A Parallel and Dynamically Adaptive 3D Cubed-Sphere Grid Framework for Hyperbolic Conservation Laws

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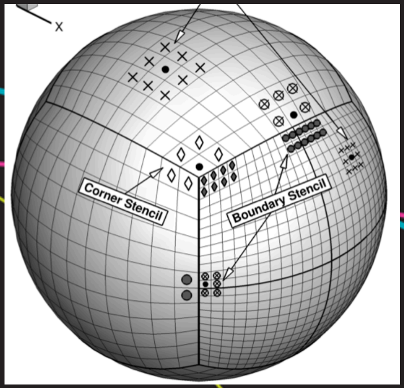
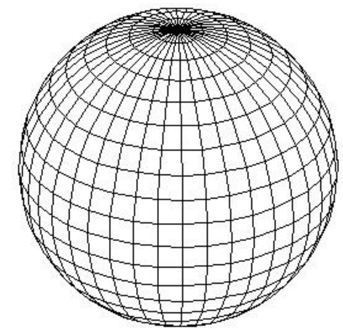


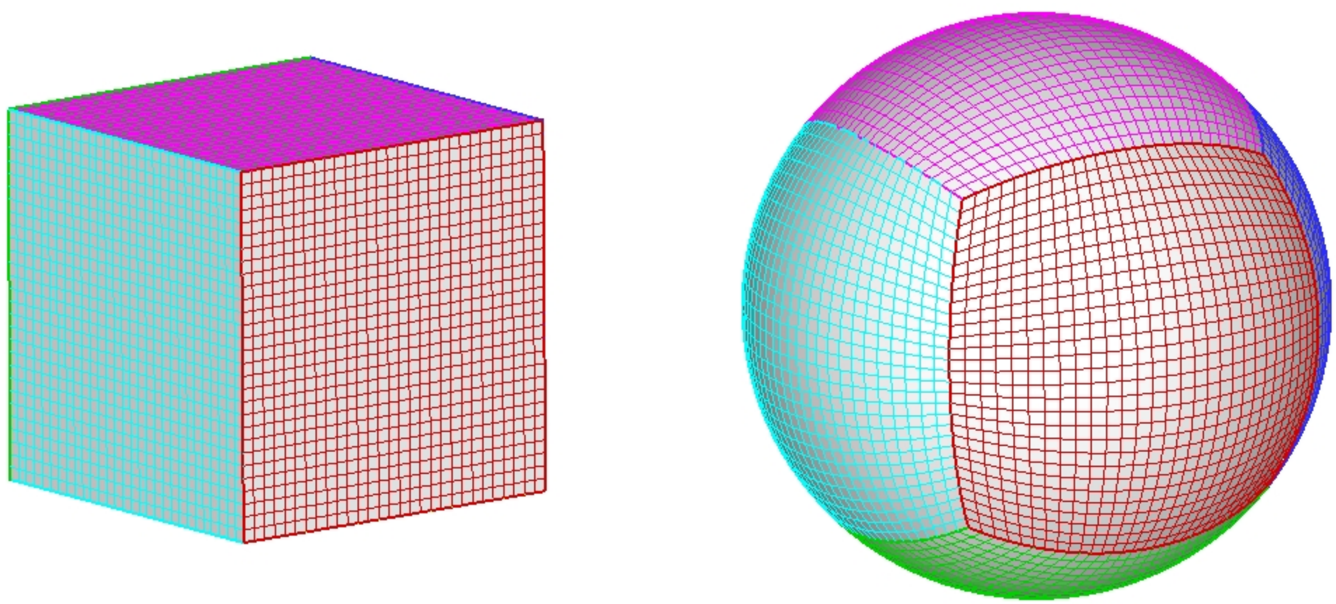
SIAM Conference on Computational Science and Engineering, February 2013

(1) cubed-sphere grids

- goal: solve PDE systems on a sphere (2D), or in a 3D domain between two concentric spheres
- cubed-sphere grids are attractive because
  - quasi-uniform (Cartesian panels)
  - no strong polar singularity



(image: mitgcm.org)



(image: Akshay Kulkarni (Harvard))

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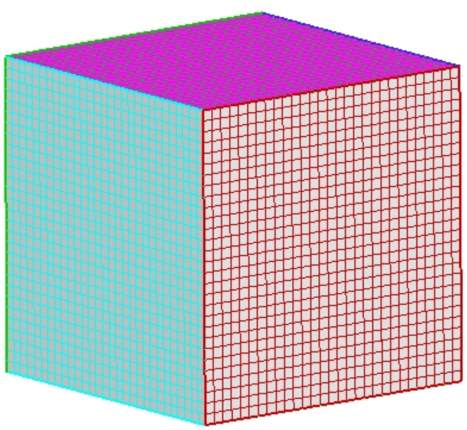
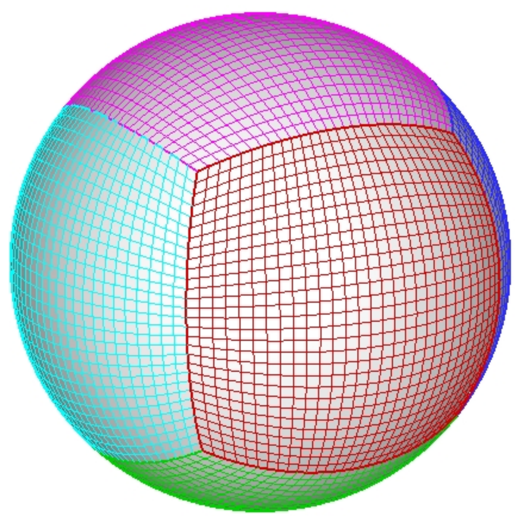
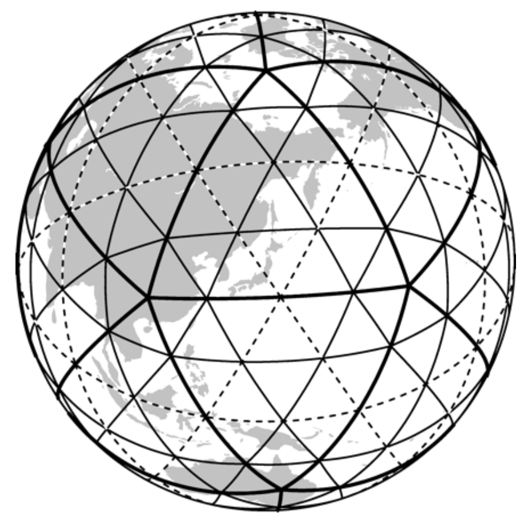
cubed-sphere grids

- cubed-sphere grids are rapidly gaining popularity in a wide area of application fields (weather, climate, oceans, astrophysics, space physics, Earth mantle, ...)
- Sadourny, 1972; Ronchi et al., 1996; and many more authors since (including Ullrich, Fragile, Cai, Erath, Zarzycki, Harris, Taylor, Johansen, Ivan, Bao, Chen, with collaborators, and many others, including several other talks and posters at this conference)





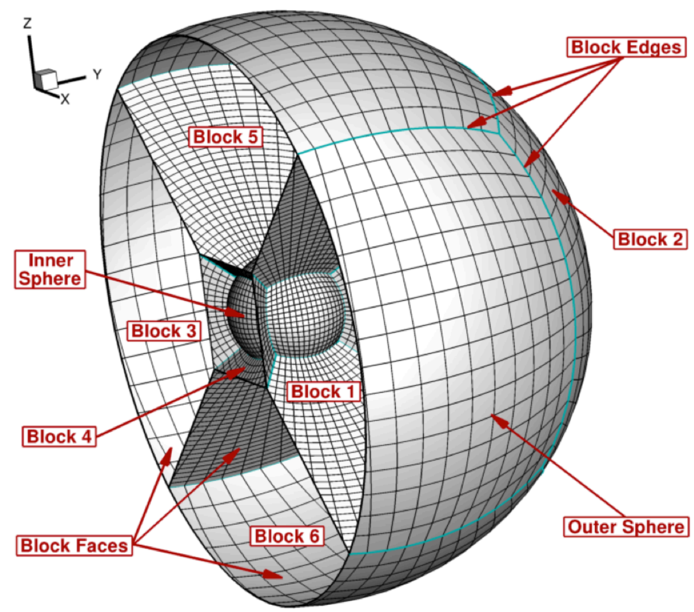
(image: Akshay Kulkarni (Harvard))

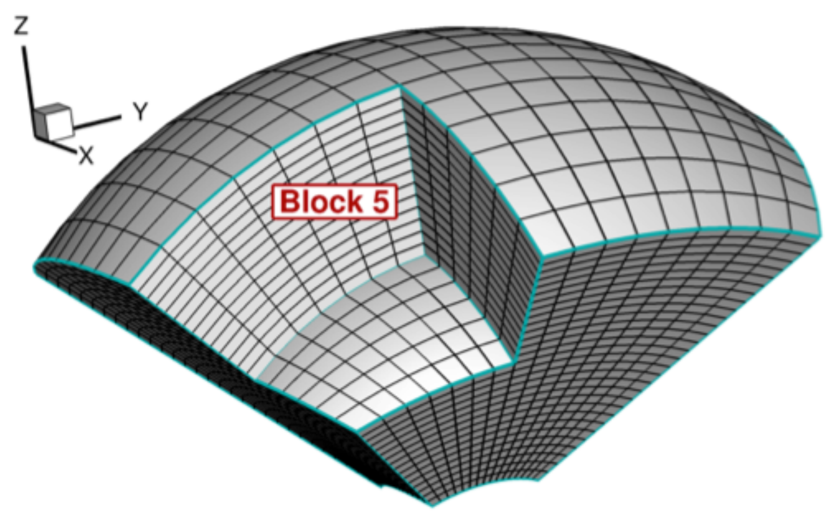


icosahedral grid
(image: Washington et al.)

this talk: 3D cubed-sphere grids

- solve PDEs in domain between two concentric spheres
- 6 ‘sectors’ of the cubed-sphere grid (in 2D: panels)
- each sector is logically Cartesian
- sector boundaries and corners can cause difficulties





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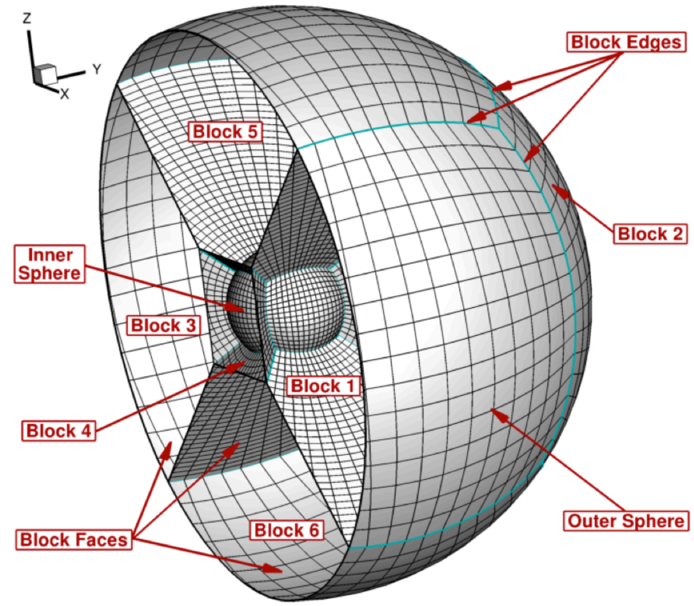
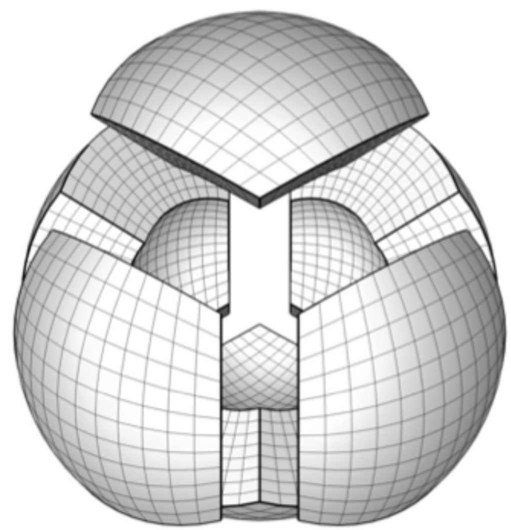
this talk: 3D cubed-sphere grids

- note: in many Earth atmosphere applications, the ‘thin’ atmosphere is approximated by stacked 2D layers (shallow water)

- solving for 2D flow in these layers requires a different coordinate system on each panel, and sophisticated coordinate transformations (extensive ongoing work in this area)

  (3rd dimension is treated separately)





