K} (x - \bar{x}_{ijk})^{p_1}(y - \bar{y}_{ijk})^{p_2}(z - \bar{z}_{ijk})^{p_3} D_{p_1p_2p_3}
\]

- Use a single (central) stencil for reconstruction
- Avoids multiple stencils, as in (W)ENO
- Calculate \( D_{p_1p_2p_3} \) (20 unknowns for cubic, \( K = 3 \)) by solving a least-squares problem \( \mathbb{L}D - B = 0 \) to recover averages \( \bar{u}_{\gamma\delta\zeta} \) in the supporting stencil
- Solve instead \( \mathbb{L}D_C D_C^{-1}D - B = 0 \) for accuracy; \( D = D_C (\mathbb{L}D_C)^\dagger B \); Store \( D_C (\mathbb{L}D_C)^\dagger \) for efficiency
- Use a solution smoothness indicator to identify non-smooth reconstructions (treat each variable individually)
- Switch to limited linear 2nd-order scheme to preserve monotonicity
5. High-Order Approaches to Deal with the Divergence Constraint Condition, $\nabla \cdot \vec{B} = 0$

Susanto et al., “High-Order Central ENO Finite-Volume Scheme with Divergence Cleaning Approach for the Ideal MHD Equations”, (JCP 2013)

**Divergence Correction Technique: Generalized Lagrange Multiplier (GLM)-MHD (Dedner et al., 2002)**

\[
\frac{\partial \vec{B}}{\partial t} + \nabla \cdot (\vec{V} \vec{B} - \vec{B} \vec{V}) + \nabla \psi = 0
\]

\[
\frac{\partial \psi}{\partial t} + c_h^2 \nabla \cdot \vec{B} = -\frac{c_h^2}{c_p^2} \psi
\]

- Solve an extra transport equation for the GLM, $\psi$
- $\lambda_{8,9} = \pm c_h$, the largest eigenvalue in the domain
- fits nicely into hyperbolic code; automatically handles grid resolution changes, high-order accuracy
- $\psi$ can be discretized with low-order accuracy
- operator splitting does not degrade accuracy
High-Order Numerical Results: CENO-GLM
Magnetohydrostatic Test Case on Cartesian Box (Warburton 1999)

\[
U(x,y,z) = \left[ 1, \vec{0}, (\cos(\pi(y+1)) - \cos(\pi z))f(x), \cos(\pi z)f(y) + \sin(\pi(y+1))f(x), \sin(\pi z)(f(y) - f(x)), 5 + 0.5 \left( B_x^2 + B_y^2 + B_z^2 \right) \right]^T
\]

\[
f(u) = e^{-\pi(u+1)}
\]

Predicted \( \|\vec{B}\| \) field obtained using the 4th-order CENO scheme with GLM-MHD on a \( 8 \times 16 \times 16 \) mesh (left). Error norms in the predicted \( B_x \) (right).
High-Order Numerical Results: CENO-GLM

Iso-Density Vortex Problem in a Periodic Cartesian Box
(MHD exact solution for a vortex in forced equilibrium)
High-Order Numerical Results

3D Rotated MHD Shu-Osher Problem (prediction of shock/entropy interaction)
High-Order Numerical Results in 2D

Orszag-Tang Vortex Problem in a Periodic Cartesian Box with Dynamic AMR IC:
\[ \rho = \gamma^2, \quad v_x = -\sin(y), \quad v_y = \sin(x), \quad B_x = -\sin(y), \quad B_y = \sin(2x), \quad p = \gamma \]
High-Order Numerical Results in 2D
Orszag-Tang Vortex Problem in a Periodic Cartesian Box with Dynamic AMR
IC: $\rho = \gamma^2$, $v_x = -\sin(y)$, $v_y = \sin(x)$, $B_x = -\sin(y)$, $B_y = \sin(2x)$, $p = \gamma$

Pressure cuts at $y = 1.9635$ at two different times ($t = 2.0$ [left], and $t = 3.0$ [right]).
6. High-Order CENO on Cubed-Sphere Grids

(1) Hexas With Nonplanar Surfaces: Use a Trilinear Interpolation to Represent Hexas Accurately
2 Special Stencils: Stencil Formed With “Rotated” Cells in Degenerated Corners

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High-Order Numerical Results

Iso-Density Vortex Problem in a Solid-Core Cubed-Sphere Grid

\( R_o = 9, \vec{V} = (1, 1, 2), \vec{X}_{\text{initial}} = (-2, -2.5, -3), \vec{X}_{\text{final}} = (1, 0.5, 3), t = 3 \)
7. Parallel Performance (2nd-order)

Strong Scaling: Fixed Total Problem Size ($p_{ref} = 48$)
Parallel Performance (2nd-order)
Weak Scaling (constant problem size per core) up to 65,536 Cores on Mira System ($p_{ref} = 1$) – Iso-Density Vortex Problem in a Periodic Cartesian Box
8. Ongoing Work and Outlook

Further numerical developments
- high-order dynamic and anisotropic AMR in 3D
- implicit time integration (Newton-Krylov-Schwarz, nonlinear convergence acceleration, multilevel preconditioners, ...)
- AMR with adjoint error estimation
- ...

