Hyperbolic Conservation Laws on 3D Cubed-Sphere Grids: A Parallel High-Order Solution-Adaptive Simulation Framework

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Project: “Solar Drivers of Space Weather: Contributions to Forecasting”

**Goal:** Develop advanced simulation methods for MHD space plasmas and apply to space-weather forecasting.

**Housed At:** Applied Math., U. Waterloo

**Collaborators:** UTIAS, NRCan, Others

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3D Parallel High-Order AMR Simulation Framework
Potential Benefits of High-Order AMR Approaches

- Linear reconstruction on uniform mesh
- Cubic reconstruction with AMR

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3D Parallel High-Order AMR Simulation Framework
1. Governing Equations
2. Parallel Implicit Solution-Adaptive Cubed-Sphere Simulation Framework
3. Extension to High-Order Accuracy
4. Numerical Results
5. Concluding Remarks & Future Research
Ideal Magnetohydrodynamics (MHD) Equations

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

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

\[
\begin{align*}
\frac{\partial}{\partial t} \begin{bmatrix} \rho \\ \rho \vec{V} \\ \rho \vec{E} \\ \vec{B} \end{bmatrix} + \vec{\nabla} \cdot \begin{bmatrix} \rho \vec{V} \\ \rho \vec{V} \vec{V} + (p + \vec{B} \cdot \vec{B}/2) \vec{I} - \vec{B} \vec{B} \\ (\rho e + p + \vec{B} \cdot \vec{B}/2) \vec{V} - (\vec{V} \cdot \vec{B}) \vec{B} \end{bmatrix} &= Q + S \\
\frac{\partial \mathbf{U}}{\partial t} + \vec{\nabla} \cdot \mathbf{F} &= Q + S, \quad \nabla \cdot \vec{B} = 0
\end{align*}
\]

**Main Challenges to the Numerical Discretization**

- Maintain physical solution (e.g. positive pressure & density)
- Provide both solution accuracy and monotonicity even in the presence of discontinuous solutions (e.g. shocks, contacts)
- Avoid shockwave instabilities (e.g. carbuncle phenomenon)
Ideal Magnetohydrodynamics (MHD) Equations

Approaches to Deal with the Divergence Constraint Condition, $\nabla \cdot \vec{B} = 0$

**Powell Source Term (Powell et al., 1999)**

$$ S = -\nabla \cdot \vec{B} \left[ 0, \vec{B}, \vec{V}, \vec{V} \cdot \vec{B} \right]^T $$

- 8-wave MHD system that is symmetric and Galilean invariant
  $\lambda_{1,2} = v_x \pm c_{fx}, \quad \lambda_{3,4} = v_x \pm c_{Ax}, \quad \lambda_{5,6} = v_x \pm c_{sx}, \quad \lambda_{7,8} = v_x$
- Numerical error in $\nabla \cdot \vec{B}$ is convected out of the domain by $\lambda_8 = v_x$

**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
Talk Outline

1. Governing Equations
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Discretizations of Spherical Domains

Several Options in the Literature

- Latitude-longitude grid constructs
- Cubed sphere
- Cartesian cut-cell approach
- Geodesic grid (e.g. icosahedron)
3D Cubed-Sphere Multi-Block Mesh in CFFC
Adequate Data Structured Required to Handle the Complex Block Connectivity

Cross-section of the cubed-sphere grid (left) and illustration of connectivity among blocks (right)
Computational Elements (Cells, Control Volumes)

Accurate Geometry Representation Required for High-Order Schemes

Representative hexa for 3D cubed-sphere grids

Examples of 2D quadrilaterals with straight and curved edges
Parallel Implicit AMR Finite-Volume Framework

Finite-Volume Formulation

General System of Conservation Laws

\[ \frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F} = \mathbf{S} + \mathbf{Q} \]

Semi-Discrete Integral Form for Hexahedral Cell \((i,j,k)\)

\[ \frac{d\mathbf{U}_{i,j,k}}{dt} = -\frac{1}{V_{i,j,k}} \sum_{m=1}^{N_f} \left( \mathbf{F} \cdot \mathbf{n} \, \Delta A \right)_{i,j,k,m} + (\mathbf{S})_{i,j,k} + (\mathbf{Q})_{i,j,k} = \mathbf{R}_{i,j,k}(\mathbf{U}) \]