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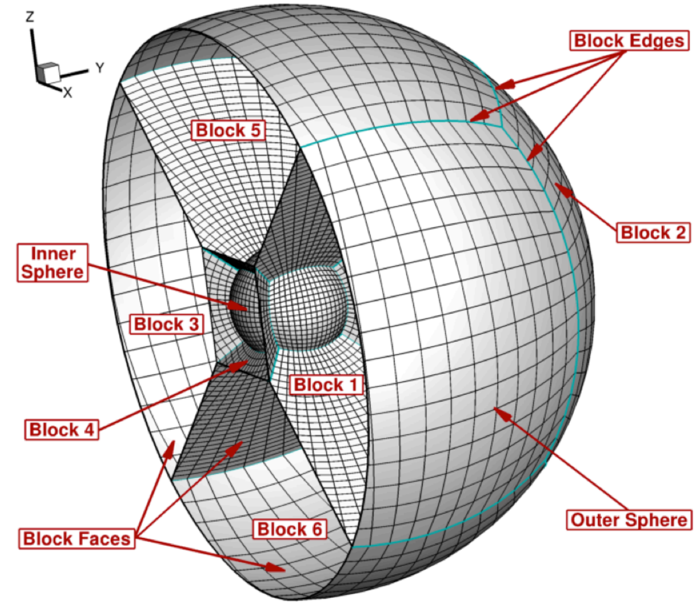
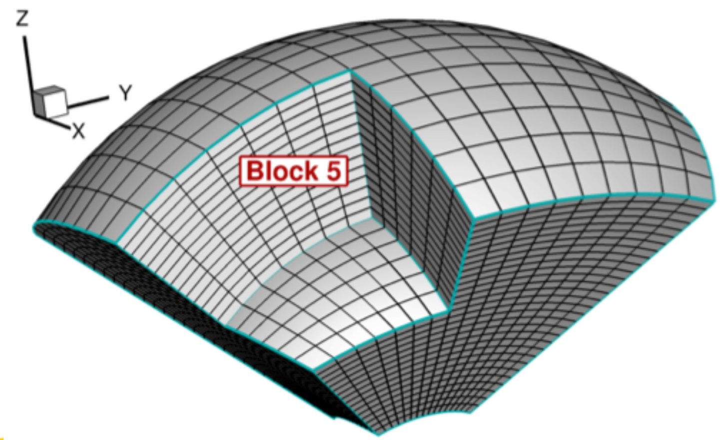
this talk: 3D cubed-sphere grids

- instead, the problems we are interested in are most easily treated in full 3D space with a single xyz coordinate system (this is a case where 3D is easier than 2D!)

- this simpler xyz setting allows us to focus on making advances in fully-3D discretizations, and in large-scale adaptivity and parallelism in 3D (rather than 2D) (astrophysics, solar and planetary physics, Earth mantle, ...)





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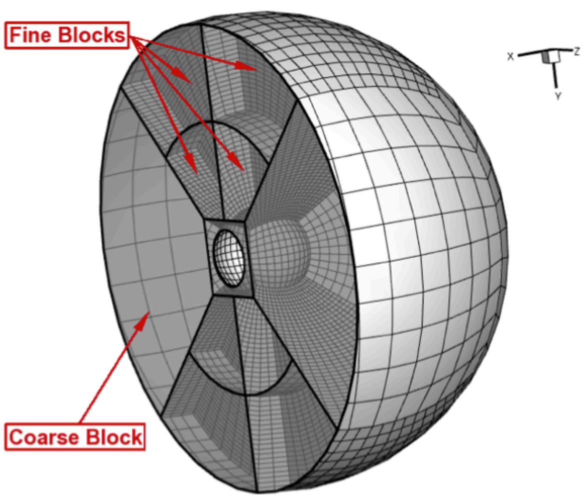
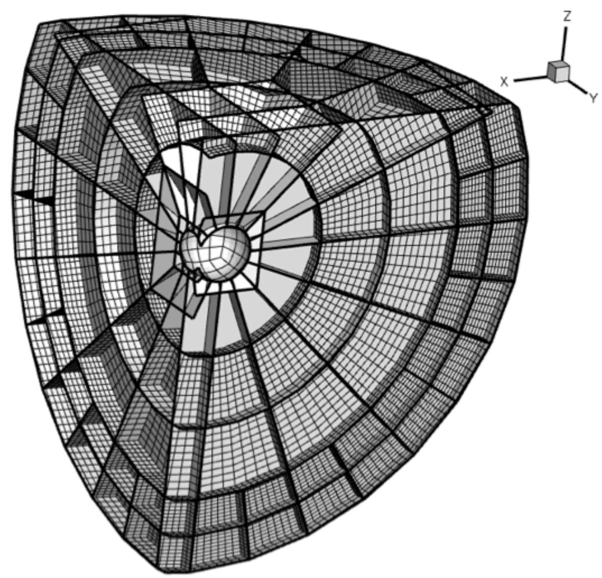
(2) our goals

- solve nonlinear hyperbolic conservation laws on 3D cubed-sphere grids, uniform second-order *accuracy*
- block-based *adaptive* grid refinement framework (logically Cartesian, self-similar blocks)
- large-scale *parallelism*: >30,000 adaptive blocks, >6,000 parallel CPU cores
- challenge: properly treat sector boundaries and corners

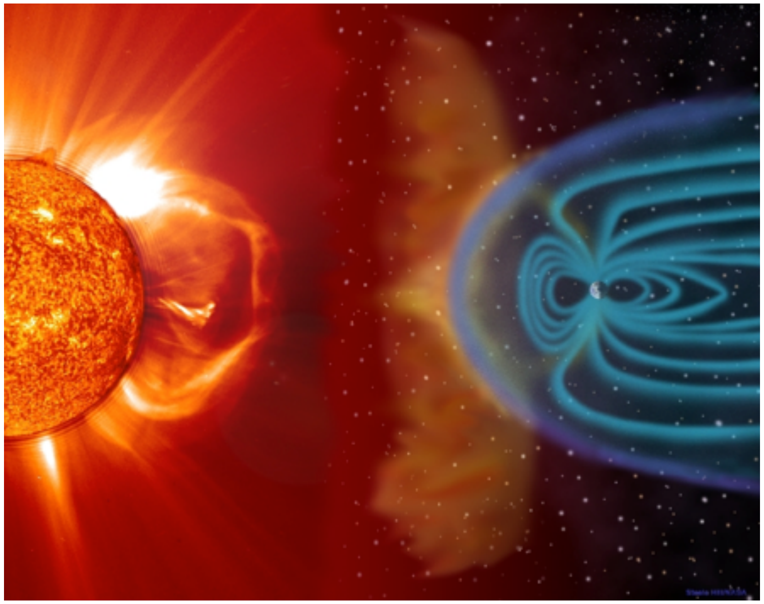




our goals

- our application areas:
  - solar wind simulation (from Sun to Earth, ‘Space Weather’)
  - simulation of magnetic environments of Moon and Mars

➔ projects sponsored by the Canadian Space Agency ("Cluster for Lunar and Planetary Sciences: Advanced Coupled Models, Scientific Mission Definition, and Data Interpretation")



(image: SOHO/EIT consortium)

our goals

- we solve nonlinear hyperbolic conservation laws:

$$\boxed{\partial_t \mathbf{U} + \vec{\nabla} \cdot \vec{\mathbf{F}} = \mathbf{S} + \mathbf{Q}}$$

  – compressible Euler

$$\mathbf{U} = \left[\ \rho,\ \ \rho\vec{V},\ \ \vec{B},\ \ \rho e\ \right]^T$$

  – compressible MHD (Magnetohydrodynamics)

$$\vec{\mathbf{F}} = \begin{bmatrix} \rho\vec{V} \\ \rho\vec{V}\vec{V} + (p + \frac{\vec{B}\cdot\vec{B}}{2})\vec{I} - \vec{B}\vec{B} \\ \vec{V}\vec{B} - \vec{B}\vec{V} \\ (\rho e + p + \frac{\vec{B}\cdot\vec{B}}{2})\vec{V} - (\vec{V}\cdot\vec{B})\vec{B} \end{bmatrix}$$

  – non-ideal effects (Navier-Stokes, resistive MHD, heat conduction, ...) are also included in our framework

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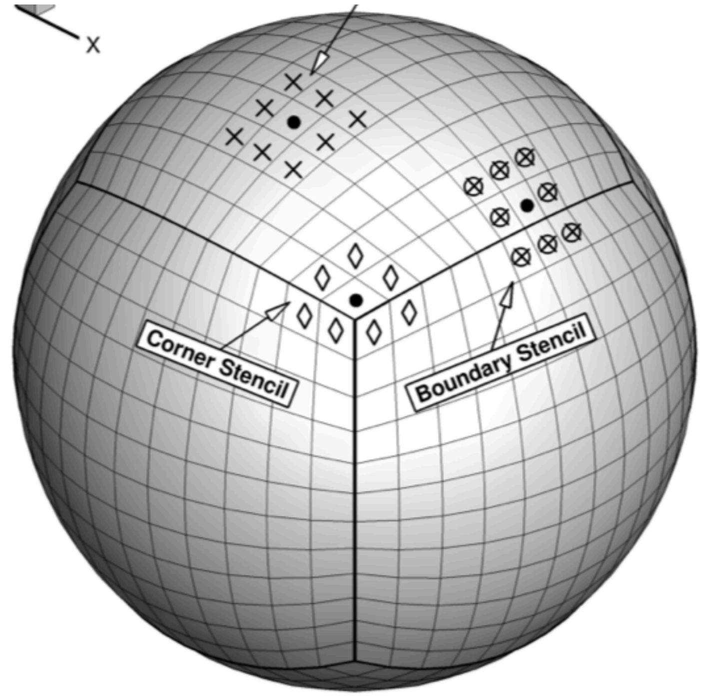
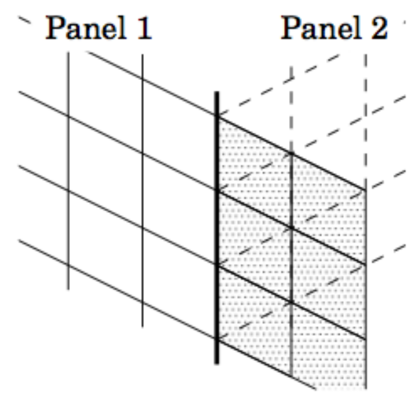
our main contributions

1. use a fully multi-dimensional finite-volume discretization (not dimension-by-dimension)
   - least-squares based
   - can automatically handle varying stencil size (at sector corners)
   - at sector boundaries, can use cells from adjacent sectors directly, without need for special interpolation or reconstruction
   - maintains uniform 2nd-order accuracy (and 3rd-, 4th-order, see Lucian Ivan's talk)
   - discretization handles sector boundaries and corners in a 'transparent' (consistent, uniform) way (important for >30,000 adaptive blocks!)





(image: Paul Ullrich)

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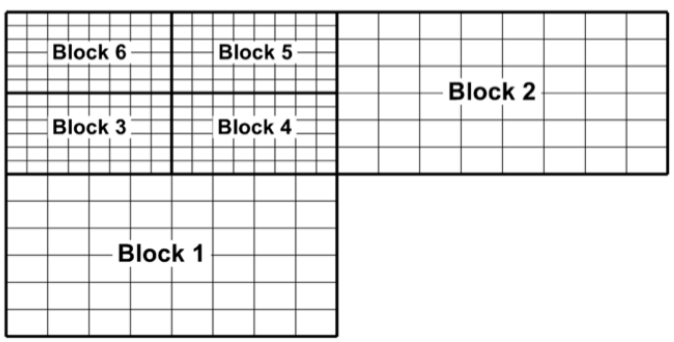
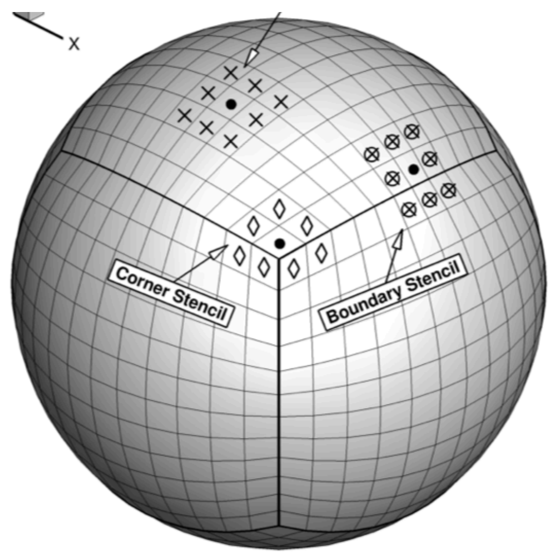
our main contributions

2. use multi-block approach where ‘all blocks are treated equally’
   - use sufficiently rich implementation concepts and data structures to make blocks ‘clever’ enough to handle sector boundaries and corners automatically/uniformly
   - sector boundaries and corners are treated ‘transparently’
   - this is a ‘software engineering’ CSE aspect, but it is crucial for managing code complexity if you want to do >30,000 adaptive blocks on >6,000 CPU cores





