A logically Cartesian, adaptively refined two-patch sphere grid for modeling transport in the atmosphere

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PDEs on the Sphere
Cambridge, UK
Sept 24-28, 2012

Start with some understanding of ...

- ☑ Finite volume schemes using the wave propagation for logically Cartesian grids (LeVeque),
- ☑ Grids and methods for solving PDEs on a sphere (Berger, DC, Helzel, LeVeque),
- ☑ Block-structured adaptive mesh refinement (Berger, Colella, DC, LeVeque), and
- ☑ Experience with several software packages for doing the above (Clawpack, AMRClaw, Chombo, ChomboClaw, Boxlib) and knowledge of many more (SAMRAI, Paramesh, Overture, ...).

Add ...

- Belief in the importance of designing numerical algorithms that from the start can be made adaptive and will scale to large number of cores,
- Appreciation of the need for domain expertise in target applications,
- A desire to be more than just a user of other people's software, but to develop my own software, and
- A full awareness of the ridiculousness of doing the above by myself, at least while in a tenure track position, in a mathematics department.

some fortuitous meetings ...

- An workshop on tracer transport on the sphere (NCAR, March 2011, Boulder CO)
- A meeting with USGS researchers from the Cascade Volcanic Observatory interested in using adaptivity to improve their forecasting of volcanic ash cloud transport (Seattle, October 2011)
- A hands-on workshop on high performance computing at the King Abdullah University of Science and Technology (KAUST) (HPC^3, March 2012, Saudi Arabia)
- An opportunity to spend the semester at the Newton Institute at a program on Multiscale Numerics for the Ocean and Atmosphere (Fall, 2012)

and we get ...

ForestClaw = p4est + Clawpack

- Adaptive, scalable, multi-block tree-code **p4est** (Carsten Burstedde, Univ. Bonn) to manage a quad- or octree of non-overlapping fixed sized grids,
- Wave propagation algorithms (R. J. LeVeque) on logically Cartesian mapped grids,

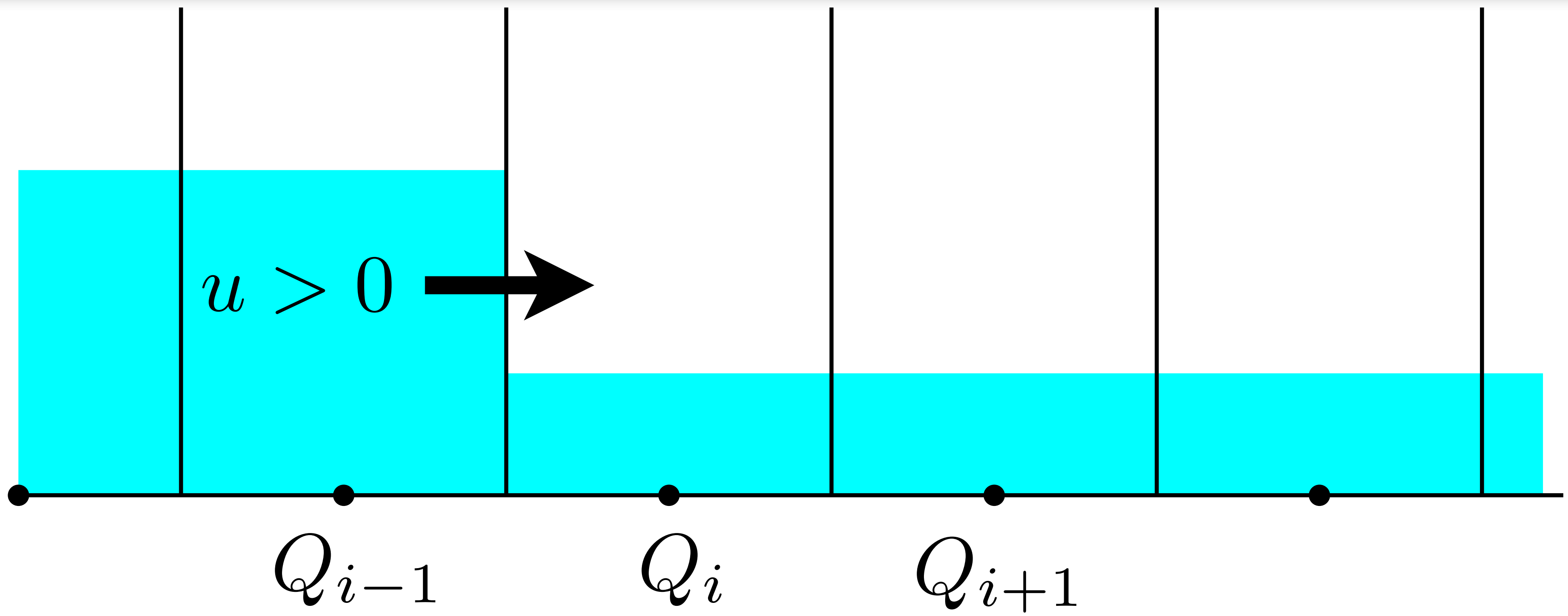
Current aim is to use adaptivity to improve forecasting capabilities of ***Ash3d****, a USGS code for modeling transport of volcanic ash in the atmosphere.*

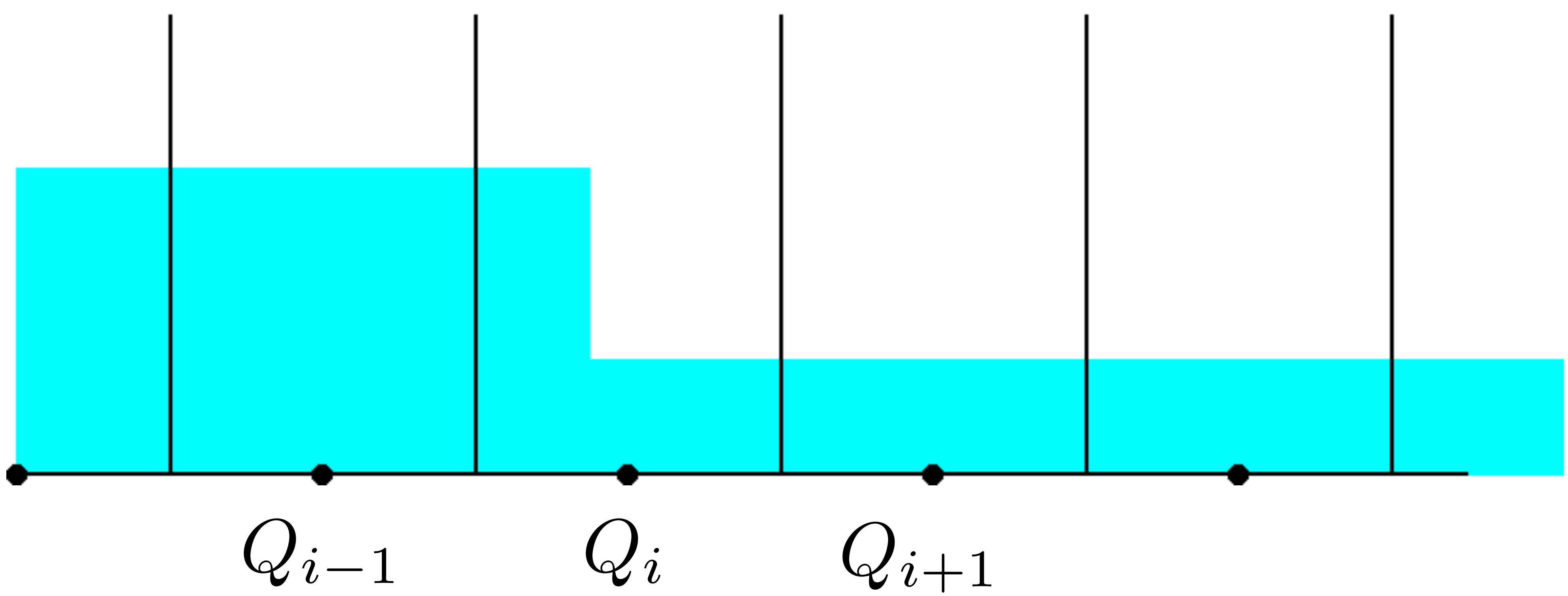
Wave propagation algorithms on the sphere

Clawpack (R. J. LeVeque) general purpose code based on the wave propagation algorithm for solving hyperbolic problems.

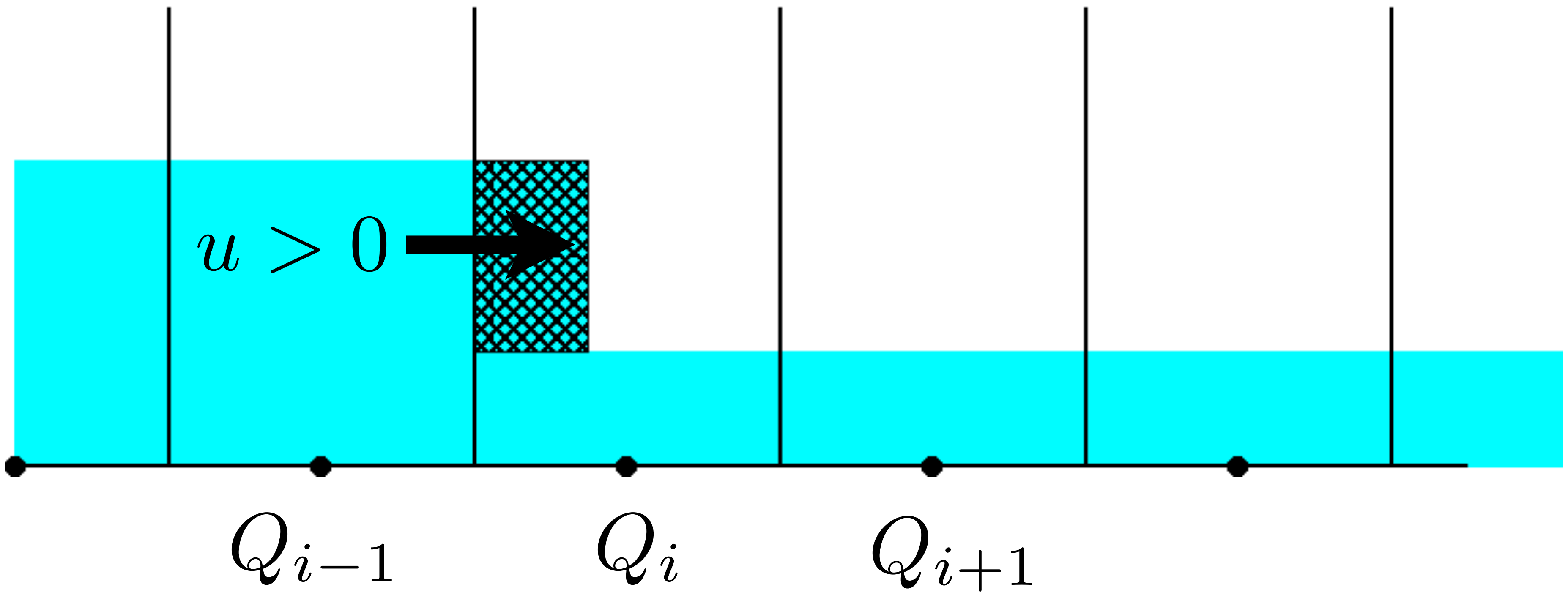
- Finite volume schemes on logically Cartesian grids
- First and second order versions, with or without limiters.
- Split and unsplit options available.
- Second order accuracy is achieved by propagating second order correction “waves” in normal and transverse directions.
- Explicit time stepping limited by CFL=1.0