Primary Steps to Obtaining Numerical Solution

- **Solution reconstruction**: limited piecewise linear approximation
- **Spatial residual computation**:
  - Interface flux evaluation: hyperbolic (& elliptic fluxes)
  - Source term integration
- **Time Integration**: evolve solution forward in time
  - Multi-stage explicit time marching schemes (e.g., RK2, RK4)
  - Parallel implicit NKS algorithm (Northrup & Groth, 2009)
Parallel Implicit AMR Finite-Volume Framework
Linear Least-Squares Reconstruction (Barth, 1993) on Cubed-Sphere Grids

Linear Reconstruction of Primitive Variables

\[ W_{i,j,k}(\vec{x}) = \overline{W}_{i,j,k} + \Phi_{i,j,k} \vec{\nabla} W \cdot (\vec{x} - \vec{x}_{i,j,k}) \]
Parallel Implicit AMR Finite-Volume Framework
Inviscid (Hyperbolic) Flux Evaluation

**Numerical Flux Evaluation for Calculating** \( R_{i,j,k}(\overline{U}) \)

- Solve a Riemann problem at each integration point to provide upwinding

\[
\vec{F}_H = \frac{1}{2} \left( \vec{F}_H (U_R, \vec{n}) + \vec{F}_H (U_L, \vec{n}) \right) - \frac{1}{2} |A (U_R, U_L, \vec{n})| (U_R - U_L)
\]

- Some Riemann solvers use only the fastest and slowest waves
- There are six flux evaluation points for a hexahedral cell

Riemann Solvers: HLLE, Lax-Friedrichs, Linde’s
Inexact Newton’s Method

- Semi-discrete form of the governing equations for steady flows
  \[ R(U) = 0 \]  \hspace{1cm} (1)

- Apply Newton’s method to solve Eq. (1) for \( U \)
  \[
  \left( \frac{\partial R}{\partial U} \right)^n \Delta U^n = J^n \Delta U^n = -R(U^n) \]  \hspace{1cm} (2)

- Solve at each Newton step the sparse linear system of Eq. (2)
  \[ Jx = b \]
  using a preconditioned iterative linear solver (GMRES) which is not fully converged
Parallel Implicit AMR Finite-Volume Framework
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)

Parallel Implicit AMR Finite-Volume Framework

3D Block-Based AMR (Berger, 1984; Gao & Groth, 2010)

- Mesh refinement by division and coarsening of self-similar structured blocks (hexahedral cells)
- Solution transfer among blocks via overlapping ghost cells
- Hierarchical octree data structure provides block connectivity
- Permits local refinement of mesh
- Physics-based refinement criteria (e.g. $\epsilon_1 \propto |\vec{\nabla} \rho|$, $\epsilon_2 \propto |\vec{\nabla} \cdot \vec{V}|$, $\epsilon_3 \propto |\vec{\nabla} \times \vec{V}|$)
- Permits parallel implementation via domain decomposition
- Highly efficient load balancing is obtained by equally distributing the solution blocks among CPUs
Parallel Implicit AMR Finite-Volume Framework

3D AMR on Cubed-Sphere Grid

CFFC Implementation

- Truly 3D AMR (also used as block-multiplication procedure)
- Body-fitted mesh by constraining the points on the boundary spheres
Parallel Implicit AMR Finite-Volume Framework

Transparent Reconstruction for Blocks of Different Resolution

\[
W_{i,j,k}(\vec{x}) = \bar{W}_{i,j,k} + \Phi_{i,j,k} \nabla W \cdot (\vec{x} - \vec{x}_{i,j,k})
\]

Linear Reconstruction of Primitive Variables

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Transparent Implementation At Block Boundaries

Goals: Have Transparency At Block Boundaries For

- high-order accurate fluxes
- adaptivity
- implicit time integration
- parallelisation
Transparent Implementation At Block Boundaries

**Technical Details**

- unstructured root block connectivity
- consistently keep track of \((i, j, k)\) orientation ordering
- \(k\)-exact least-squares with variable stencil size
- collapsed ghost cells at degenerated corners
- limit mesh resolution change to factor 2
- parallel domain decomposition with self-similar solution blocks
Talk Outline

1. Governing Equations
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Overview Idea of the High-Order MHD Algorithm