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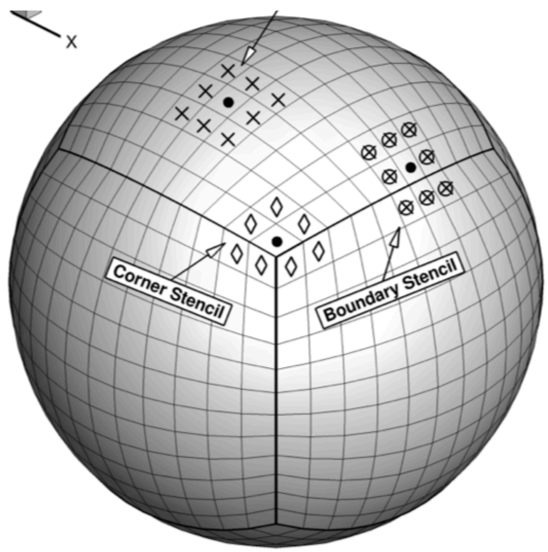
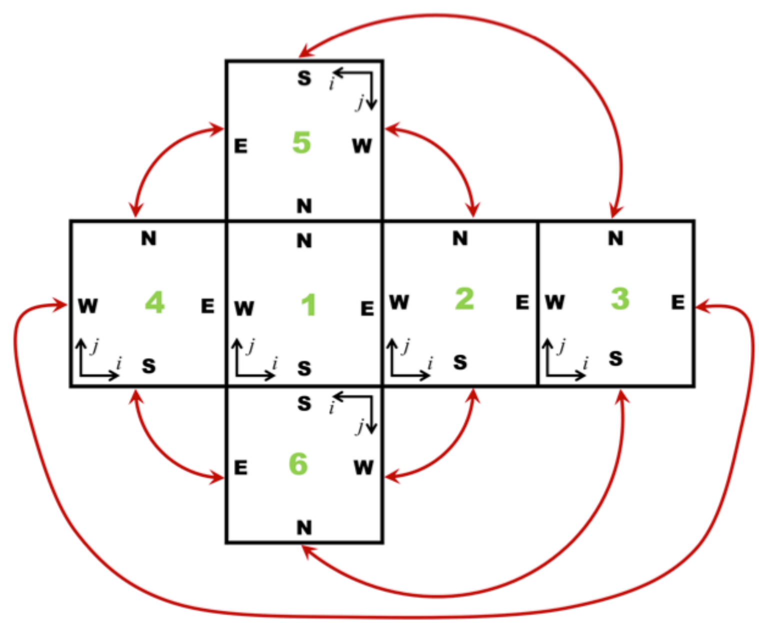
our main contributions

use multi-block approach where 'all blocks are treated equally'

in particular:

- multi-dimensional discretization
- 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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our main contributions

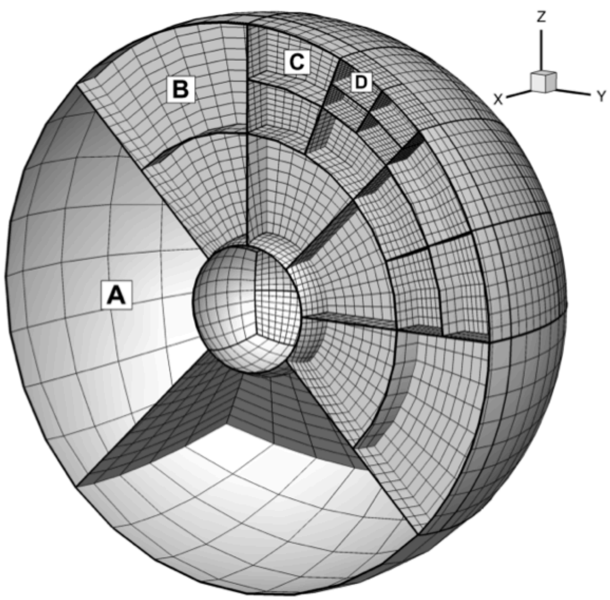
- L. Ivan, S. Northrup, C. Groth, and H. De Sterck, ‘Adaptive Cubed-Sphere Simulation Framework for Space-Physics Flows’, in Proceedings of the 18th Annual **Conference of the CFD Society of Canada, May 2010**

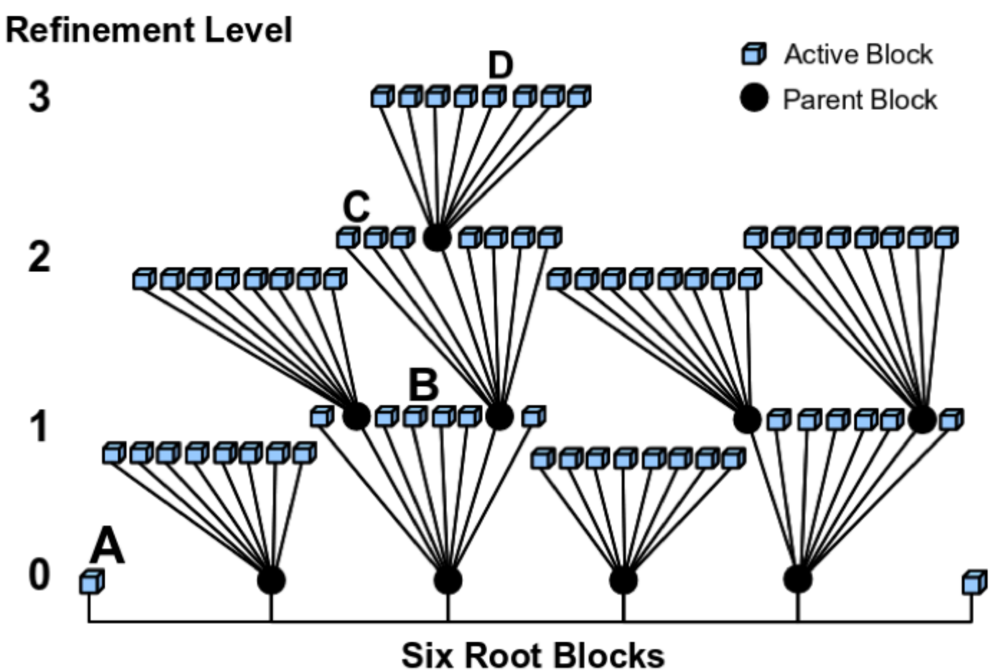
- L. Ivan, H. De Sterck, S. Northrup, and C. Groth, ‘Three-Dimensional MHD on Cubed-Sphere Grids: Parallel Solution-Adaptive Simulation Framework’, **AIAA CFD Conference, 2011, AIAA paper 2011-3382**

- Lucian Ivan, Hans De Sterck, Scott A. Northrup, and Clinton P. T. Groth, ‘Multi-Dimensional Finite-Volume Scheme for Hyperbolic Conservation Laws on Three-Dimensional Solution-Adaptive Cubed-Sphere Grids’, **submitted to Journal of Computational Physics, 2012**

(3) block-based adaptive grid framework

- use self-similar, logically Cartesian blocks (e.g., 8x8x8)
- use octree data structure with six root blocks
- implemented in C++, templated
- the same framework is also used in Groth's group for combustion simulations (Groth's CFFC framework was starting point for our work) (Gao and Groth, 2010)





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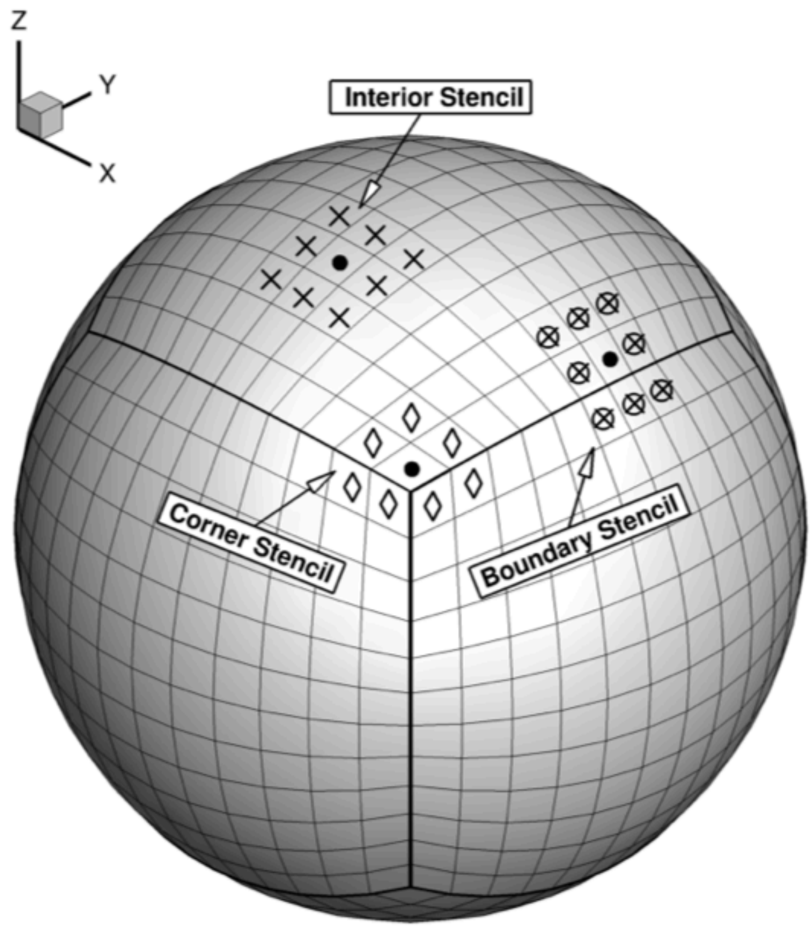
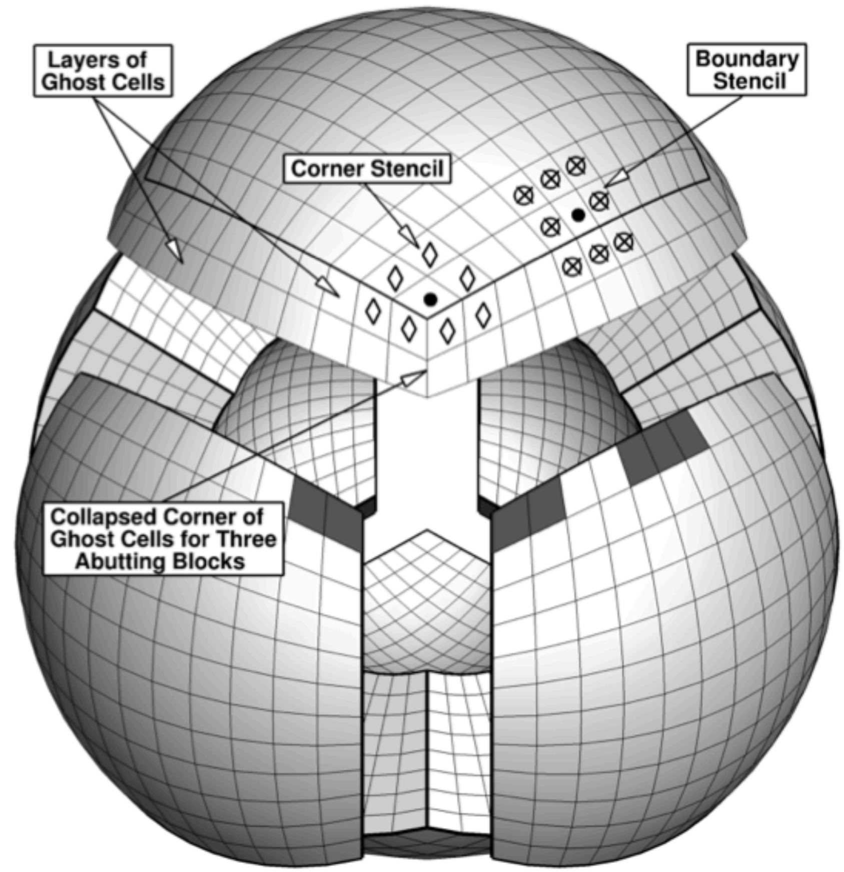
block-based adaptive grid framework