Wave propagation algorithms





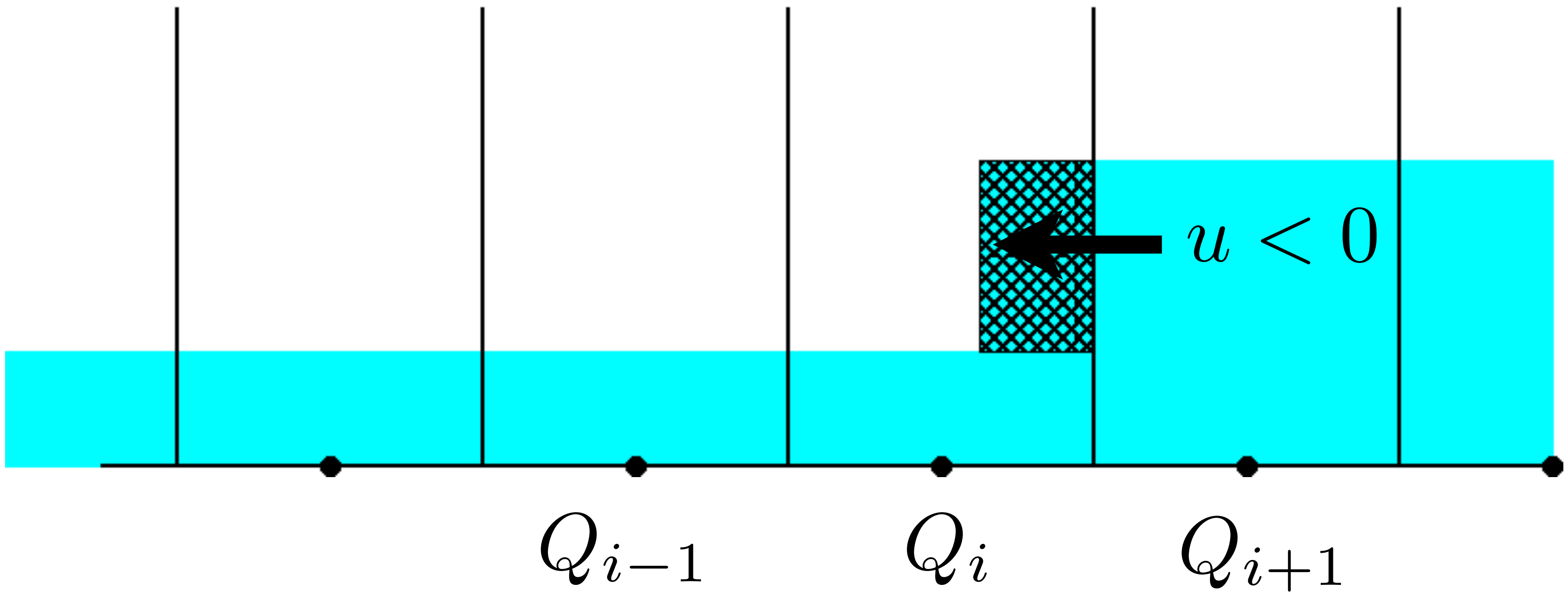
Wave propagation algorithms



In time Δt, total mass in the cell increases by shaded area :

$$\Delta x Q_i^{n+1} = \Delta x Q_i^n - u\,\Delta t\left(Q_i^n - Q_{i-1}^n\right)$$

Wave propagation algorithms



In time Δt, total mass in the cell increases by shaded area :

$$\Delta x Q_i^{n+1} = \Delta x Q_i^n - u\,\Delta t\left(Q_{i+1}^n - Q_i^n\right)$$

Upwind scheme

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x}\left(u^+(Q_i^n - Q_{i-1}^n) + u^-(Q_{i+1}^n - Q_i^n)\right)$$

where

$$u^+ = \max(u, 0), \qquad u^- = \min(u, 0)$$

We can define waves at each interface as :

Waves : $\mathcal{W}_{i-1/2} \equiv Q_i - Q_{i-1}$

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x}\left(u^+\mathcal{W}_{i-1/2} + u^-\mathcal{W}_{i+1/2}\right)$$

Upwind scheme for systems

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x}\left(\sum_{p=1}^{m}(\lambda^p)^+\mathcal{W}_{i-1/2}^p + \sum_{p=1}^{m}(\lambda^p)^-\mathcal{W}_{i+1/2}^p\right)$$

where the waves are now defined as from an eigenvalue decomposition of the jump in value at each interface

Waves : $$\widetilde{\mathcal{W}}_{i-1/2}^p = \alpha^p r^p$$

Written in terms of *fluctuations* :

$$\mathcal{A}^+\Delta Q_{i-1/2} \equiv \sum_{p=1}^{m}(\lambda^p)^+\mathcal{W}_{i-1/2}$$

$$\mathcal{A}^-\Delta Q_{i-1/2} \equiv \sum_{p=1}^{m}(\lambda^p)^-\mathcal{W}_{i-1/2}$$

Solve Riemann problems

Second order correction terms

High resolution terms gives better accuracy (2nd order for smooth solutions)

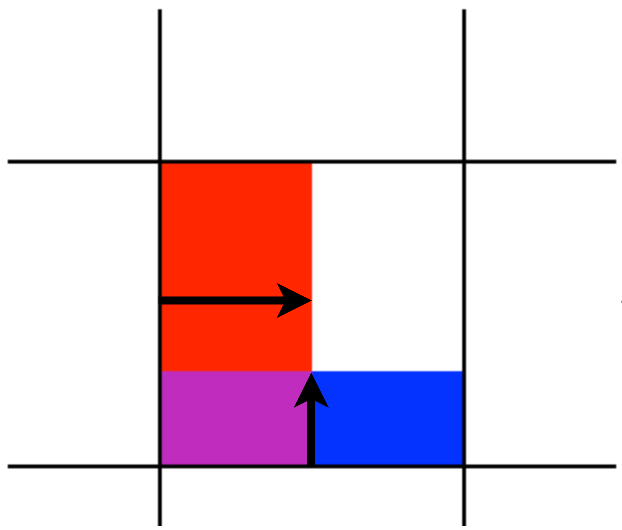
$$
\begin{aligned}
Q_i^{n+1} = Q_i^n \quad & - \quad \frac{\Delta t}{\Delta x} \left(\mathcal{A}^+ \Delta Q_{i-1/2} + \mathcal{A}^- \Delta Q_{i+1/2} \right) \\
& - \quad \frac{\Delta t}{\Delta x} \left(\widetilde{F}_{i+1/2} - \widetilde{F}_{i-1/2} \right)
\end{aligned}
$$

where

$$
\widetilde{F}_{i-1/2} = \frac{1}{2} \sum_{p=1}^{m} |\lambda^p| \left(1 - \frac{\Delta t}{\Delta x} |\lambda^p| \right) \widetilde{\mathcal{W}}_{i-1/2}^p
$$

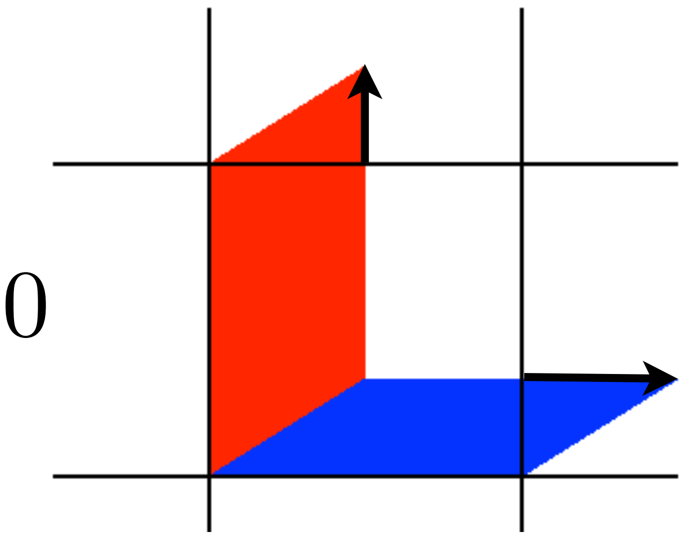
where $\widetilde{\mathcal{W}}_{i-1/2}^p$ are *limited* waves.