- Apply a high-order CENO approach (Ivan & Groth, 2007) (initially proposed for 2D inviscid and viscous flows, but not for MHD)
- Use CENO + GLM-MHD (Dedner et al., 2002) to satisfy $\nabla \cdot \vec{B} = 0$

Central Essentially Non-Oscillatory (CENO) Idea

- ENO Property: **Spurious oscillations** proportional to the size of the jump at points of discontinuity are **NOT allowed** (i.e. no Gibbs-like phenomenon) but **they may exist** on the order of truncation error.
- Combine an **unlimited** $k$-exact reconstruction with a monotonicity preserving **limited linear** ($k = 1$) scheme
- Use a **single (central) stencil** for reconstruction
- Hybrid method: use a **smoothness indicator** to switch between reconstruction procedures

Note: ENO scheme on a fixed central stencil have been explored in 1D by Harten & Chakravarthy, 1991
CENO High-Order Finite-Volume Formulation
2D Algorithm on Quadrilateral Elements

General System of Conservation Laws
\[
\frac{\partial U}{\partial t} + \vec{\nabla} \cdot \vec{F} = S + Q
\]

Semi-Discrete Integral Form for Quadrilateral Element
\[
\frac{d\overline{U}_{i,j}}{dt} = -\frac{1}{A_{i,j}} \oint_{\Omega} \vec{F} \cdot \vec{n} \, d\ell + \frac{1}{A_{i,j}} \iint_{A} (S + Q) \, da = R_{i,j}(\overline{U})
\]

Primary Steps to Obtaining Numerical Solution
- **Solution reconstruction**: high-order piecewise polynomials
- **High-order spatial residual computation**:
  - Interface flux evaluation: hyperbolic & elliptic fluxes
  - Source term integration
- **Time Integration**: evolve solution forward in time
  - Multi-stage explicit time marching schemes (e.g., RK2, RK4)
High-Order Spatial Discretization Procedure

Requires More Accurate Evaluation of $\mathbf{R}_{i,j}(\mathbf{U})$

- More accurate calculation of flux and source term integrals
  \[
  \frac{1}{A_{i,j}} \int_{\Omega} \mathbf{F} \cdot \mathbf{n} \, d\ell = \frac{1}{A_{i,j}} \sum_{l=1}^{N_f} \sum_{m=1}^{N_G} \left( \omega \mathbf{F} \cdot \mathbf{n} \Delta \ell \right)_{i,j,l,m}
  \]

- **Solution** ⇒ Use more Gauss quadrature points ($N_G \geq 2$)

- More accurate numerical flux at each integration point
  
  Upwinding hyperbolic flux by solving a Riemann problem
  \[
  \mathbf{F}_H = \mathcal{F}_H (\mathbf{U}_L, \mathbf{U}_R, \mathbf{n})
  \]

- **Solution** ⇒ Evaluate $\mathbf{U}$ more accurately at faces of computational cells (i.e., high-order solution reconstruction)
Central ENO (CENO) Reconstruction in 3D

- Piecewise polynomial approximation for solution:

\[
W_{i,j,\kappa}^k(\vec{r}) = \sum_{p_1=0}^{k} \sum_{p_2=0}^{k} \sum_{p_3=0}^{k} (x - \bar{x}_{i,j,\kappa})^{p_1} (y - \bar{y}_{i,j,\kappa})^{p_2} (z - \bar{z}_{i,j,\kappa})^{p_3} D_{p_1 p_2 p_3}^k
\]

- Use a trilinear interpolation to represent skewed hexas accurately
- Compute all volume and face integrals based on the trilinear mapping
- Use a supporting stencil to determine \( D_{p_1 p_2 p_3} \) (e.g., maximum 125 cells for cubic and quartic polynomials)
Numerical Results in 2D
Supersonic Flow Past Cylinder at $M_\infty = 2.1$

Final mesh: 2,150 $10 \times 10$ blocks

Predicted pressure distribution obtained using the 4th-order CENO scheme on final refined AMR mesh and regions of limited and unlimited reconstruction
Numerical Results in 2D
Superfast Rotating Outflow from the Cylinder
$R_i = 1, R_o = 6$, Inflow: $\rho = 1, p = 1, V_r = 3, V_\theta = 1, B_r = 1$

