Parallel, adaptive framework for mapped, multi-block domains

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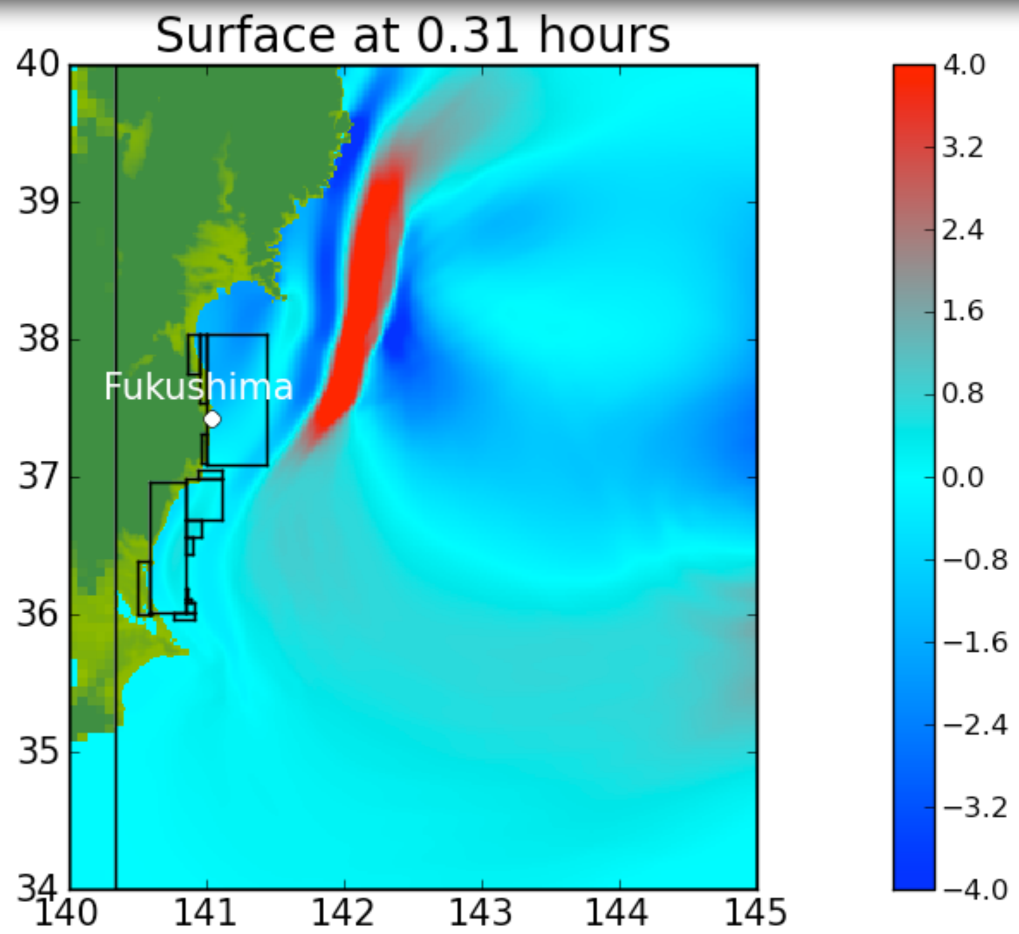
Randall J. LeVeque (Univ. of WA), Marsha Berger (NYU), David George (USGS)