- self-similar blocks have two layers of ghost cells





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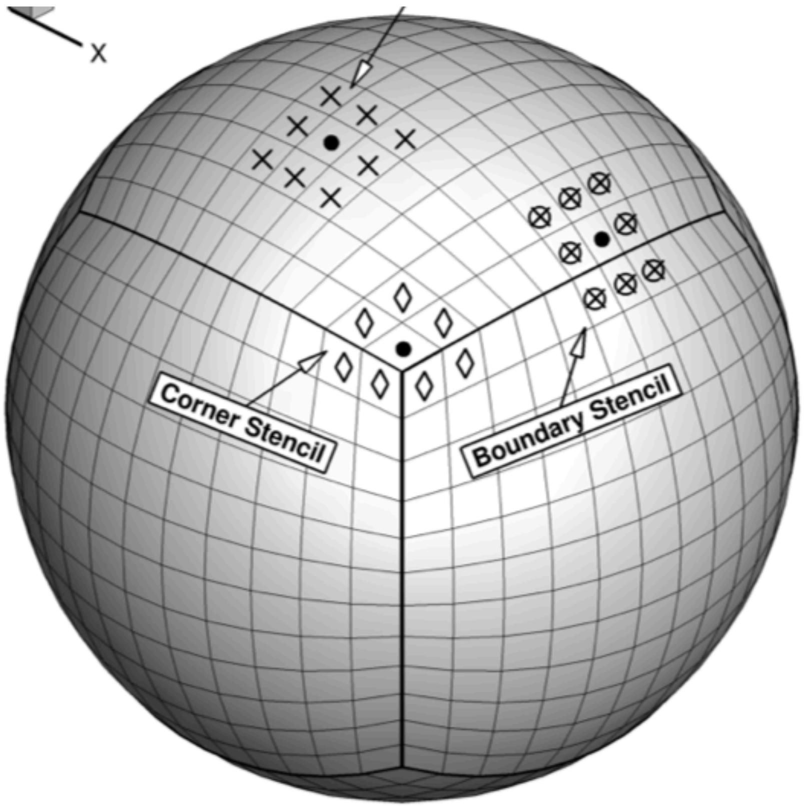
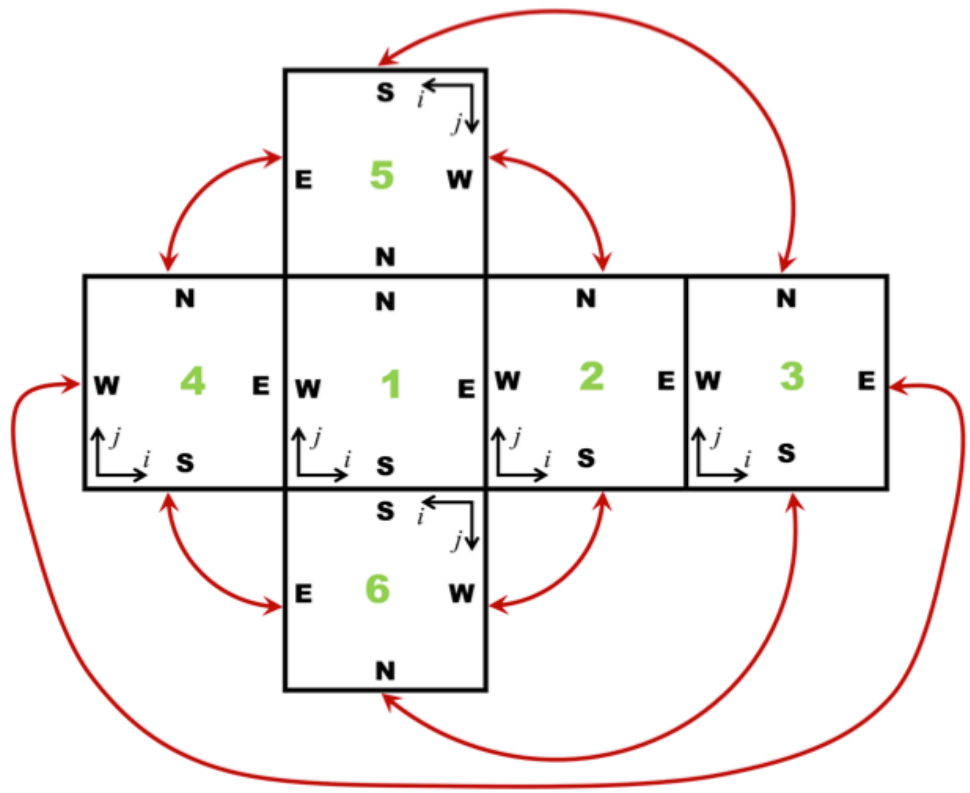
block-based adaptive grid framework

- unstructured root block connectivity (Gao and Groth, 2010)
- collapsed ghost cells in degenerate corners





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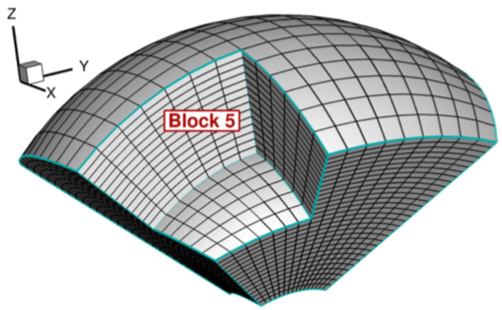
(4) numerical scheme: multi-dimensional finite volume method

- based on Barth's *k*-exact approach
- finite-volume method on hexahedrals



$$\boxed{\partial_t \mathbf{U} + \vec{\nabla} \cdot \vec{\mathbf{F}} = \mathbf{S} + \mathbf{Q}}$$

$$\frac{d\overline{\mathbf{U}}_{ijk}}{dt} = \frac{1}{V_{ijk}} \left[-\oint_{\partial \mathcal{V}_{ijk}} \vec{\mathbf{F}} \cdot \vec{n} \, \mathrm{d}a + \iiint_{\mathcal{V}_{ijk}} (\mathbf{S} + \mathbf{Q}) \, \mathrm{d}v \right]$$

$$\frac{d\overline{\mathbf{U}}_{ijk}}{dt} = -\frac{1}{V_{ijk}} \sum_{f=1}^{6} \sum_{m=1}^{N_g} \left(\tilde{\omega} \vec{\mathbf{F}}_{\mathrm{num}} \cdot \vec{n} \right)_{i,j,k,f,m} + (\overline{\mathbf{S}})_{ijk} + (\overline{\mathbf{Q}})_{ijk} = \mathbf{R}_{ijk}(\overline{\mathbf{U}})$$

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numerical scheme: multi-dimensional finite volume method

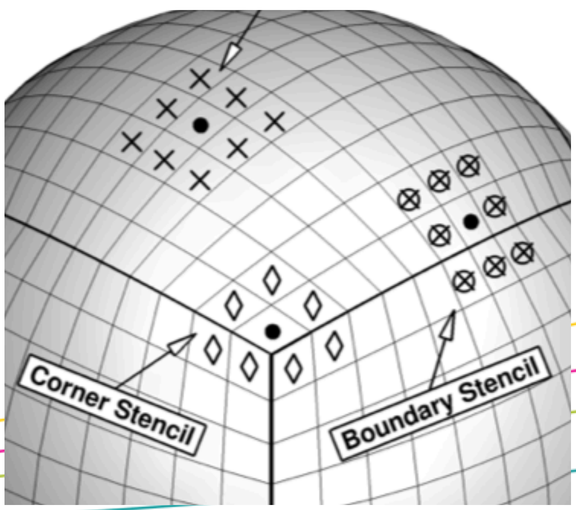
$$\frac{d\overline{\mathbf{U}}_{ijk}}{dt} = -\frac{1}{V_{ijk}} \sum_{f=1}^{6} \sum_{m=1}^{N_g} \left(\tilde{\omega}\vec{\mathbf{F}}_{\mathrm{num}} \cdot \vec{n}\right)_{i,j,k,f,m} + \left(\overline{\mathbf{S}}\right)_{ijk} + \left(\overline{\mathbf{Q}}\right)_{ijk} = \mathbf{R}_{ijk}(\overline{\mathbf{U}})$$

- 2nd-order polynomial reconstruction in each cell

$$u_I^K(\vec{X}) = \sum_{p_1=0}^{K} \sum_{p_2=0}^{K} \sum_{\substack{p_3=0 \\ (p_1+p_2+p_3 \le K)}}^{K} (x-\bar{x}_I)^{p_1} (y-\bar{y}_I)^{p_2} (z-\bar{z}_I)^{p_3} D^K_{p_1 p_2 p_3}$$

- least-squares problem: find reconstruction polynomials such that

$$(\mathbb{A}\mathbf{D} - \mathbf{B})_{\gamma\delta\zeta} = \left(\frac{1}{V_{\gamma\delta\zeta}} \iiint_{\mathcal{V}_{\gamma\delta\zeta}} u^K_{ijk}(\vec{X})\, \mathrm{d}\upsilon \right) - \bar{u}_{\gamma\delta\zeta} = 0$$



(stencil size is 3x3x3, or less at sector corners)

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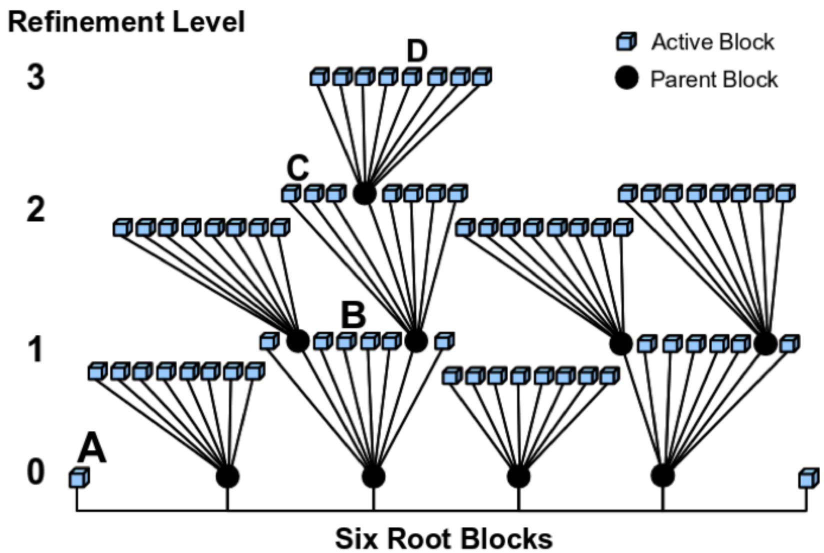
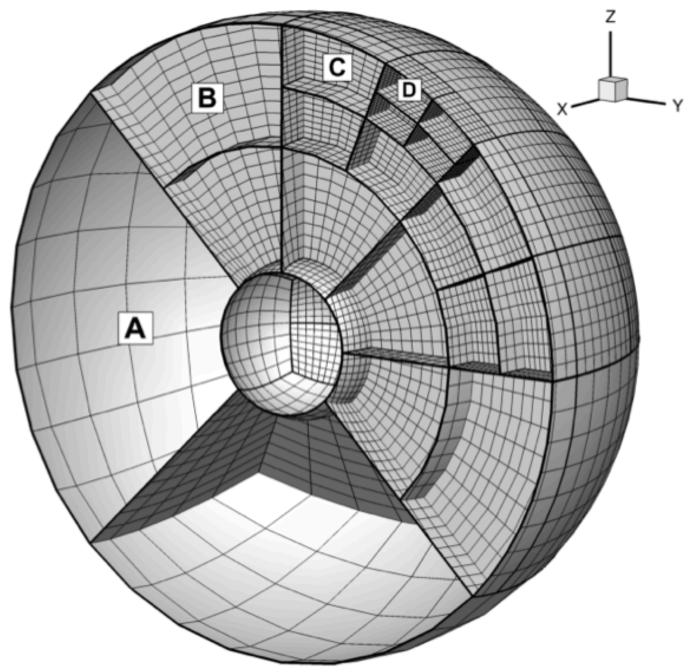
(5) adaptive grid refinement

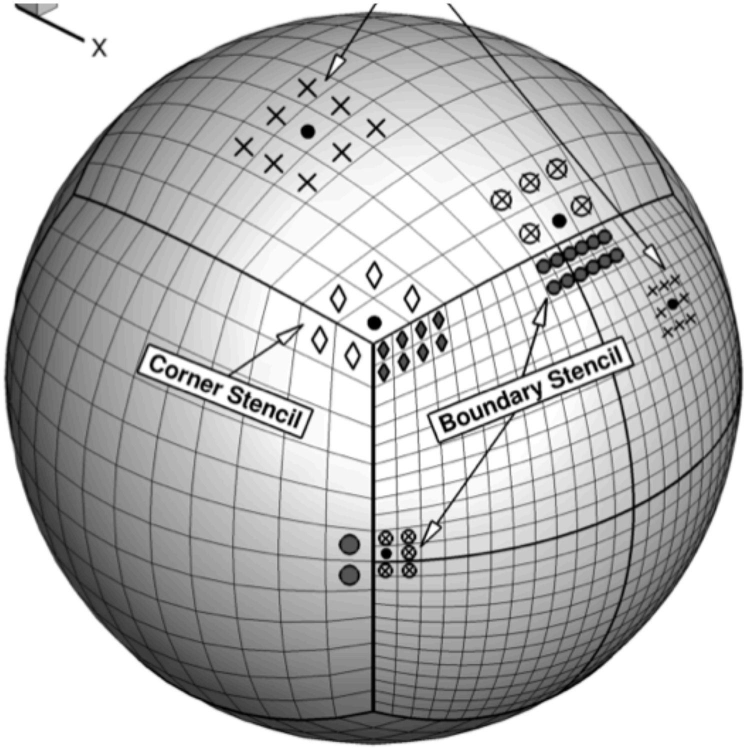
- adaptive refinement (1➔8 blocks) and coarsening (8➔1 block)
- physics-based refinement criteria (e.g., density gradient)
- dynamic refinement and coarsening (refinement follows moving features)