Predicted density distribution obtained using the 4th-order CENO scheme with GLM-MHD on a $80 \times 80$ mesh (left). Error norms in the predicted solution entropy (right).
Numerical Results in 2D

MHD Shu-Osher’s Shock Tube at $45^\circ$ Relative to Grid

Interaction of sinusoidal density variation with moving shockwave

Comparison of predicted density distributions obtained using the 4th-order CENO and the 2nd-order schemes in combination with GLM-MHD.
Numerical Results in 3D

Transonic Wind on AMR Mesh

$R_i = 1$, $R_o = 10$, $GM_* = 14$, Inflow: $\rho = 5$, $p = 23$

Predicted Mach number distribution obtained on the adapted cubed-sphere mesh (left). Comparison of flow properties in the X-axis direction relative to a highly-accurate 1D “exact solution” (right).
Numerical Results in 3D

Time-Invariant Solar Wind \( R_i = 1, R_o = 100, \gamma = 5/3, n_s = 1.4 \times 10^8 \text{cm}^{-3}, T_s = 2.0 \times 10^6 \text{K} \)

Solar wind conditions based on the model of Groth et al., 2000

- Magnetic field strength: 8.4 G at the poles and 2.2 G at the equator.
- Differential heating in closed and open field line regions
- The actual simulation had the magnetic and rotational axes aligned.

Magnetic field strength: 8.4 G at the poles and 2.2 G at the equator.
Differential heating in closed and open field line regions
The actual simulation had the magnetic and rotational axes aligned.
Numerical Results in 3D

Time-Invariant Solar Wind $R_i = 1, R_o = 30, \gamma = 5/3, n_s = 1.4 \times 10^8 \text{cm}^{-3}, T_s = 2.0 \times 10^6 \text{K}$

Prediction of solar-wind speed and magnitude of $\vec{B}$ obtained on 96 $20 \times 20 \times 20$ blocks and 768,000 cells.
Numerical Results in 3D

Time-Invariant Solar Wind \( R_i = 1, R_o = 30, \gamma = 5/3, n_s = 1.4 \times 10^8 \text{cm}^{-3}, T_s = 2.0 \times 10^6 \text{K} \)

Close-up view of magnetic field lines and multi-block mesh
Numerical Results in 3D
CFFC Parallel Strong Scaling Performance on SciNet GPC (Nehalem processors)

Solar Wind Flow; Limited 2nd-order FV Scheme;
6,144 Blocks of 8x8x8 Cells; 2,000 5-stage Explicit Time Steps

Speedup ($S_p$)

Efficiency ($E_p$)

Number of Processor Cores ($p$)

Ideal Speedup
Ideal Efficiency
Numerical Speedup
Numerical Efficiency
Solution reconstruction obtained using the 4th-order CENO scheme on a mesh with 8 blocks of $4 \times 8 \times 8$ and 2,048 cells (left) and error norms (right).
Numerical Results in 3D Magnetohydrostatic Test Case on Cartesian Box (Warburton 1999)

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

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

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).
Talk Outline

1. Governing Equations
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Concluding Remarks & Future Research

Parallel Solution-Adaptive Simulation Framework

- Developed for 3D cubed-sphere grids and space-physics flows
- Uses multi-dimensional FVM and gnomonic cubed-sphere grids
- Permits local solution-directed mesh refinement
- Extended to 4th-order accuracy using CENO + GLM-MHD
- Handles and resolves regions of strong discontinuities/shocks
- Accuracy assessment based on several test problems
- Excellent parallel performance on thousands of CPUs
- Applied to realistic solar winds for distances up to 1AU

On-Going Research

- Further investigation of the adaptive cubed-sphere algorithm in conjunction with high-order accuracy (e.g., dynamic AMR)
- Application to more complex space-physics problems (e.g., CME propagation, solar wind-magnetosphere interaction)
Acknowledgments

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Appendix
Central ENO (CENO) Reconstruction
Compromise Between Accuracy, Efficiency and Robustness


- Combine an unlimited $k$-exact reconstruction with a monotonicity preserving limited linear ($k = 1$) scheme, both using fixed central stencils.
- Hybrid method: use a smoothness indicator to switch between the two reconstruction procedures.