PDEs on the Sphere

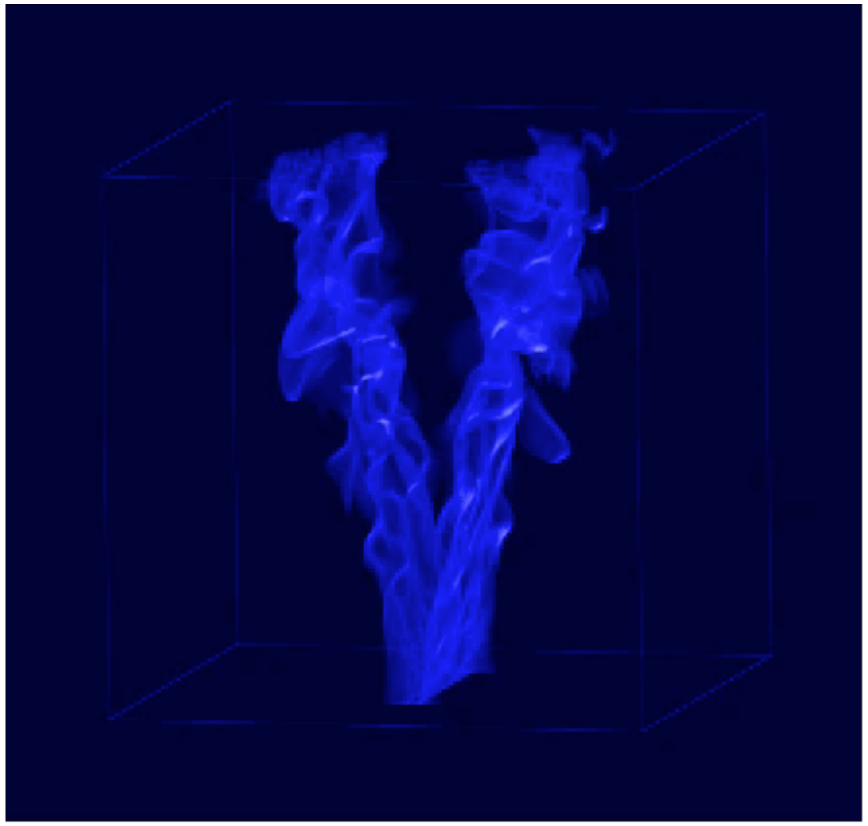
April 7-11, 2014

Boulder, CO

Applications of AMR



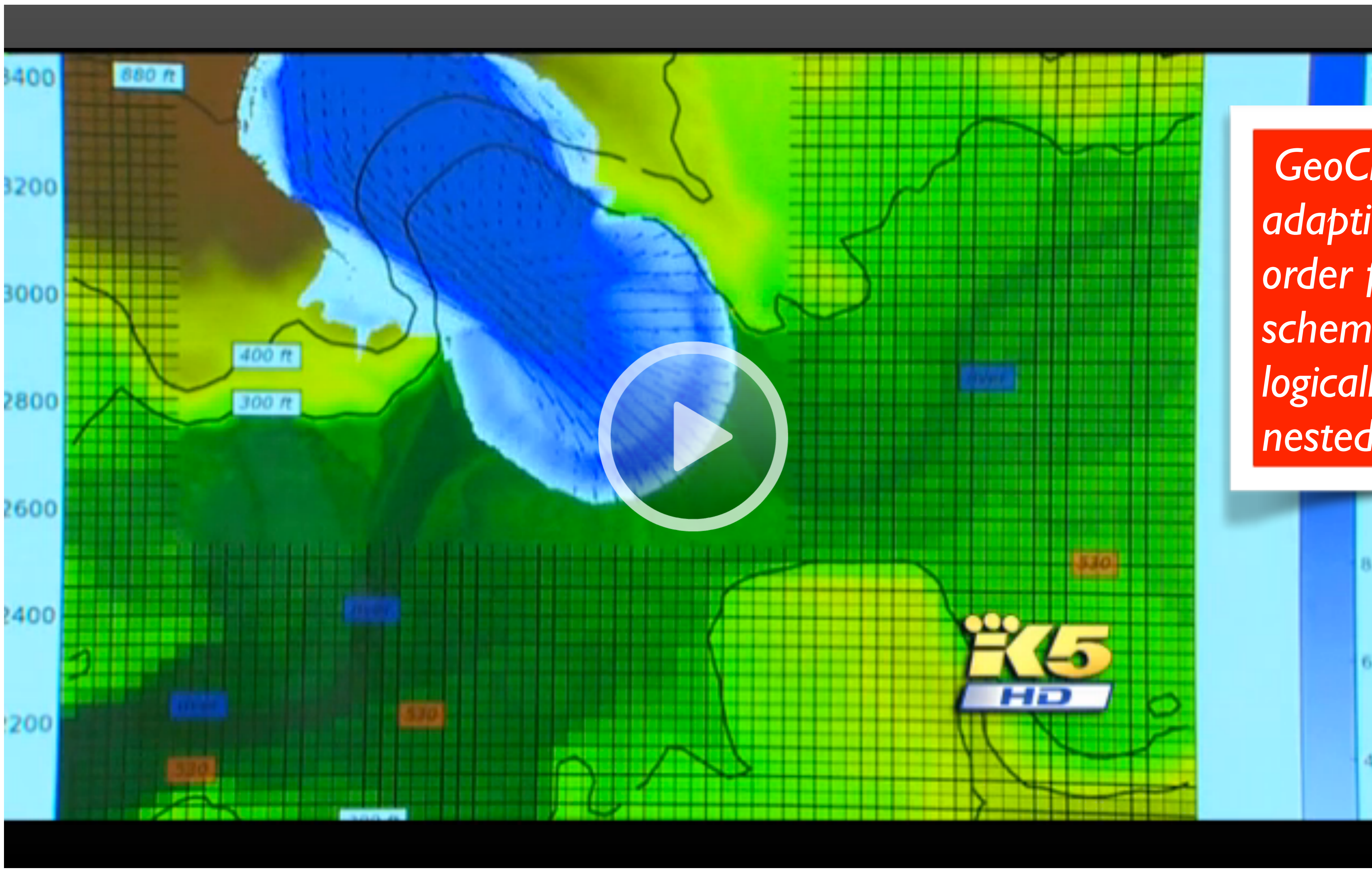
Tsunami modeling (R. LeVeque, D. George, M. Berger)