Wave-propagation method in two dimensions



Normal waves

$$u > 0, \quad v > 0$$



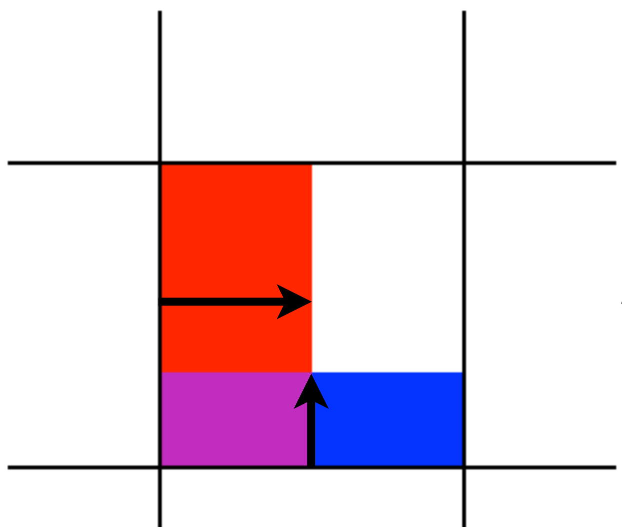
Transverse waves

Wave propagation algorithm

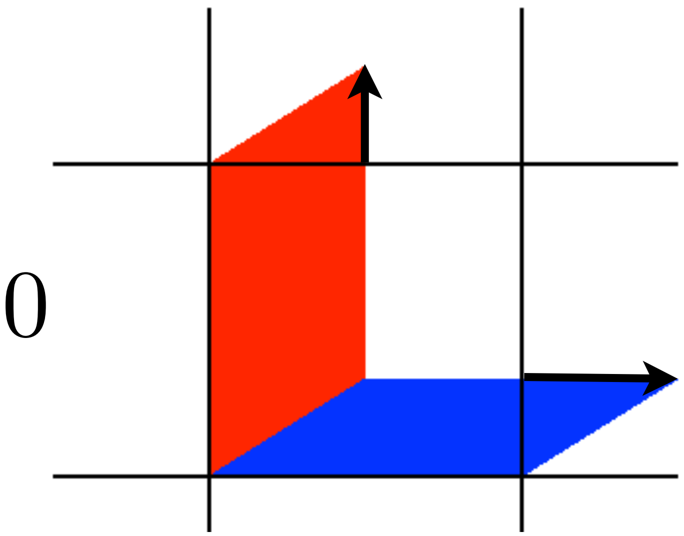
$$
\begin{aligned}
Q_{ij}^{n+1} = Q_{ij}^{n} - \frac{\Delta t}{\Delta x}\left[u^{+}\mathcal{W}_{i-1/2,j} + u^{-}\mathcal{W}_{i+1/2,j}\right] - \frac{\Delta t}{\Delta y}\left[v^{+}\mathcal{W}_{i,j-1/2} + v^{-}\mathcal{W}_{i+1/2,j}\right] \\
-\frac{\Delta t}{\Delta x}\left[\widetilde{\mathcal{F}}_{i+1/2,j} - \widetilde{\mathcal{F}}_{i-1/2,j}\right] - \frac{\Delta t}{\Delta y}\left[\widetilde{\mathcal{G}}_{i,j+1/2} - \widetilde{\mathcal{G}}_{i,g-1/2}\right]
\end{aligned}
$$

Correction terms come from linear terms and transverse propagation

Wave-propagation method in two dimensions



$$u > 0, \qquad v > 0$$



Normal waves *Transverse waves*

Wave propagation algorithm

$$
\begin{aligned}
Q_{ij}^{n+1} = Q_{ij}^{n} &- \frac{u\Delta t}{\Delta x}\left(Q_{ij}^{n} - Q_{i-1,j}^{n}\right) - \frac{v\Delta t}{\Delta y}\left(Q_{ij}^{n} - Q_{i,j-1}^{n}\right) \\
&+ \frac{1}{2}(\Delta t)^2 \left\{ \frac{u}{\Delta x}\left[\frac{v}{\Delta y}(Q_{ij}^{n} - Q_{i,j-1}^{n}) - \frac{v}{\Delta y}(Q_{i-1,j}^{n} - Q_{i-1,j-1})\right]\right. \\
&\qquad \left. + \frac{v}{\Delta y}\left[\frac{u}{\Delta x}(Q_{ij}^{n} - Q_{i-1,j}^{n}) - \frac{u}{\Delta x}(Q_{i,j-1}^{n} - Q_{i-1,j-1})\right]\right\}
\end{aligned}
$$

Forms of equations handled by Clawpack

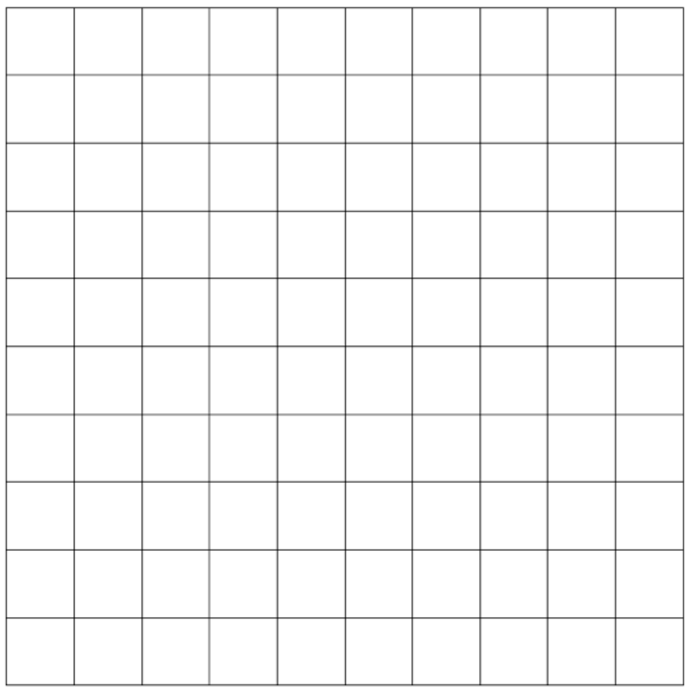
Conservative form	$q_t + f(q)_x = 0$
Quasi-linear form	$q_t + f'(q)\, q_x = 0$
Transport equation	$q_t + u(x) q_x = 0$
Spatially varying flux functions	$q_t + f(q, x)_x = 0$
Source terms	$q_t + f(q)_x = \Psi(q, \ldots)$

Finite volume schemes on curvilinear grids

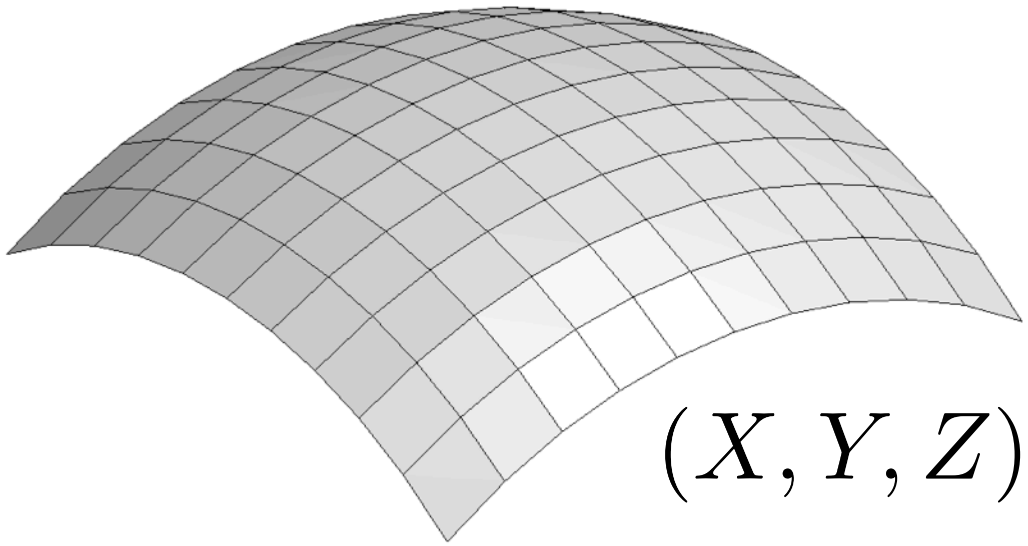
Assume an underlying logically Cartesian computational grid and a smooth mapping given by

$$\mathbf{T}(\xi,\eta) = (X(\xi,\eta), Y(\xi,\eta), Z(\xi,\eta))^T$$

η



ξ



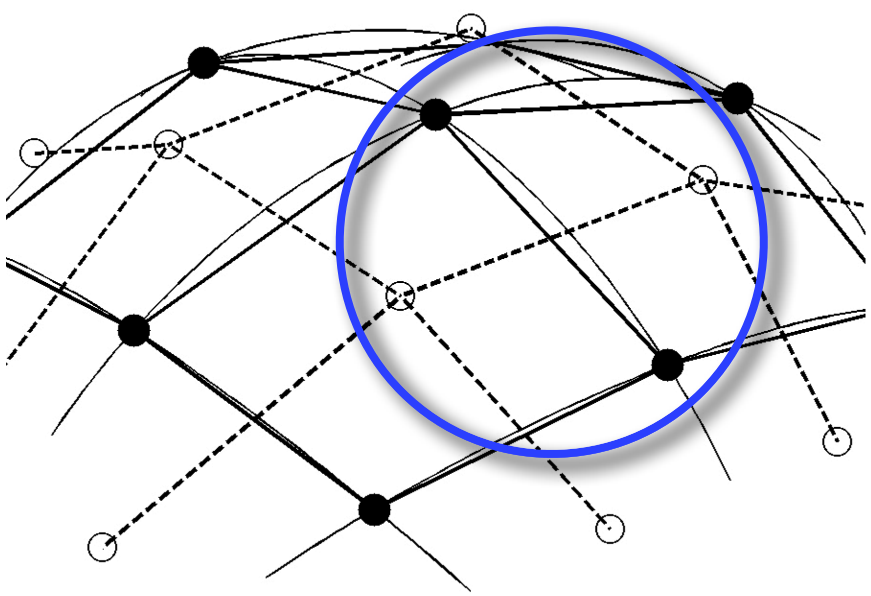
(X, Y, Z)