Note: Hybrid ENO on fixed stencil explored in 1D by Harten & Chakravarthy, 1991

Advantages of CENO Reconstruction:

- Provides **ENO-like accuracy** in smooth regions & strictly ensures **monotonicity** near discontinuities.
- Always uses the **same central stencil**, avoids complexities of ENO and WENO schemes (i.e., multiple and possibly poorly conditioned stencils).
- Readily extendable to multiple dimensions & variables, unstructured mesh.
- Identifies regions of **under-resolved** and **non-smooth data** (may be useful for mesh adaptation).
Central ENO (CENO) Reconstruction
Compromise Between Accuracy, Efficiency and Robustness


- Combine an **unlimited \( k \)-exact reconstruction** with a monotonicity preserving **limited linear \((k = 1)\)** scheme, both using fixed central stencils.
- Hybrid method: use a smoothness indicator to switch between the two reconstruction procedures.

Note: Hybrid ENO on fixed stencil explored in 1D by Harten & Chakravarthy, 1991

**Disadvantages of CENO Reconstruction:**

- Loss of uniform accuracy (not, in the strict sense, an ENO scheme)
- Requires two solution reconstructions for non-smooth stencils
Determination of Smoothness Indicator in 3D

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

$$
\alpha = 1 - \frac{\sum_{\gamma} \sum_{\delta} \sum_{\zeta} \left( u_{\gamma,\delta,\zeta}^k \left( \vec{r}_{\gamma,\delta,\zeta} \right) - u_{i,j,\kappa}^k \left( \vec{r}_{\gamma,\delta,\zeta} \right) \right)^2}{\sum_{\gamma} \sum_{\delta} \sum_{\zeta} \left( u_{\gamma,\delta,\zeta}^k \left( \vec{r}_{\gamma,\delta,\zeta} \right) - \bar{u}_{i,j,\kappa} \right)^2}
$$

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

$$
S = \frac{\alpha}{\max \left( (1 - \alpha), \epsilon \right)} \frac{(SOS - DOF)}{(DOF - 1)}
$$

$SOS$ : Size of Stencil; $DOF$ : Degrees of Freedom; $\epsilon = 10^{-8}$

- **Step 3:** Compare to a pass/no-pass cutoff value $S_c$

- if $S > S_c \Rightarrow$ smooth/fully-resolved solution
- if $S < S_c \Rightarrow$ non-smooth/discontinuous solution
- $1000 \leq S_c \leq 5000$ (determined from numerical experiments)
Behaviour of the Smoothness Indicator: \( f(\alpha) = \frac{\alpha}{1 - \alpha} \)
Numerical Results

Transonic Wind on Fixed Mesh

\[ R_i = 1, \quad R_o = 10, \quad GM_* = 14, \quad \text{Inflow: } \rho = 5, \quad p = 23 \]

Mach Prediction for an Inviscid Compressible Diatomic Fluid Expanding in Gravitational Field

Predicted Mach number distribution obtained on a uniform mesh with 1,228,800 total cells and 128 cells in the radial direction.
Numerical Results

Transonic Wind on Fixed Mesh

$R_i = 1$, $R_o = 10$, $GM_* = 14$, Inflow: $\rho = 5$, $p = 23$

Comparison of flow properties along X-axis for M1 (19,200), M2 (153,600) and M3 (1,228,800) meshes relative to a 1D “exact solution” obtained with Newton Critical Point (NCP) method (De Sterck et. al. 2009).
Numerical Results

Supersonic Flow Past a Sphere

\( M_\infty = 2.0, R_i = 1, R_o = 32, GM_* = 0 \)

Predicted density distribution on the final refined AMR mesh with 10,835 blocks and 8,321,280 computational cells (7 levels of refinement, \( \eta = 0.993 \))
Numerical Results in 3D
Solution to Manufactured Problem

\[ R_i = 2, \quad R_o = 3.5, \quad M_{cf} > 1 \quad \text{everywhere} \]

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

Error norms in the predicted solution density (left). Comparison of explicit and NKS implicit algorithms for the number of equivalent residual evaluations and the computational time on Intel Xeon E5540 (right).
Numerical Results in 3D
Magnetically Dominated Bow Shock

$R_i = 1, R_o = 8, M_{Ax} = 1.49, \theta_{vB} = 5^\circ$

Cubed-sphere grid formed by only five root blocks (left). Predicted acoustic Mach number distribution in the (x,y) plane after 7 refinement levels and with 22,693 blocks and 14,523,520 computational cells (right).