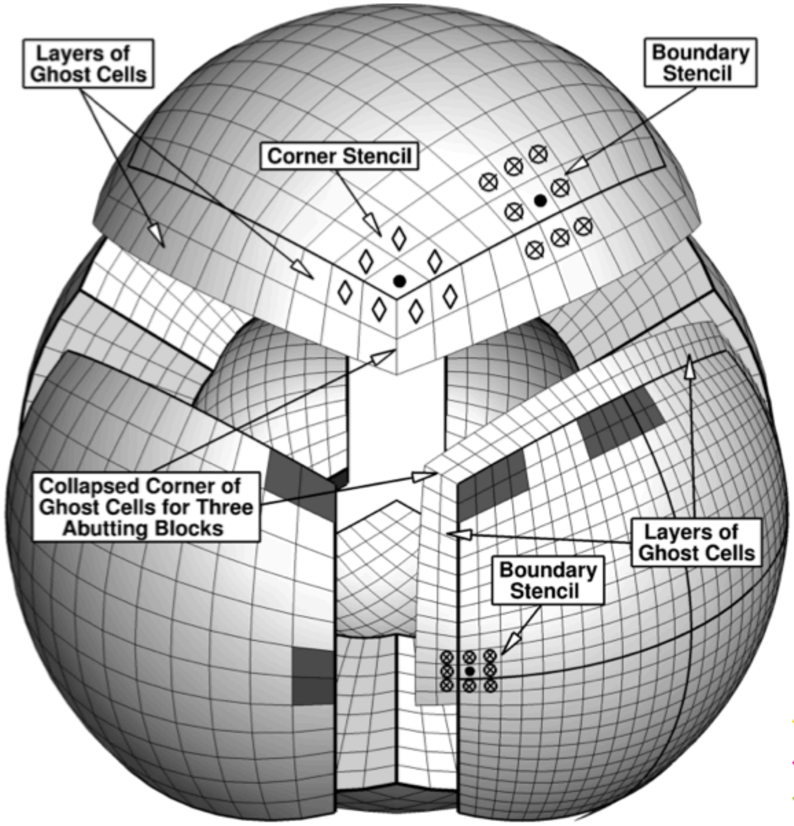




adaptive grid refinement

- adjacent blocks cannot differ in resolution by more than a factor of two
- implementation for cubed-sphere greatly facilitated by ‘all blocks are treated equally’ (dynamic refinement!)





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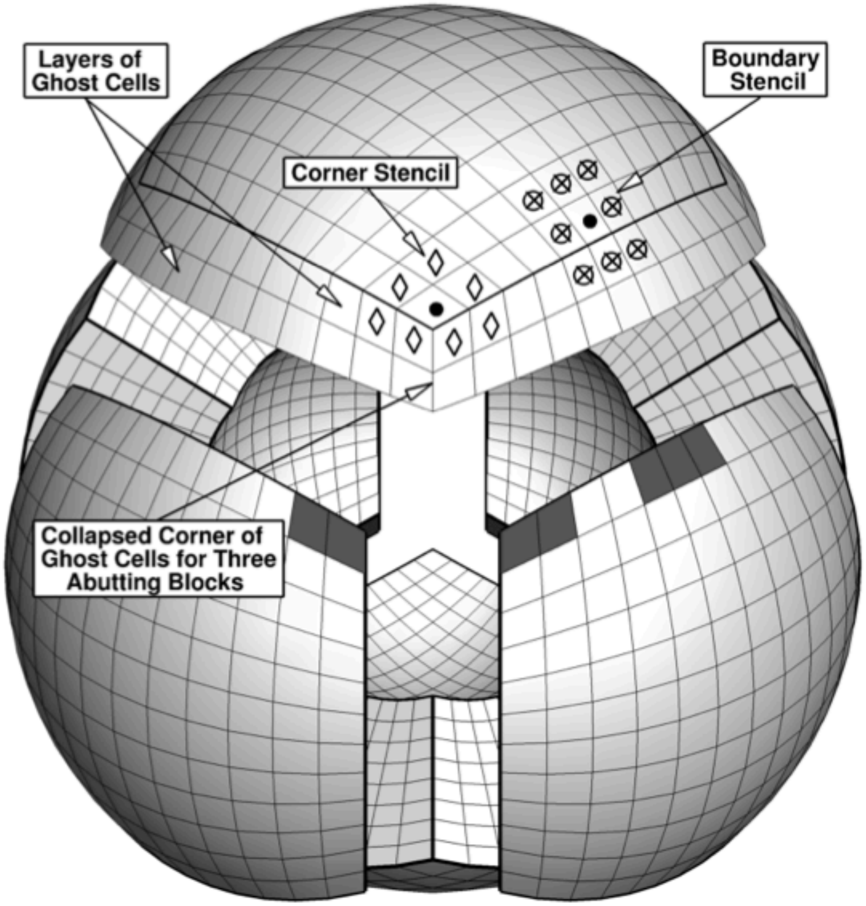
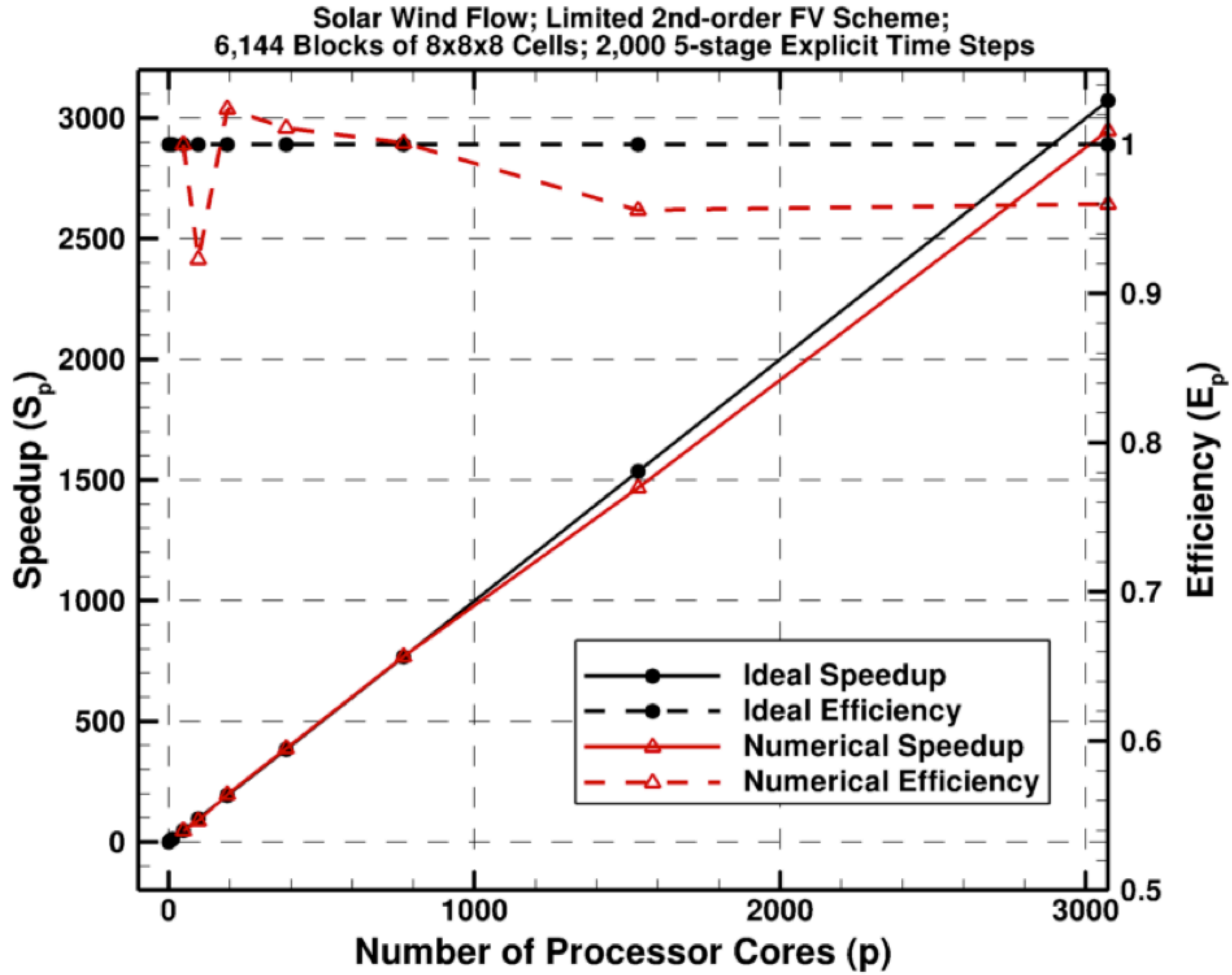
(6) parallelisation

- two layers of ghost cells for each block
- MPI message passing

- many more blocks than processors
- self-similar blocks: load-balancing by equally distributing blocks over CPU cores (Morton ordering can be employed)





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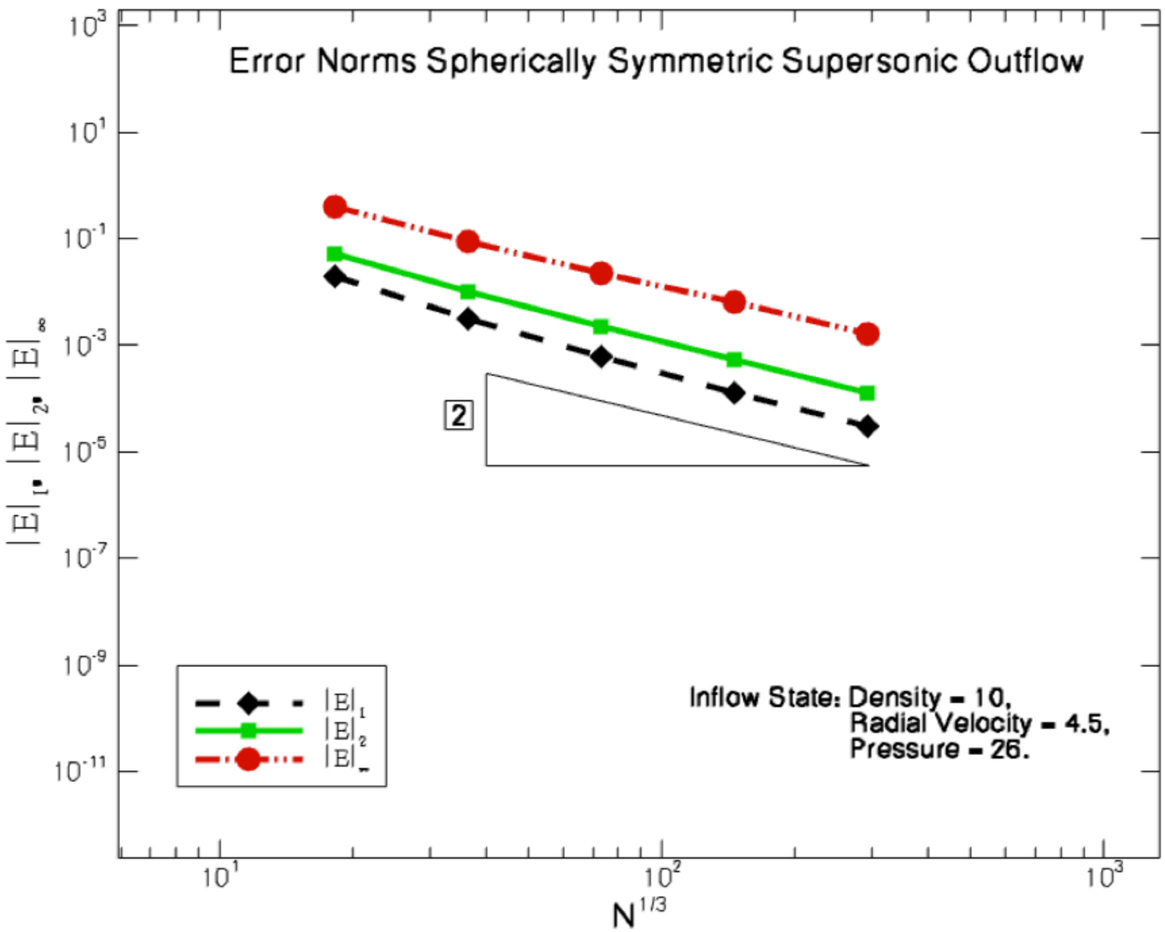
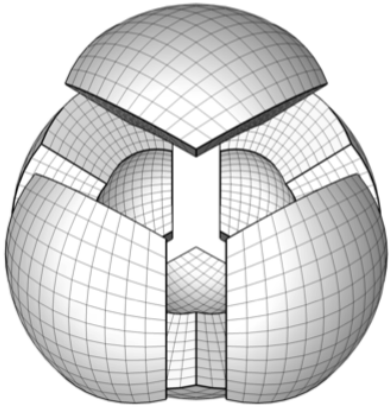
(7) validation tests