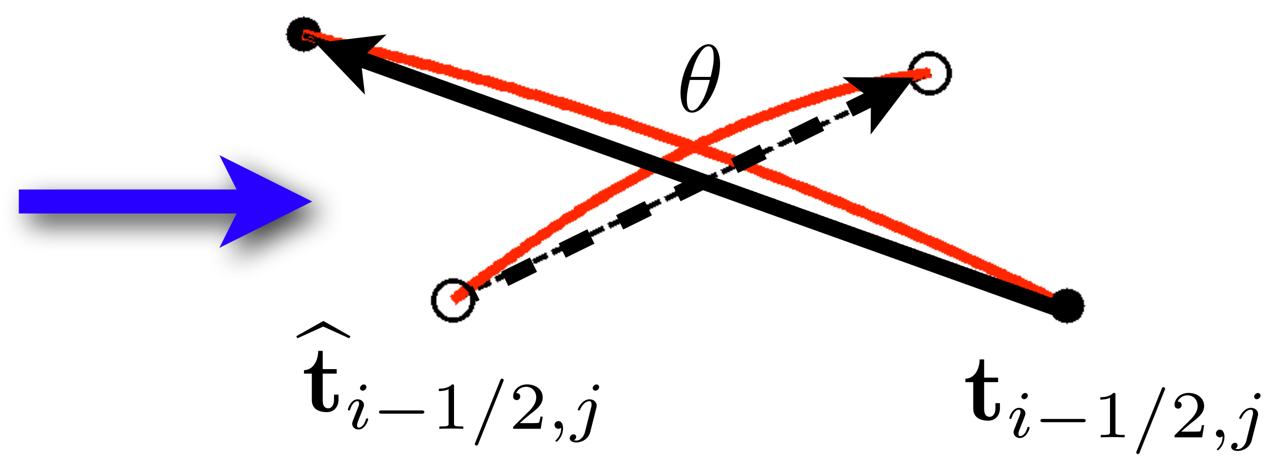
Computational space

Physical space

Wednesday, October 3, 12

Discrete metric terms





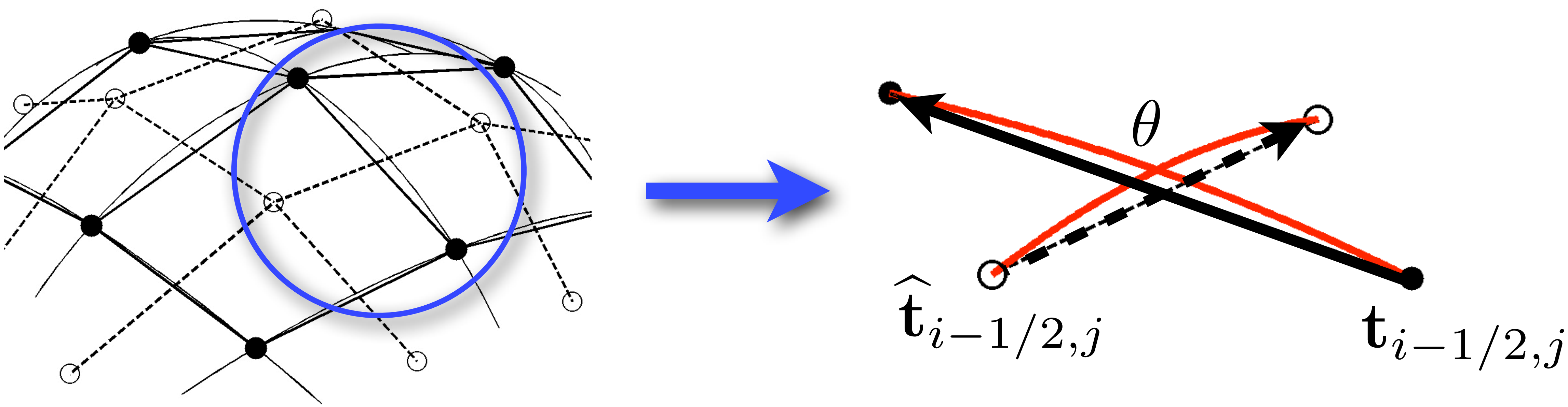
$$a_{11} = \mathbf{T}_\xi \cdot \mathbf{T}_\xi \approx \mathbf{t} \cdot \mathbf{t} = \|\mathbf{t}\|^2$$

$$a_{12} = a_{21} = \mathbf{T}_\xi \cdot \mathbf{T}_\eta \approx \mathbf{t} \cdot \widehat{\mathbf{t}} = \|\mathbf{t}\|\|\widehat{\mathbf{t}}\| \cos(\theta)$$

$$a_{22} = \mathbf{T}_\eta \cdot \mathbf{T}_\eta \approx \widehat{\mathbf{t}} \cdot \widehat{\mathbf{t}} = \|\widehat{\mathbf{t}}\|^2$$

$$\sqrt{a} = \| \mathbf{T}_\xi \times \mathbf{T}_\eta \| \approx \| \mathbf{t} \times \widehat{\mathbf{t}} \| = \|\mathbf{t}\|\|\widehat{\mathbf{t}}\| \sin(\theta)$$

Normals and lengths



Lengths

$$\ell_{i-1/2,j} = \int_{\eta_{j-1/2}}^{\eta_{j+1/2}} \| \mathbf{T}_\eta \| \; d\eta \approx \| \mathbf{t}_{i-1/2,j} \|$$

Edge normals tangent to the surface

$$\mathbf{n}_{i-1/2,j} \approx \frac{\mathbf{t}^{(1)}}{\| \mathbf{t}^{(1)} \|} \approx \frac{1}{\| \mathbf{t} \|} \left(\frac{\| \mathbf{t} \|}{\| \widehat{\mathbf{t}} \|} \csc(\theta)\, \widehat{\mathbf{t}} - \cot(\theta) \mathbf{t} \right)$$

Discrete mesh cell areas

$$A_{ij} = \int_{C_{ij}} \| \mathbf{T}_\xi \times \mathbf{T}_\eta \| \; d\xi \, d\eta$$

Approximate mesh cell surface as a ruled surface :

$$\mathbf{S}(u,v) = \mathbf{a}_{00} + \mathbf{a}_{01} u + \mathbf{a}_{10} v + \mathbf{a}_{11} uv, \qquad 0 \le u, v \le 1$$

where the coefficients $\mathbf{a}_{\ell m} \in \mathcal{R}^3$ are computed from four corners of the mesh cell. Then

$$\begin{aligned} A_{ij} &\approx \int_{C_{ij}} \| \mathbf{S}_u \times \mathbf{S}_v \| \; du dv \\ &\approx \| \, (\mathbf{a}_{01} + \frac{1}{2}\mathbf{a}_{11}) \times (\mathbf{a}_{10} + \frac{1}{2}\mathbf{a}_{11}) \, \| \end{aligned}$$

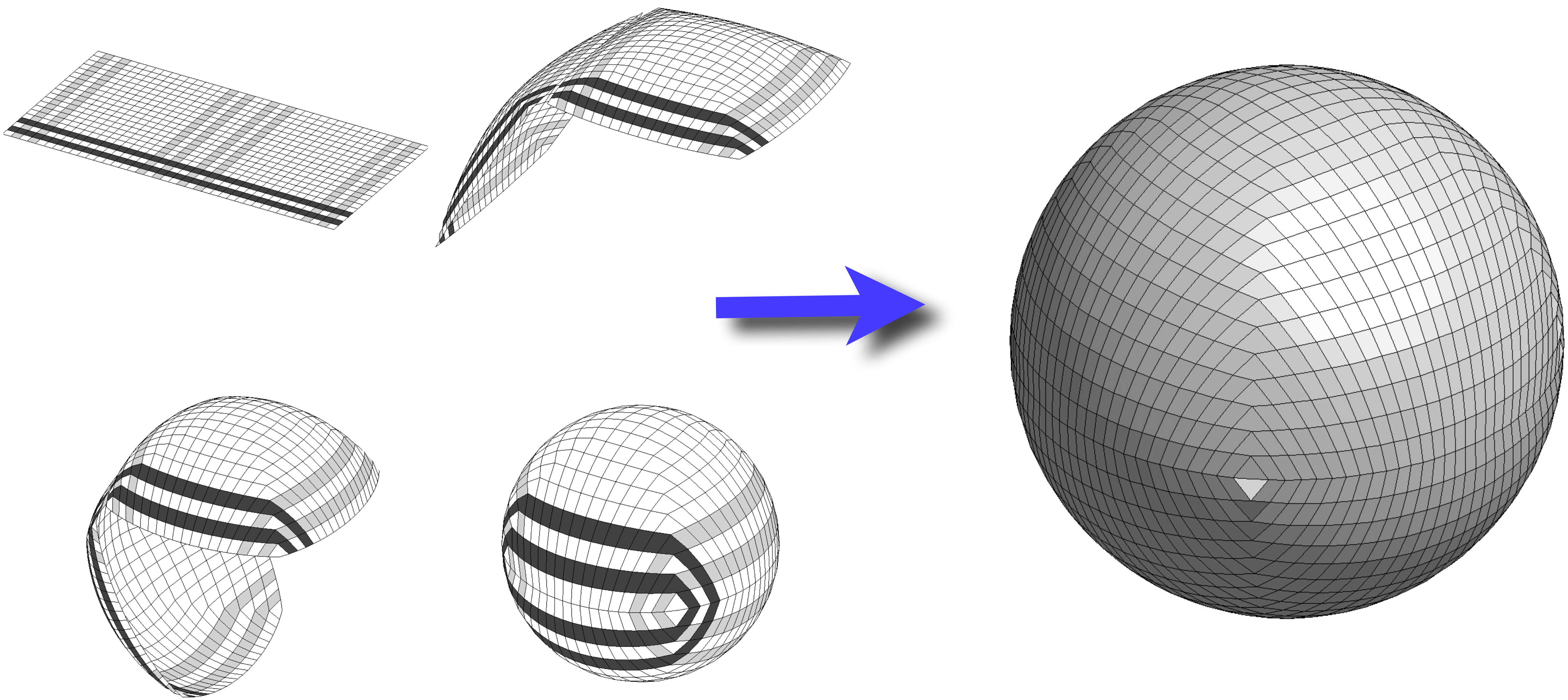
FV update formula for curvilinear grids

$$
\begin{aligned}
Q_{ij}^{n+1} \quad = \quad & Q_{ij}^{n} - \frac{\Delta t}{\kappa_{ij}\Delta\xi}\left(u^{+}\Delta Q_{i-1/2,j} + u^{-}\Delta Q_{i+1,j}\right) - \\
& \frac{\Delta t}{\kappa_{ij}\Delta\eta}\left(v^{+}\Delta Q_{i,j-1/2} + v^{-}\Delta Q_{i,j+1}\right) - \\
& \frac{\Delta t}{\kappa_{ij}\Delta\xi}\left(\widetilde{F}_{i+1/2,j} - \widetilde{F}_{i-1/2,j}\right) - \frac{\Delta t}{\kappa_{ij}\Delta\eta}\left(\widetilde{G}_{i,j+1/2} - \widetilde{G}\right.
\end{aligned}
$$

where

$$
\begin{aligned}
u_{i-1/2,j} \quad &= \quad \frac{\ell_{i-1/2,j}}{\Delta\eta}\widetilde{u}_{i-1/2,j} \\
v_{i,j-1/2} \quad &= \quad \frac{\ell_{i,j-1/2}}{\Delta\xi}\widetilde{v}_{i,j-1/2} \\
\kappa_{ij} \quad &= \quad \frac{A_{ij}}{\Delta\xi\Delta\eta}
\end{aligned}
$$