Current and Potential Applications
- Solar waves (coupled Solar interior-exterior, helioseismology)
- Stellar waves (asteroseismology)
- Solar wind interaction with Earth’s magnetosphere (space weather)
- supersonic escape from extrasolar planets (need radiative transfer)
- applications in geophysics (mantle flow), weather, climate, ...
Second-Order Numerical Results in 3D

Interaction of Solar-Wind and Moon With a Dipole Field Anomaly Near Surface

Inner sphere: **magnetic diffusion** $\partial_t \vec{B} = \eta \nabla^2 \vec{B}$; Outer domain: **ideal MHD**

Ghost-cell BCs: absorb wind on dayside; reflect $\vec{V}$ on nightside; $\vec{B}$ continuous

Setup and simulation (25,427,968 cells) performed by A. Susanto in PhD work
Anisotropic Refinement and Coarsening

Williamschen & Groth, “Parallel Anisotropic Block-Based Adaptive Mesh Refinement Algorithm For Three-Dimensional Flows”, AIAA, 2013
Steady Supersonic Spherical Outflow

Williamschen & Groth, “Parallel Anisotropic Block-Based Adaptive Mesh Refinement Algorithm For Three-Dimensional Flows”, AIAA, 2013, (Non-conductive Fluid)

Left: Isotropic AMR with 11,796,480 cells
Right: Anisotropic AMR with 442,368 cells
Two cubed-sphere grids embedded in a multi-block Cartesian grid

Extended 3D Cubed-Sphere Multi-Block Mesh
Thank you

Questions?
Numerical Results in 3D

Error Distribution for Reconstructed Solution of $f(x, y, z) = r^{-\frac{5}{2}}$, where $r$ is radius.

Error Norms of Cubic Reconstruction at $r=2.6$ for $f(r)=r^{-2.5}$

33 cells

57 cells

125 cells
Central Stencils for Reconstruction \((K = 3, 4)\)

81 Cells

57 Cells

33 Cells
Step 1: Calculate $\alpha$ (exploit the assumption of valid Taylor series expansion in the neighbourhood)

$$\alpha = 1 - \frac{\sum\sum\sum (u^K_{\gamma\delta\zeta}(\vec{r}_{\gamma\delta\zeta}) - u^K_{ijk}(\vec{r}_{\gamma\delta\zeta}))^2}{\sum\sum\sum\sum (u^K_{\gamma\delta\zeta}(\vec{r}_{\gamma\delta\zeta}) - \bar{u}_{ijk})^2}$$

Step 2: Evaluate $S$ (inspired by the definition of multiple-correlation coefficients, Lawson, 1974)

$$S = \frac{\alpha}{\max((1 - \alpha), \epsilon)} \frac{(\mathcal{N}_{SOS} - \mathcal{N}_D)}{(\mathcal{N}_D - 1)}$$

$\mathcal{N}_{SOS}$ : Size of Stencil; $\mathcal{N}_D$ : Degrees of Freedom/Unknowns; $\epsilon = 10^{-8}$

Step 3: Compare to a pass/no-pass cut-off value $S_c$

- if $S > S_c$ ⇒ smooth/fully-resolved solution
- if $S < S_c$ ⇒ non-smooth/discontinuous solution
- $1000 \lesssim S_c \lesssim 5000$ (determined from numerical experiments)
Behaviour of the Smoothness Indicator: \( f(\alpha) = \frac{\alpha}{1 - \alpha} \)
CENO Reconstruction of Smooth and Discontinuous Function on Cubed-Sphere Grid

Function Plot

Smoothness Indicator Distribution

Limited 2nd-order Reconstruction

4th-order Reconstruction

Block Mesh: 40^3 cells

F(x,y,z)

3.2
3
2.8
2.6
2.4
2.2
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
High-Order Numerical Results

Solution to Manufactured Problem

\[ U(x, y, z) = \begin{bmatrix} r^{-\frac{5}{2}}, & \frac{x}{\sqrt{r}}, & \frac{y}{\sqrt{r}}, & \frac{z}{\sqrt{r}} + \kappa r^{\frac{5}{2}}, & \frac{x}{r^3}, & \frac{y}{r^3}, & \frac{z}{r^3} + \kappa, & r^{-\frac{5}{2}} \end{bmatrix}^T, \quad \kappa = 0.017 \]

\[ R_i = 2, R_o = 3.5, M_{cf} > 0 \text{ everywhere} \]
High-Order CENO Results in Three Dimensions:
- Convergence Studies of Reconstructions
- Reconstruction of Smooth and Discontinuous Function
- Convergence Studies for MHD Manufactured Solution: Superfast Axisymmetric Inflow
Numerical Results in 3D

Reconstruction of \( f(x, y, z) = (1 - R + R^2)e^{x+y+z} \) on Cubed-Sphere Grids