- radial supersonic outflow on cubed-sphere grid:





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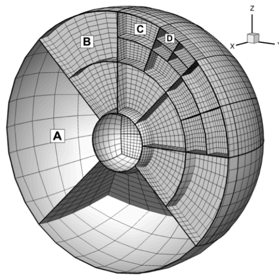
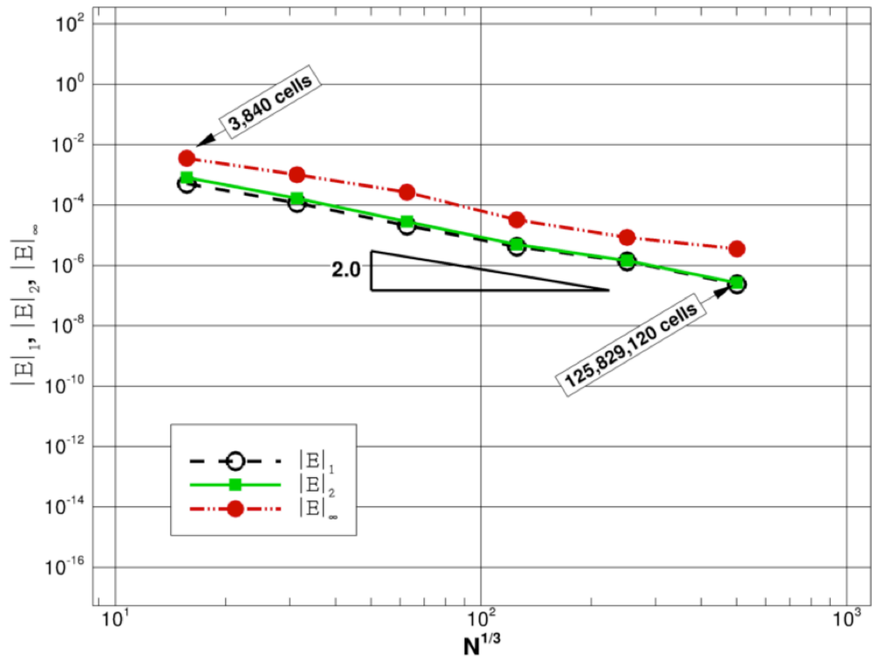
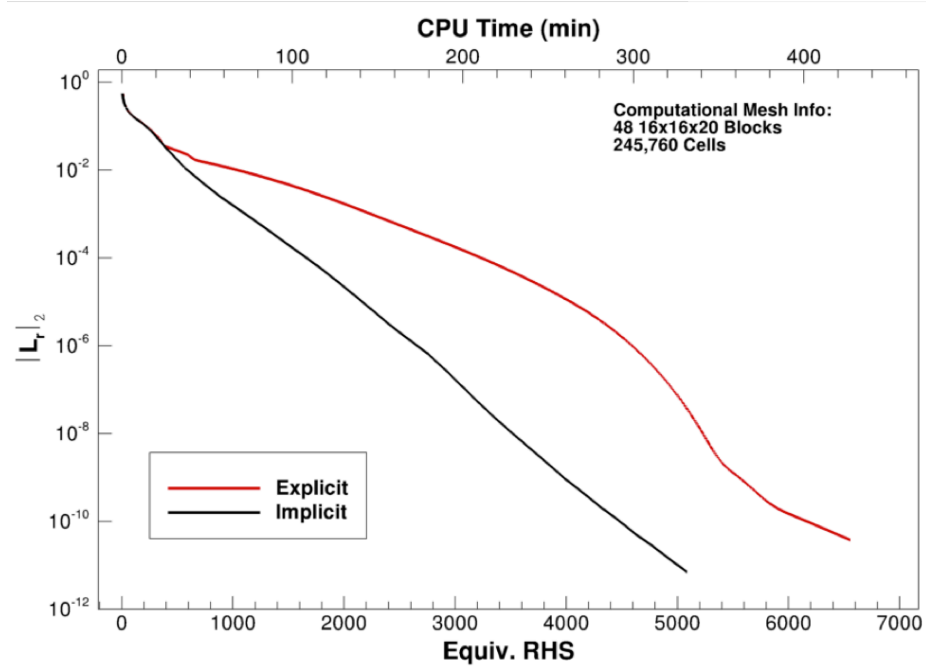
validation tests

- MHD manufactured solution on cubed-sphere grid (axi-symmetric) (also implicit, NKS)

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







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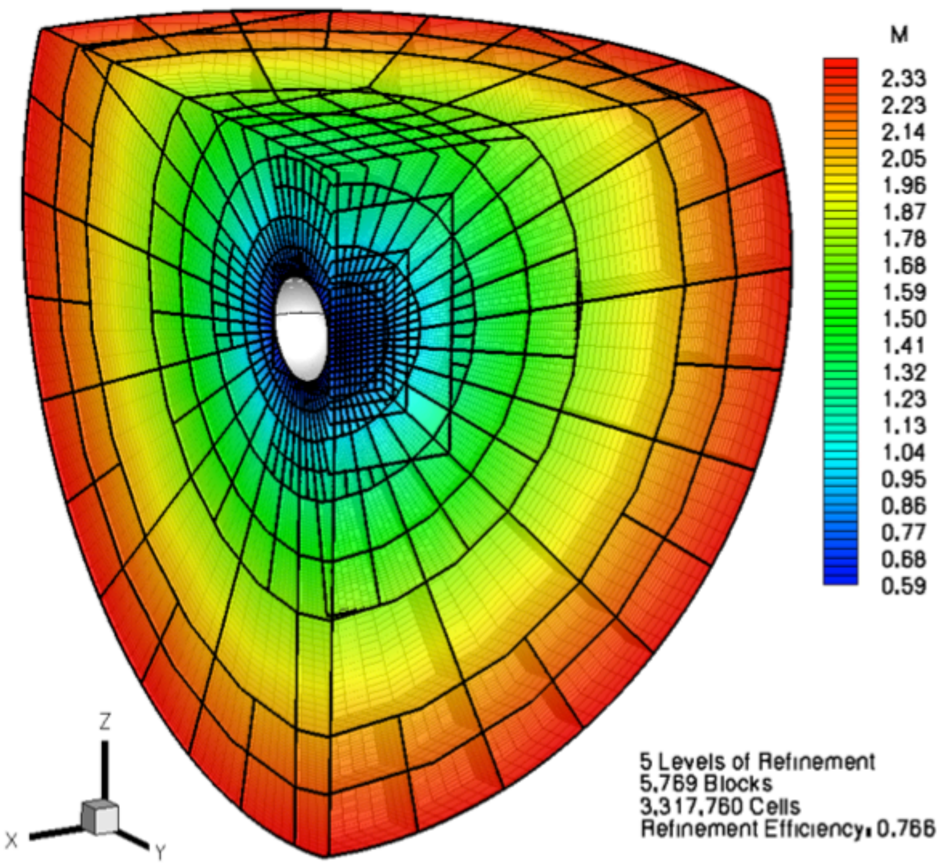
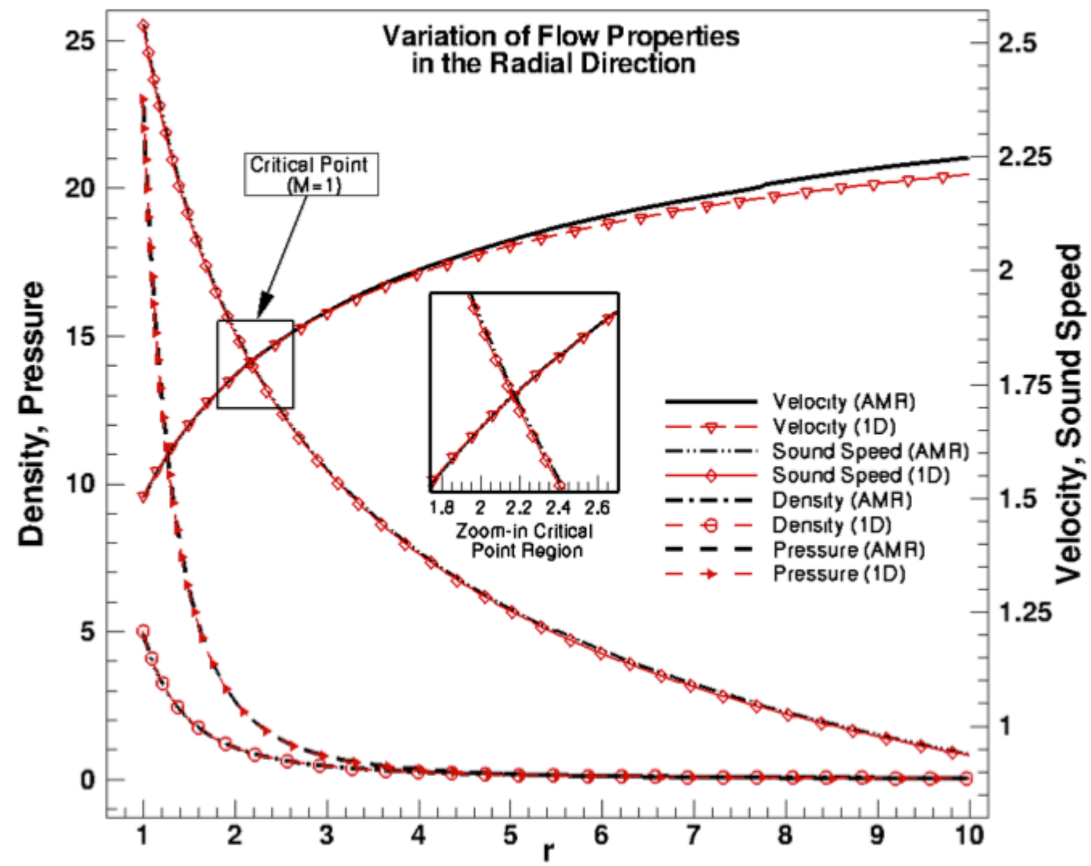
validation tests

- transonic wind on adaptive mesh





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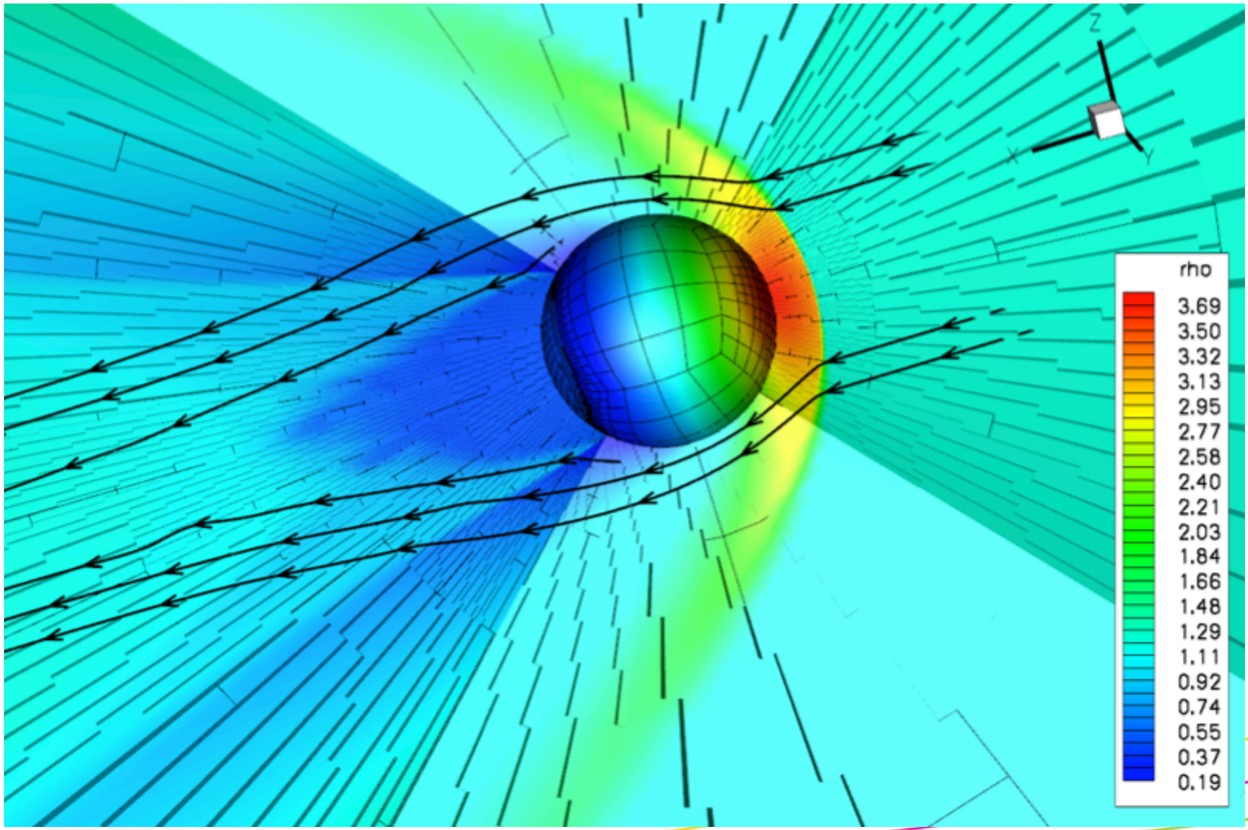
(8) large-scale results