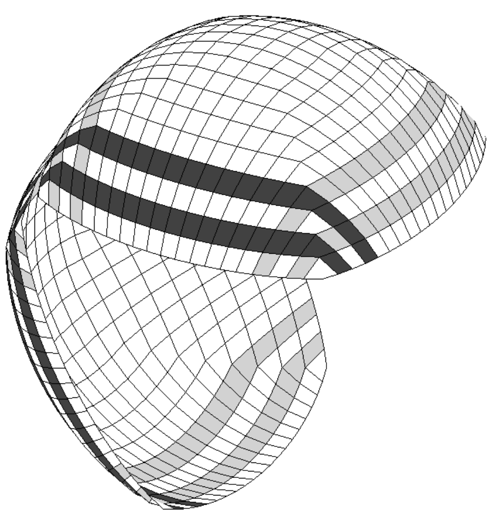
Single logically Cartesian sphere grid

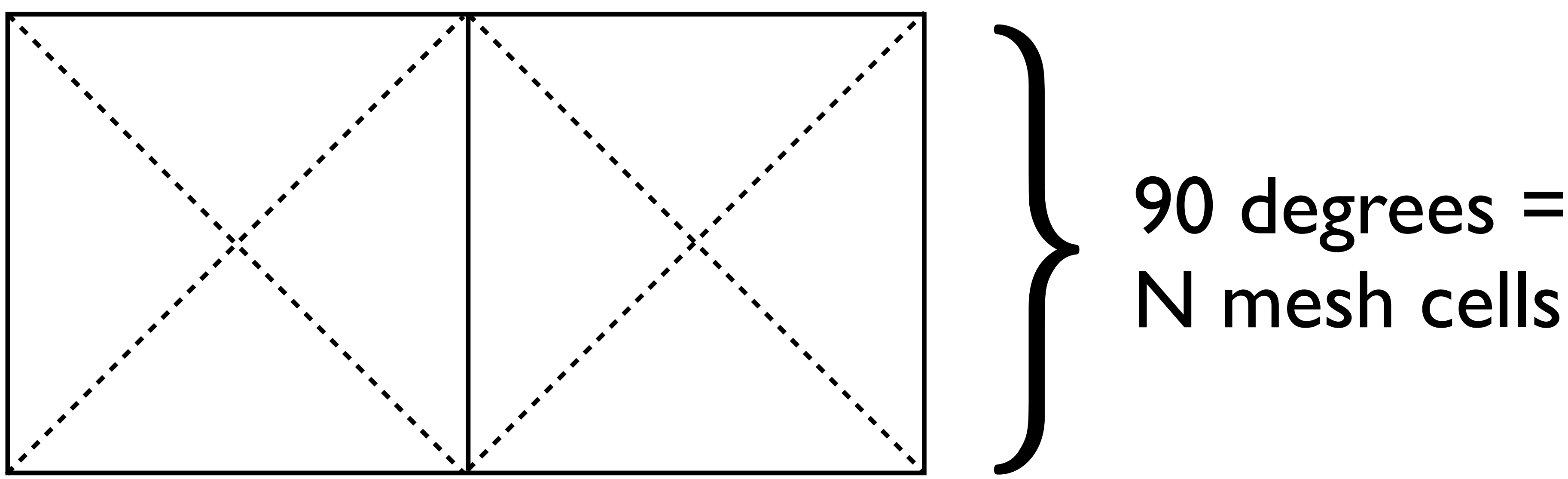


D. Calhoun, C. Helzel, and R. LeVeque, SIAM Review, 50 (2008)

A two-patch sphere grid?

- Our sphere grid is like the cubed-sphere grid, but with two patches
- We will refer to the grid resolution by the number of grid cells on a patch edge, which is approximately 90 degrees.