Solution reconstruction obtained using the 4th-order CENO scheme on a mesh with 196,608 cells (left) and error norms for 2nd- and 4th-order (right).
High-Order 3D CENO-GLM Formulation for MHD

Accurate Evaluation of $R_{ijk}(\bar{U})$

- Use **CENO + GLM-MHD** (Dedner *et al.*, 2002) to satisfy $\nabla \cdot \vec{B} = 0$
- Susanto *et al.*, “High-Order Central ENO Finite-Volume Scheme with Divergence Cleaning Approach for the Ideal MHD Equations”, *(JCP 2013)*

**More accurate numerical flux at each integration point**

- Upwinding **hyperbolic flux** by solving a Riemann problem

$$\vec{F}_H = \vec{F}_H (U_L, U_R, \vec{n})$$

- Evaluate $U_L, U_R$ more accurately using a CENO reconstruction
- Evaluate **elliptic flux** using high-order solution gradients

$$\vec{F}_E \cdot \vec{n} = \vec{F}_E (U, \vec{\nabla}U, \vec{n})$$

$$U = \frac{1}{2} (U_L + U_R) \quad \vec{\nabla}U = \frac{1}{2} (\vec{\nabla}U_L + \vec{\nabla}U_R)$$

- Evaluate $\vec{\nabla}U_L, \vec{\nabla}U_R$ using the same high-order reconstruction
- Achieve $O(\Delta x^{K+1})$ solution by selecting $K$ and $N_G$ appropriately (e.g., $K = 4$ with $N_G = 2$)
High-Order CENO with 3D AMR

High-order solution transfer from coarse to fine cells and vice-versa

- Evaluate volumetric integral over the cell domain:

\[
I = \int \int \int g(\vec{X}(p, q, s)) \det J \, dp \, dq \, ds \approx \sum_{m=1}^{N_v} g(\vec{X}(p_m, q_m, s_m)) \left( \det J \right)_m \omega_m = \sum_{m=1}^{N_v} g(\vec{X}_m) \tilde{\omega}_m
\]

- High-order prolongation of coarse \( u_{ijk}^{K} (\vec{X}) \) to each fine cell (e.g., octant 1):

\[
\bar{u}_1 = \frac{1}{V_1} \int \int \int u_{ijk}^{K} (\vec{X}(p, q, s)) \det J \, dp \, dq \, ds = \sum_{m=1}^{N_v} u_{ijk}^{K} (\vec{X}_m) \tilde{\omega}_m (\tilde{\omega}_m)_1 = \frac{(\tilde{\omega}_m)_1}{\omega_m}
\]

Key Elements of High-Order AMR

- Use the coarse-cell \( \vec{X}_m \) points; it avoids computing 8 trilinear mappings
- Derive weights \( (\tilde{\omega}_m)_s \) s.t. to integrate exactly \( u_{ijk}^{K} (\vec{X}) \) on subdomain \( s \)
- Weights \( (\tilde{\omega}_m)_s \) are specific to each canonical octant (i.e., subdomain)
- For cubic \( (K = 3) \) there are 64 \( \vec{X}_m \) (i.e., \( 4 \times 4 \times 4 \) tensor product)
- Restriction operator is based on conservation of fine-cell mean solutions
Second-Order FV AMR Simulation Framework

Ivan et al., “Multi-Dimensional Finite-Volume Scheme for Hyperbolic Conservation Laws on Three-Dimensional Solution-Adaptive Cubed-Sphere Grids”, (JCP 2013)
High-Order Numerical Results

Left: Euler Bow Shock \[ R_i = 1, R_o = 3.7, M = 2.8 \]
Right: Magnetically Dominated Bow Shock \[ R_i = 1, R_o = 6, M_{Ax} = 1.49, \theta_{vB} = 5^\circ \]
Prediction of Mach and total magnetic field, \( B_T \), by 4th-order CENO on 320 blocks

1,966,080 cells

2,621,440 cells
High-Order Numerical Results

Iso-Density Vortex Problem in a Cubed-Sphere Grid with AMR

\( R_i = 1, \quad R_o = 17, \quad \vec{V} = (1, 1, 2), \quad \vec{X}_{\text{initial}} = (0, -7, -7), \quad \vec{X}_{\text{final}} = (5, -2, 3), \quad t = 5 \)
Concluding Remarks & Future Research

Parallel High-Order AMR Simulation Framework

- Developed for 3D cubed-sphere grids and space-physics flows
- Applicable to general hexahedral as well as unstructured grids
- Achieves 4th-order accuracy for MHD using CENO + GLM-MHD
- Permits local solution-directed mesh refinement
- Relatively adequate refinement driven by smoothness-based refinement criteria
- Handles and resolves regions of strong discontinuities/shocks
- Accuracy and computational cost assessment based on test problems with analytical solutions
- Assessment of parallel performance on thousands of CPUs cores

On-Going Research

- Application to more complex space-physics problems
- Coupling of high-order scheme with anisotropic AMR