- supersonic flow past a sphere
- 10,835 adaptive blocks and 8,321,280 computational cells (7 levels of refinement)



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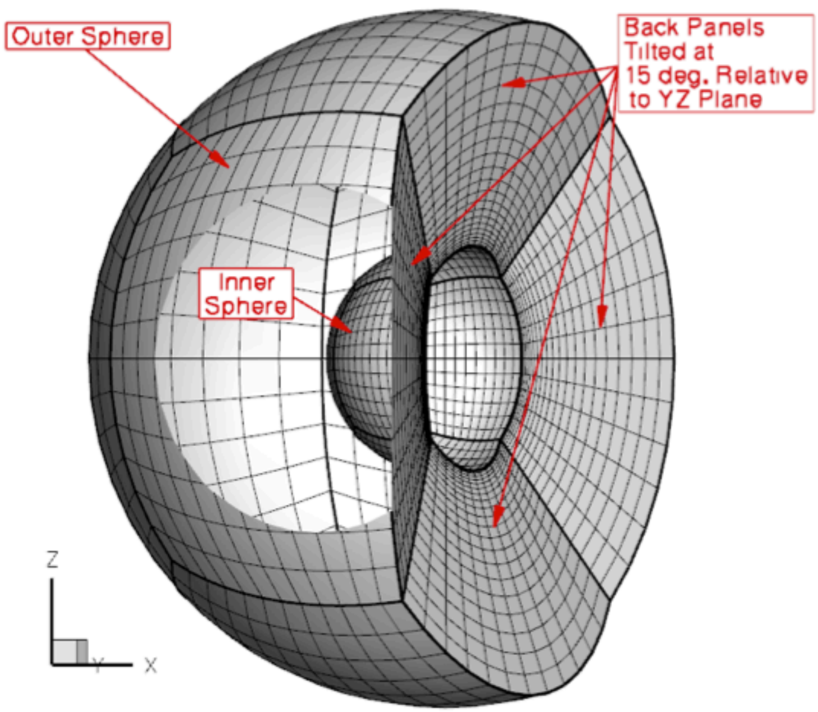
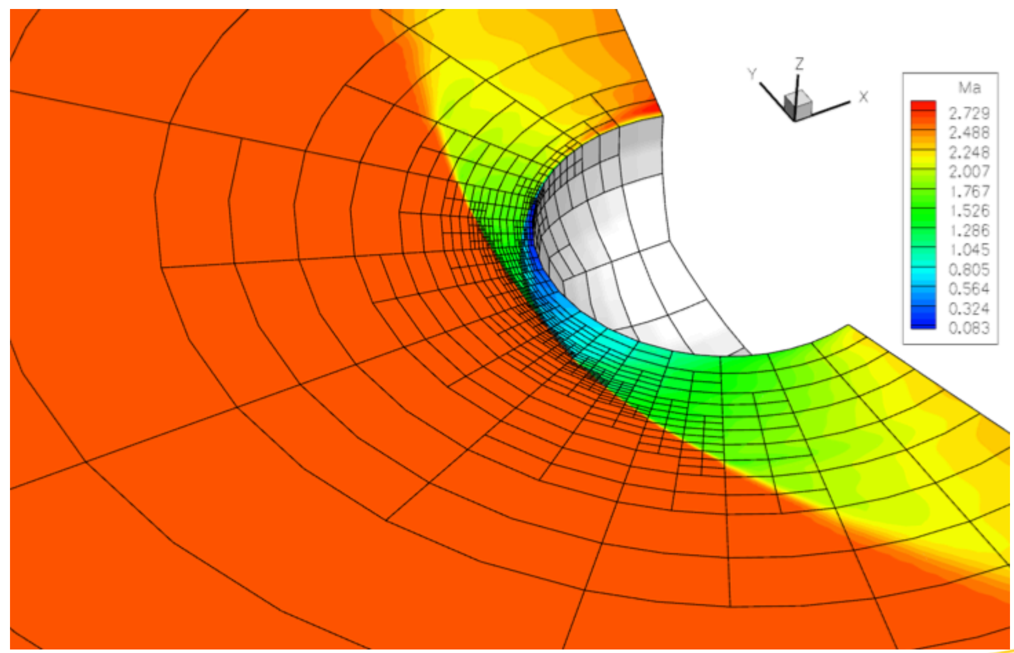
large-scale results

- ‘magnetically dominated’ MHD bow shock flow
- we only use 5 root blocks!
- 7 refinement levels with 22,693 blocks and 14,523,520 computational cells





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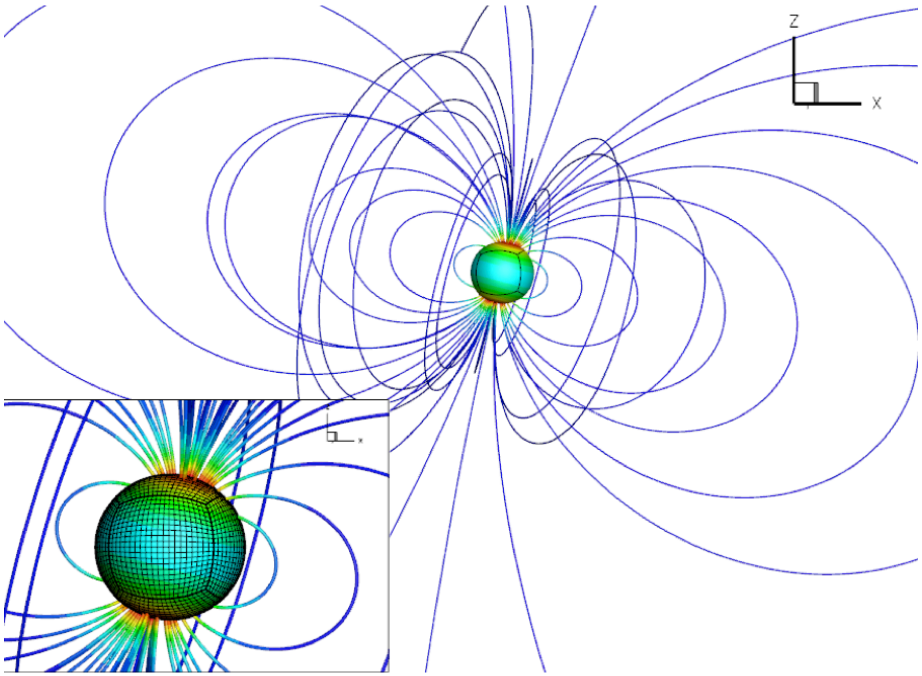
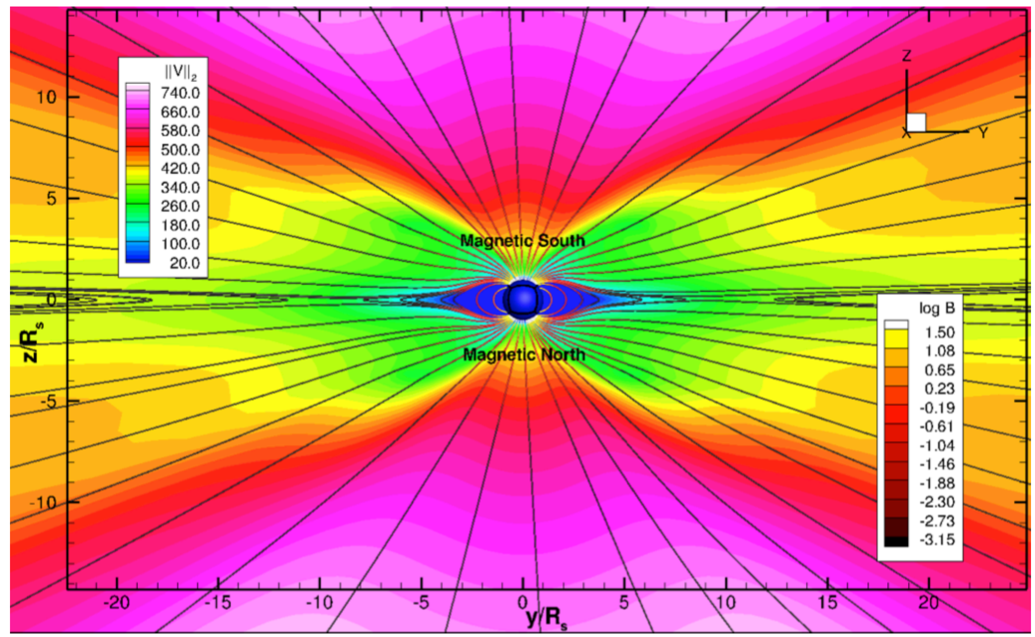
large-scale results

- MHD solar wind (Groth et al. model)





large-scale results

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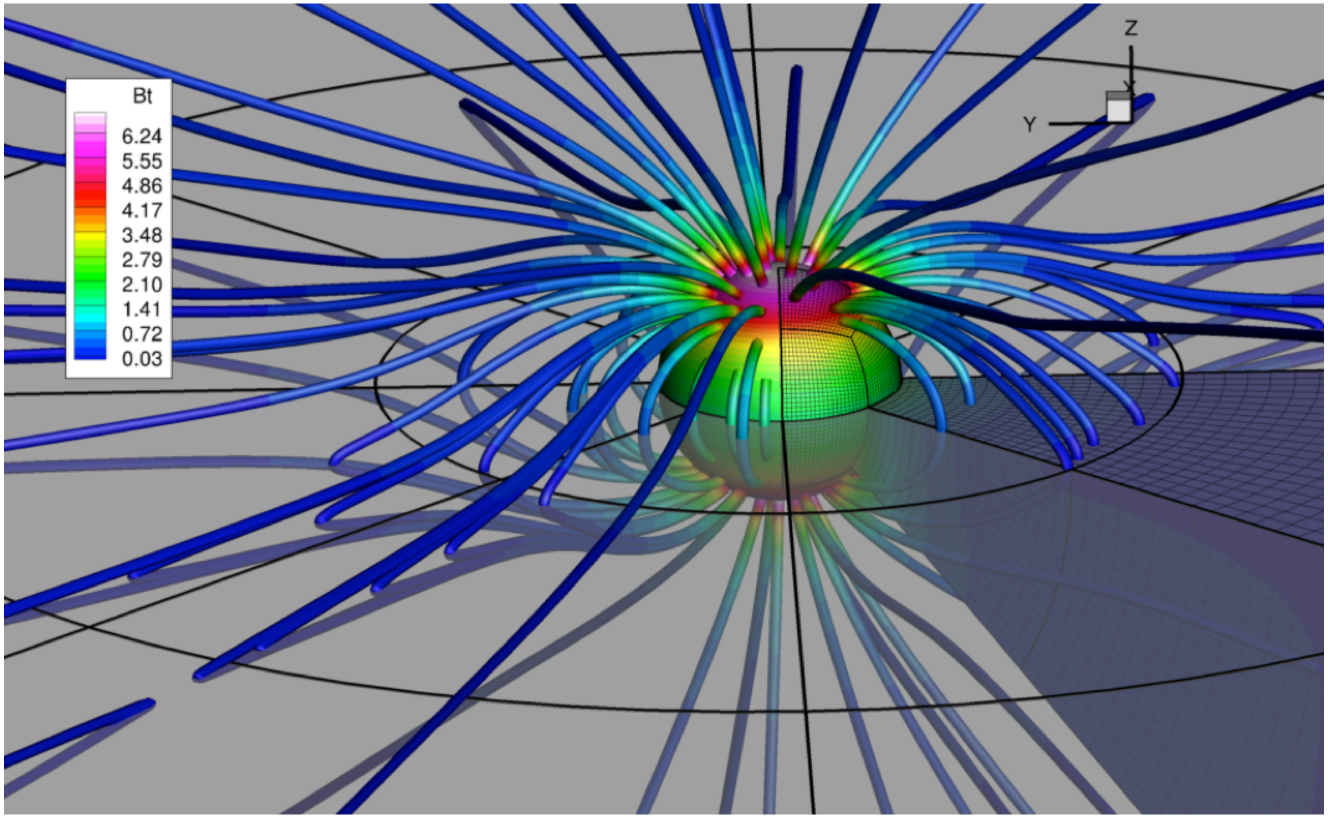
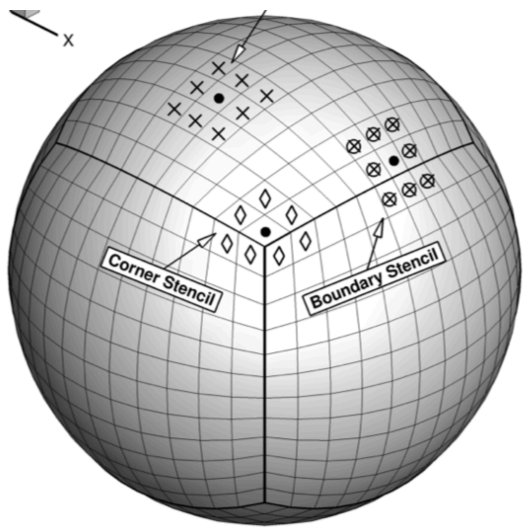