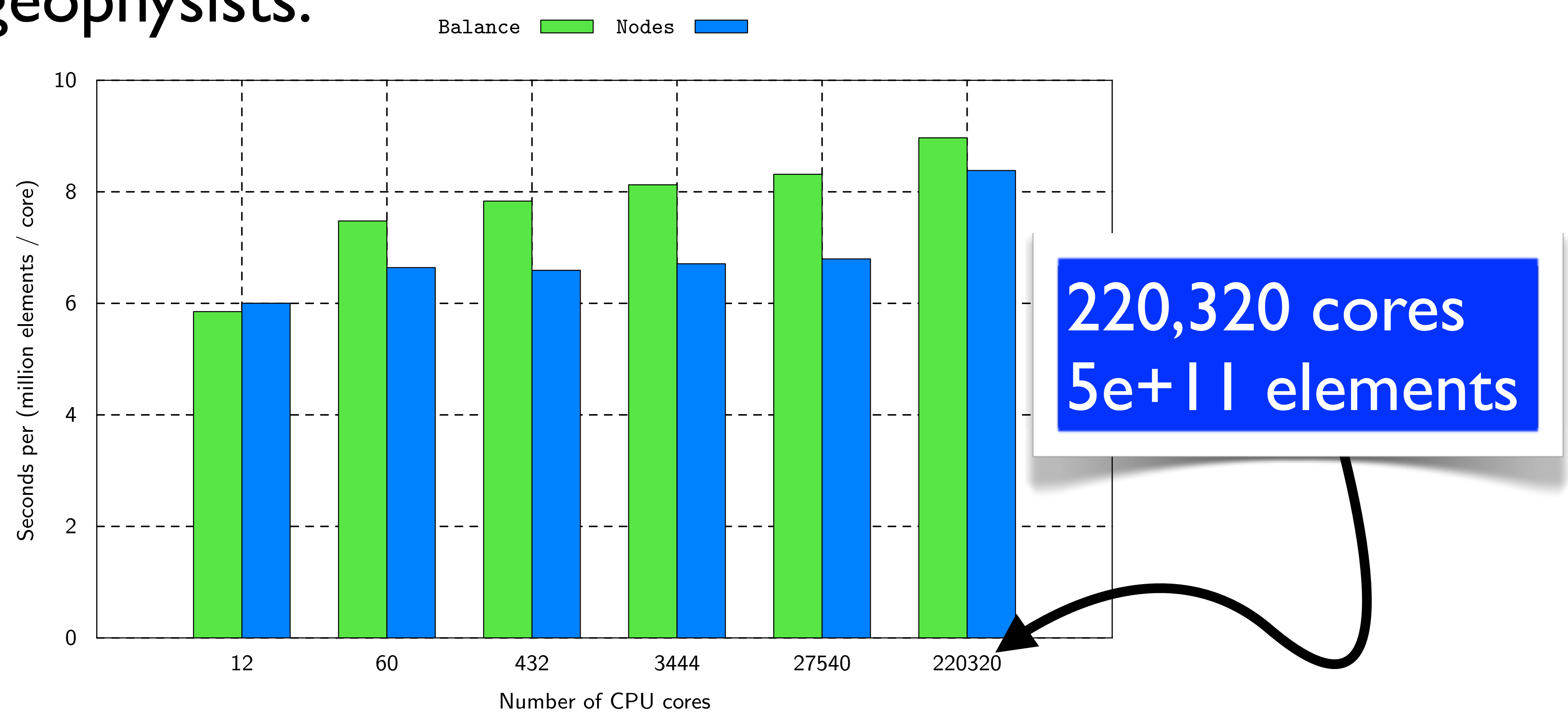


Dashed and solid lines are discontinuities in the mapping

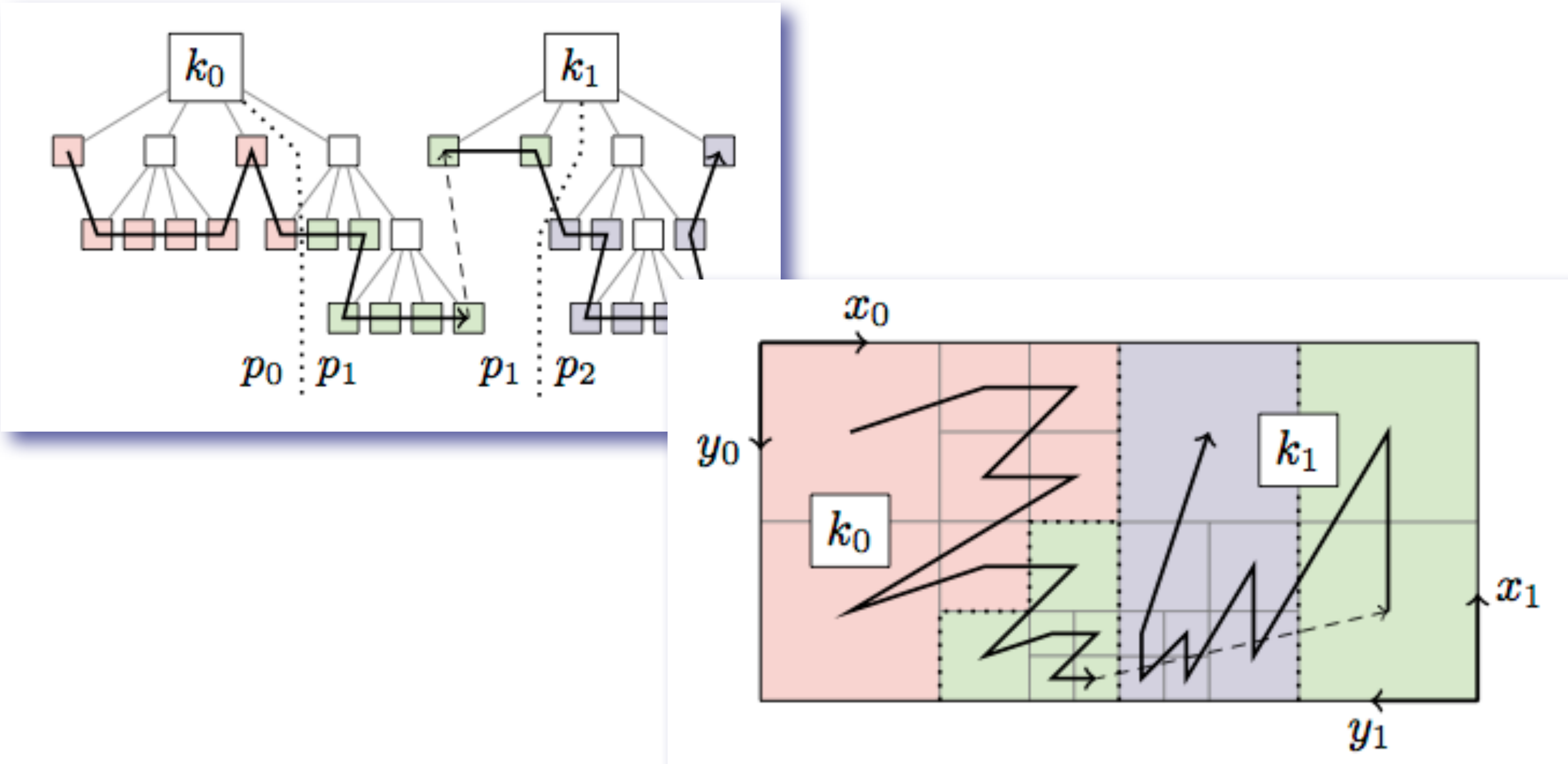
A Pillow grid?

p4est

- Parallel, multiblock code for managing a forest of adaptive quad- or octrees.
- Developed by Carsten Burstedde (Univ. of Bonn), with Wilcox, Ghattas and others
- Highly scalable on realistic applications of interest to geophysists.

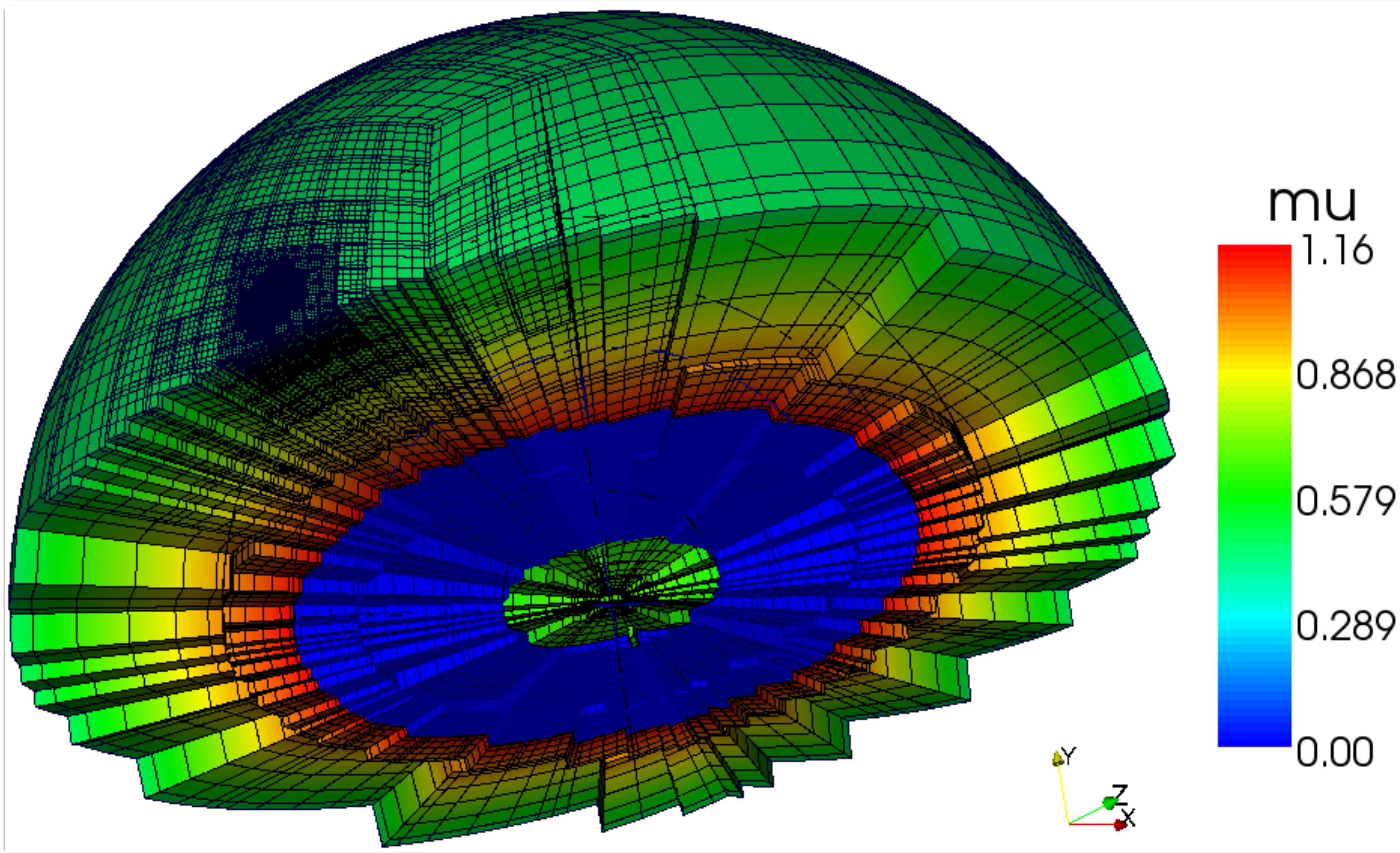


p4est



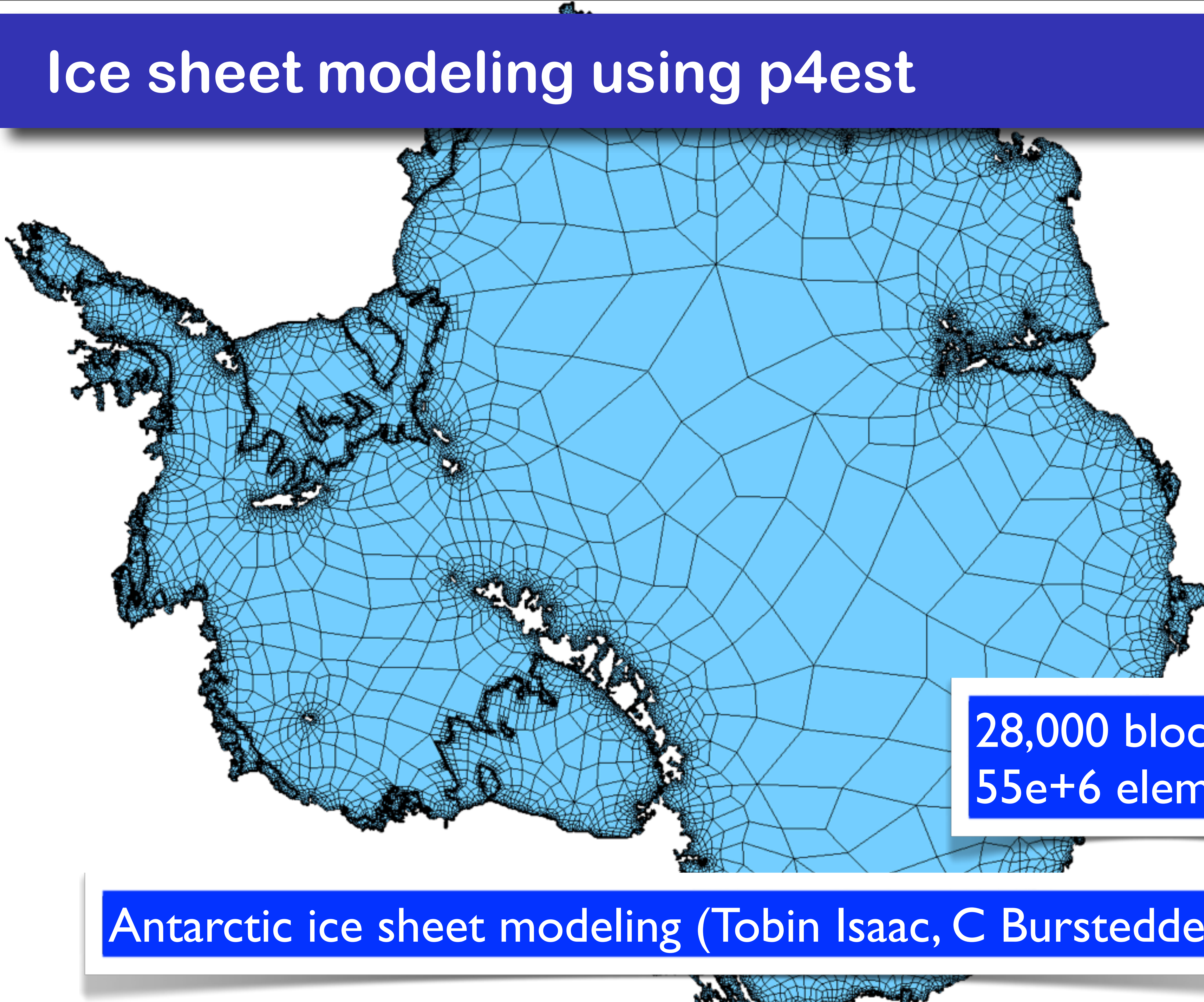
High scalability is achieved while preserving data locality

p4est



Earthquake simulation using p4est on a cubed sphere mesh. (Burstedde, Wilcox, Ghattas, SISC, 2011)

Ice sheet modeling using p4est



28,000 blocks
55e+6 elements

Antarctic ice sheet modeling (Tobin Isaac, C Burstedde)

ForestClaw = p4est + Clawpack

- Use p4est to manage the parallel multiblock of quad- or octree whose leaves are non-overlapping, fixed size grids.
- Implement basic block-structured AMR algorithm (Berger, Colella, LeVeque and others)
- Reuse existing patch based solvers for single grids
- Do subcycling in time on finer grids to improve scalability and accuracy,
- Ensure mass conservation at coarse/fine interfaces
- p4est guides parallel transfers,
- p4est provides information about face orientations.

Similar approaches

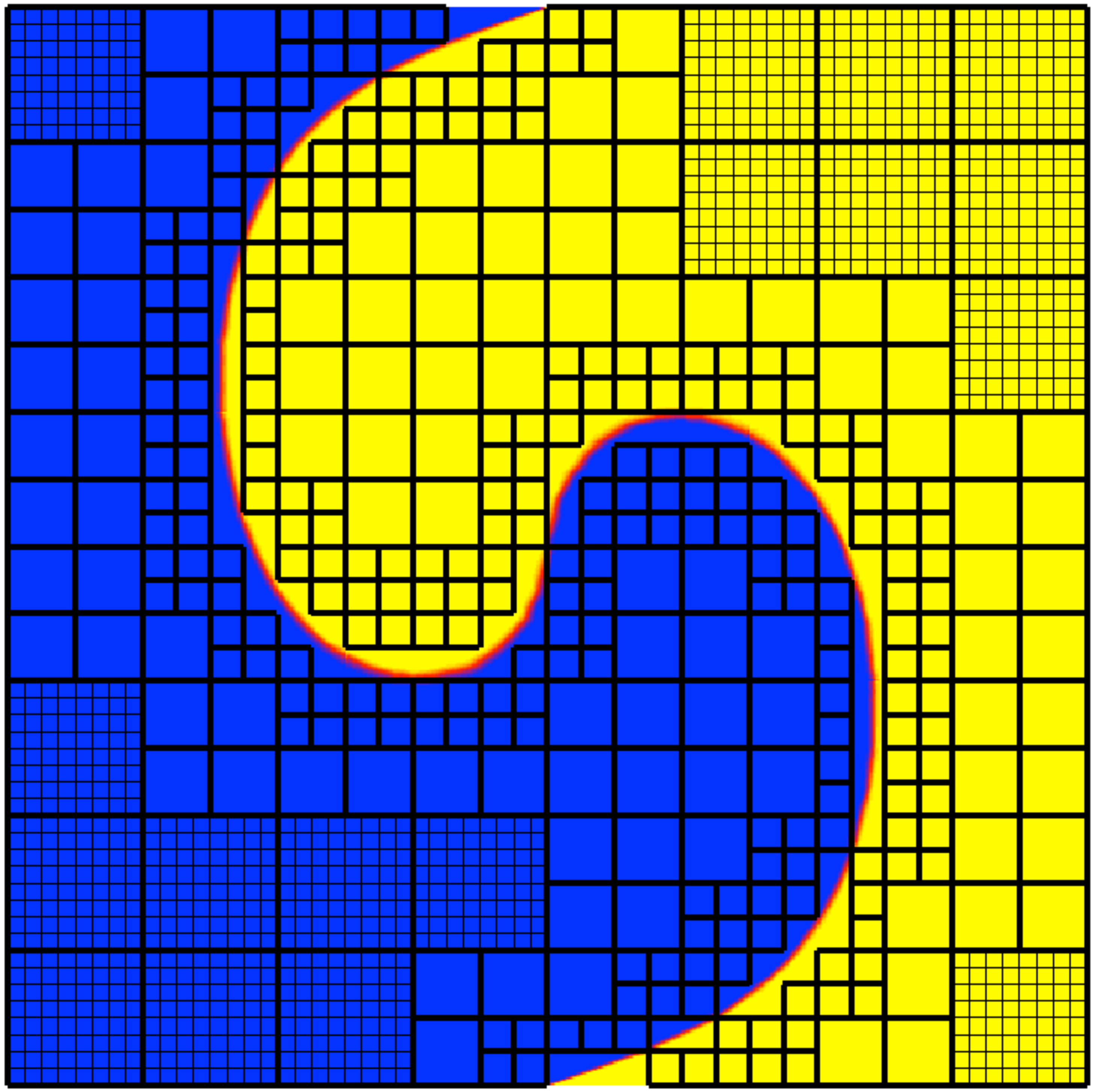
Similar approaches based on fixed size grids and/or octrees...

- "Building Cubes Method" (Sasaki, Akahito, Yamazaki, et al.)
- Parallel adaptive methods for weather prediction C. Jablonowski, Oehmke, Stout and others
- Gerris Flow solver - cell-based octree approach (S. Popinet)
- NIRVANA (U. Ziegler)
- Block-structured AMR codes (Chombo, Boxlib, AMRClaw, SAMRAI, AMROC, Agrif, ...) could all be run in an "octree" like mode.