(9) conclusions and future work

- our contributions:

1. we have proposed a fully multi-dimensional finite-volume approach for cubed-sphere grids (handles sector boundaries and corners in a consistent way, naturally maintaining uniform 2nd-order accuracy without need for special interpolation or reconstruction)



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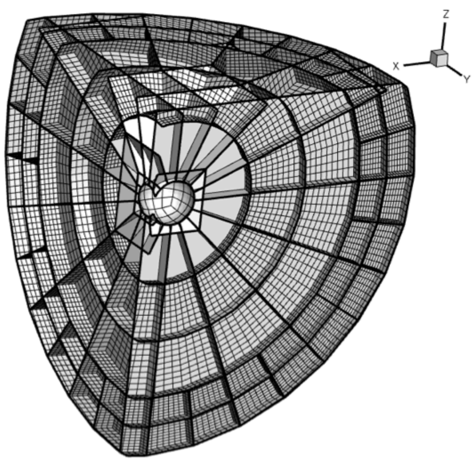
conclusions and future work

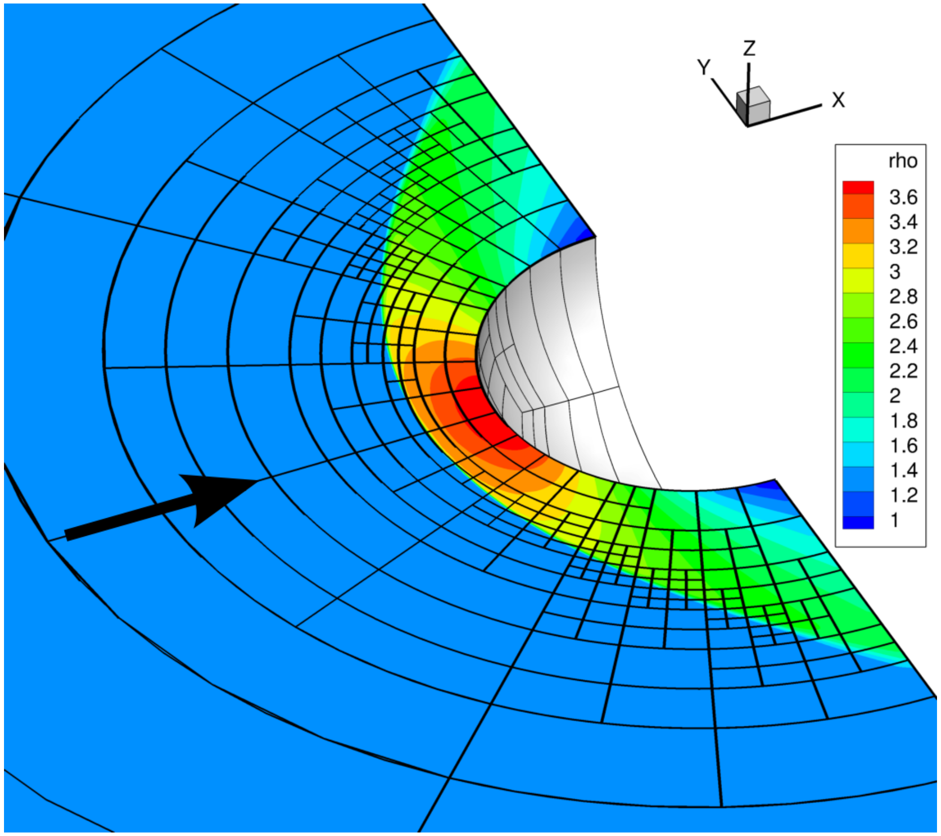
- our contributions:
  2. we have developed a 3D cubed-sphere framework with unprecedented capabilities in terms of full 3D adaptivity (dynamic) and parallelism, with >30,000 adaptive blocks and >6,000 CPU cores
     - multi-block approach where 'all blocks are treated equally' is a crucial ingredient (unstructured connectivity)

       ➔ sector boundaries and corners are treated consistently/ transparently/uniformly



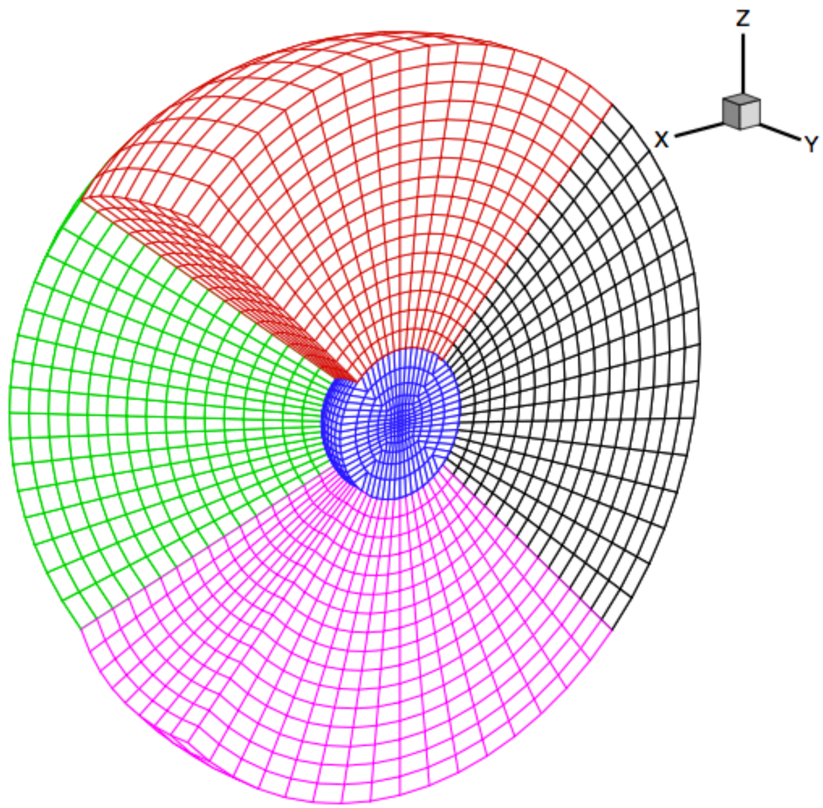
ongoing and future work

- 3rd and 4th order accuracy (Lucian Ivan's talk tomorrow, **ICCFD7 2012**)
- anisotropic refinement (2D: one 4x4 block → two 4x4 blocks)



ongoing and future work

- 3rd and 4th order accuracy (Lucian Ivan's talk tomorrow, **ICCFD7 2012**)
- Mars/Moon simulations (need to solve PDE inside the spherical object ➔ 7 root blocks!)



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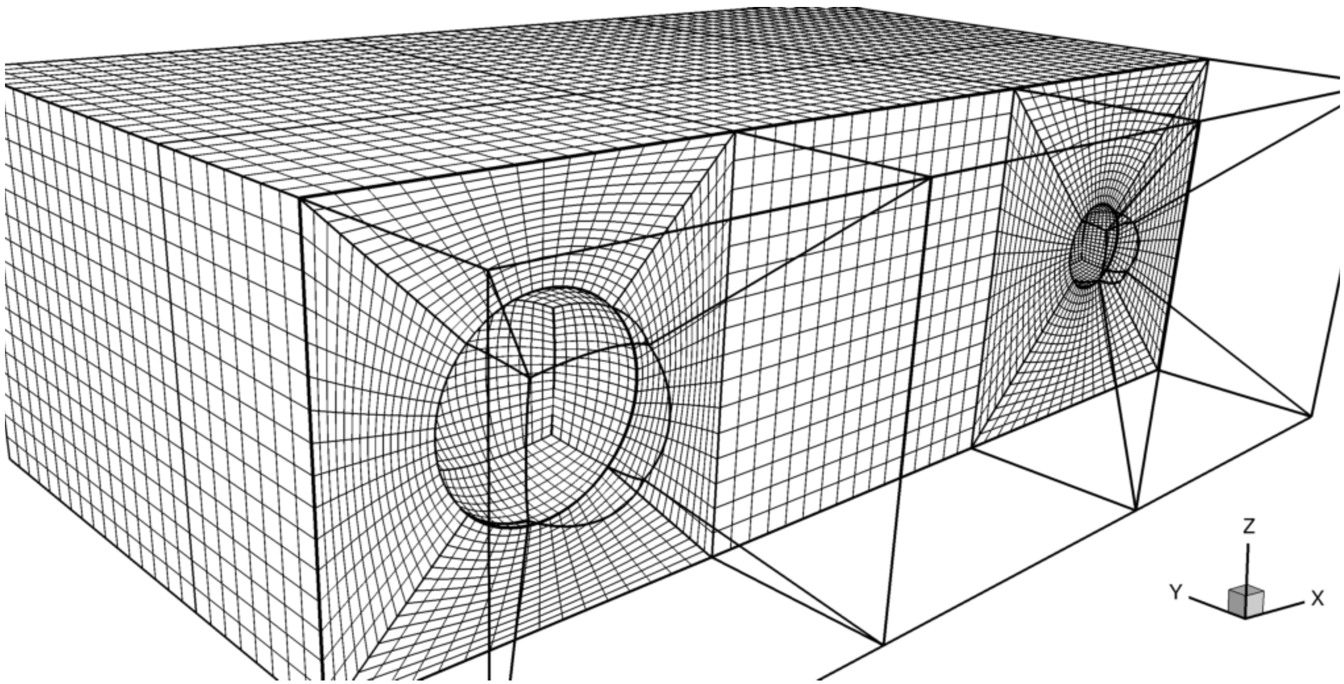
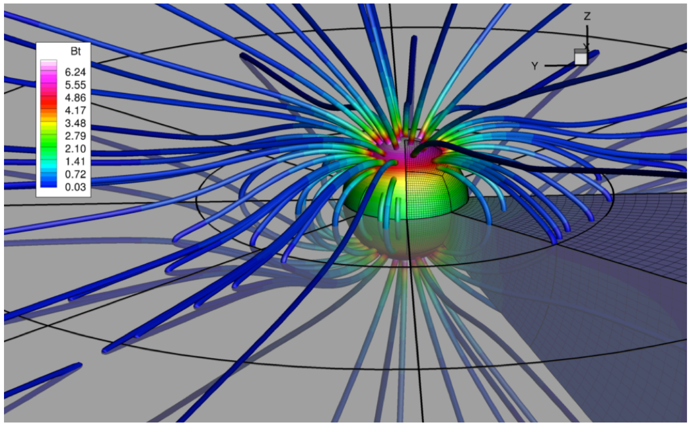
ongoing and future work

- our framework is flexible enough to handle multiple spherical objects (e.g., Earth and Moon)



- we're also interested in potentially exploring weather/climate-type applications using our framework (perhaps fully 3D, non-hydrostatic)
- Earth mantle convection is another area of potential interest



thank you

- L. Ivan, S. Northrup, C. Groth, and H. De Sterck, ‘Adaptive Cubed-Sphere Simulation Framework for Space-Physics Flows’, in Proceedings of the 18th Annual **Conference of the CFD Society of Canada, May 2010**
- L. Ivan, H. De Sterck, S. Northrup, and C. Groth, ‘Three-Dimensional MHD on Cubed-Sphere Grids: Parallel Solution-Adaptive Simulation Framework’, **AIAA CFD Conference, 2011, AIAA paper 2011-3382**
- Lucian Ivan, Hans De Sterck, Scott A. Northrup, and Clinton P. T. Groth, ‘Multi-Dimensional Finite-Volume Scheme for Hyperbolic Conservation Laws on Three-Dimensional Solution-Adaptive Cubed-Sphere Grids’, **submitted to Journal of Computational Physics, 2012**

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