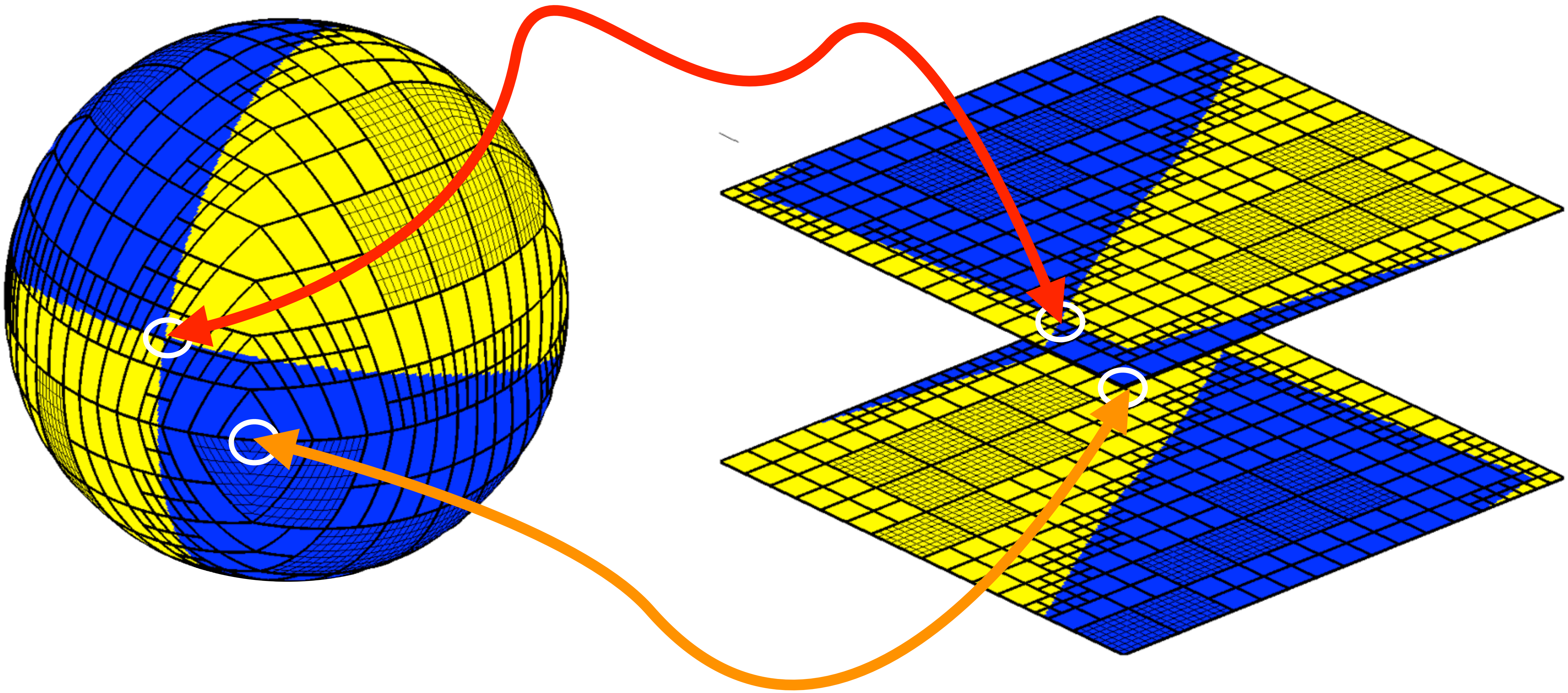
Results

Results

q(1) at time 2.5009

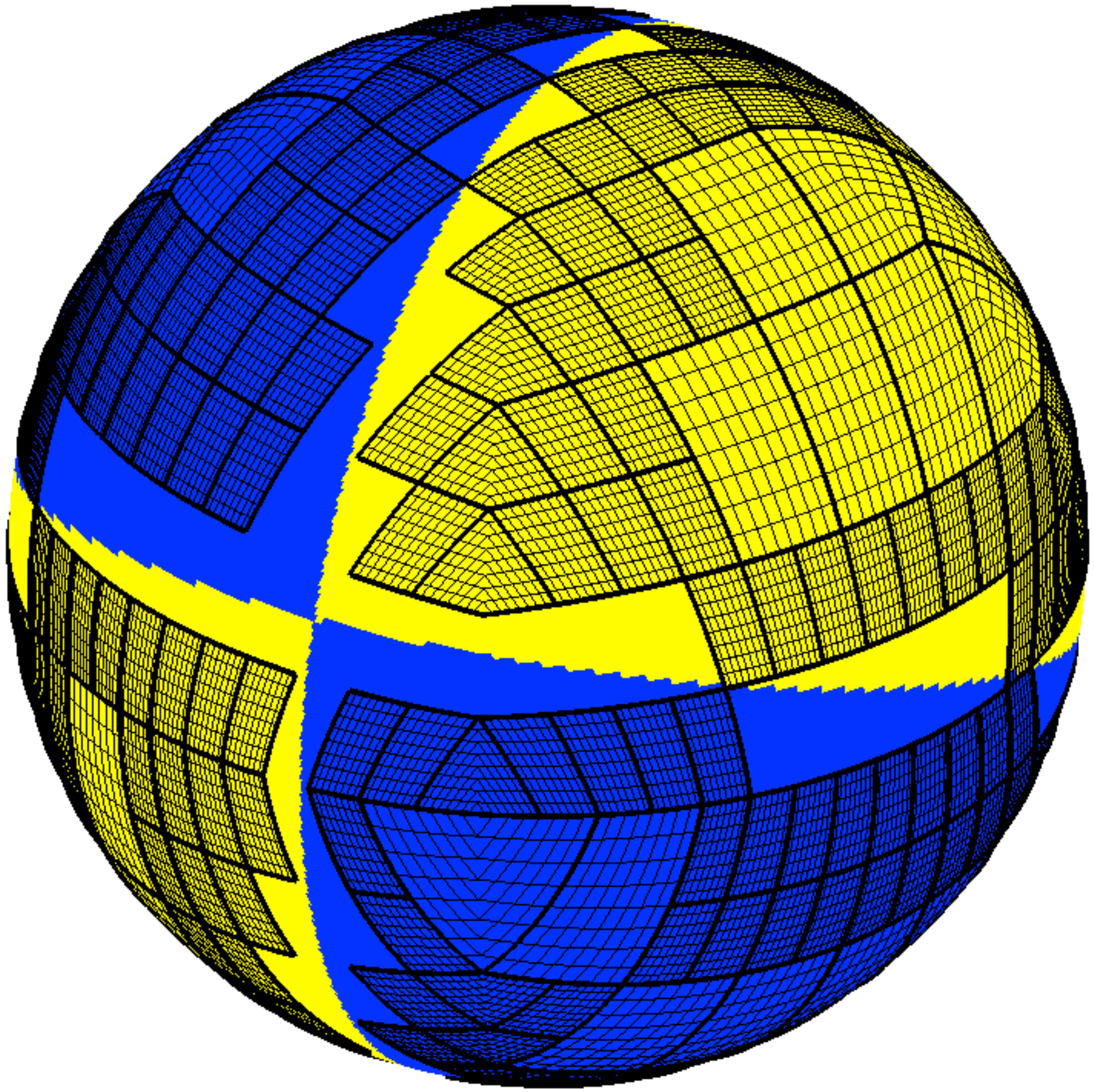


Scalar transport on the sphere



Scalar advection

Scalar advection



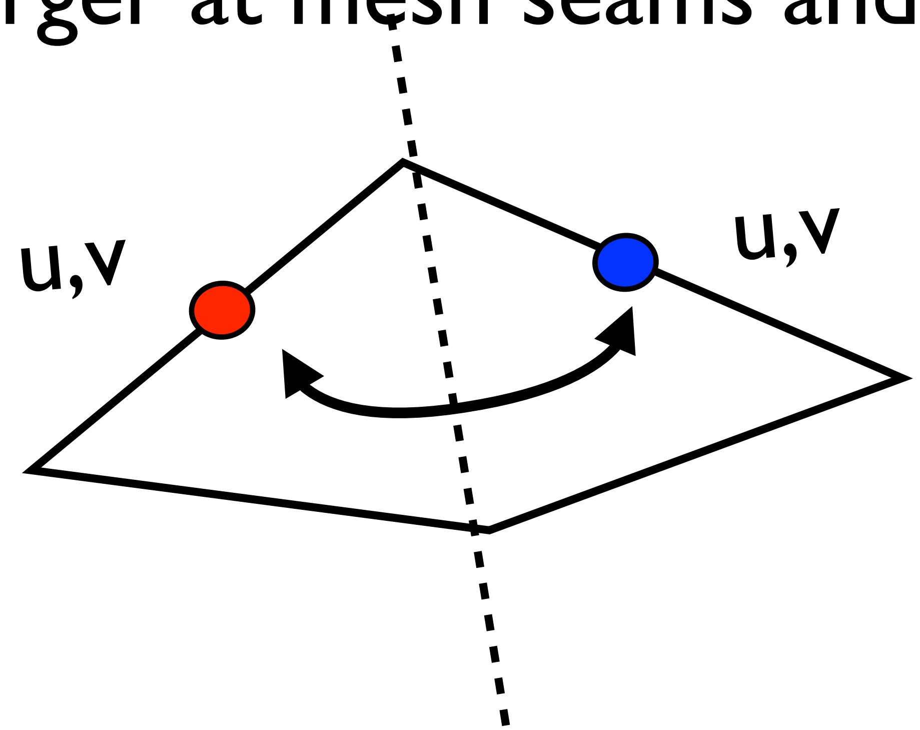
Refinement criteria

- Feature-based refinement - refine near boundaries, where a tracer is highly concentrated, large gradients
- Extrapolate from coarser grid solutions to estimate truncation error
- A posteriori error estimation
- Adjoint methods
- ....

A code should be flexible enough to allow the user to experiment with different choices.

Current issues

- Convergence is between 1 and 2, depending on where error is measured, what norm, what problem, ...
- Accuracy of our methods depends on the smoothness of the mesh.
- Errors are larger at mesh seams and along the diagonals



Transverse propagation uses velocities on two sides of a discontinuity, introducing O(1) errors in the truncation error.

Future work

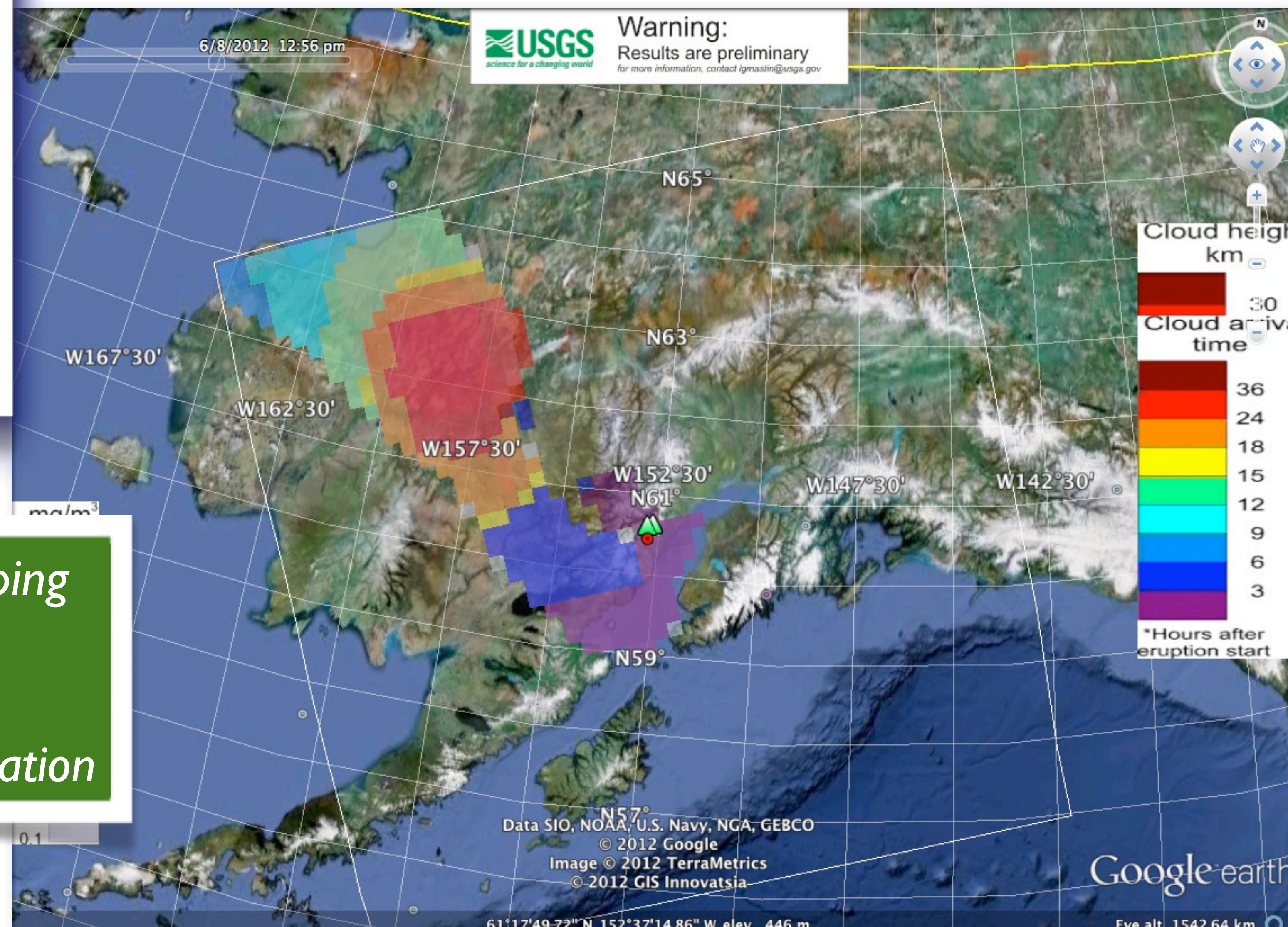
(Future work from NCAR Tracer Transport 2011 meeting)

- ☑ Adaptive Mesh Refinement
- ☑ ~~Implementation in AMRClaw or ChomboClaw~~

- Develop general way to handle face orientations in the multiblock setting.
- More general approach to handling user input, including specification of block layout and orientations,
- Scaling tests,
- Accuracy tests
- Applications...

Ash cloud modeling

Ash3d



- *Split horizontal, vertical time stepping*
- *Fully conservative,*
- *Eulerian, finite volume*
- *Algorithms based on wave propagation*

Ash3d :A finite-volume, conservative numerical model for ash transport and tephra deposition, Schwaiger, Denlinger, Mastin, JGR (2012)