Rod stabilized V-flame (J. B. Bell, Lawrence Berkeley Lab)

- Astrophysics, combustion
- Shock capturing for aerodynamic applications
- Storm surges, debris flow, porous media flow
- Ice sheet modeling, tsunami modeling

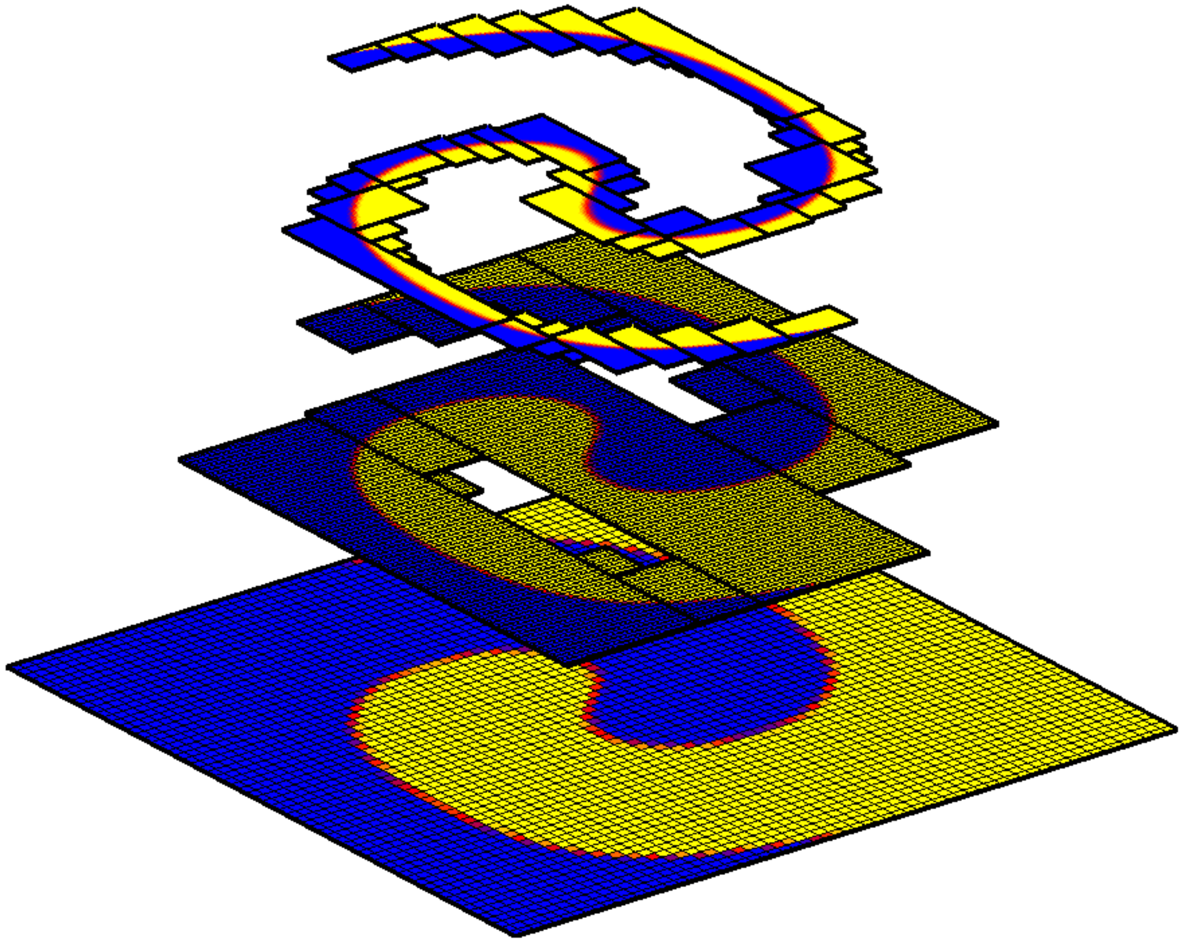
GeoClaw in the news (4/8/2014)

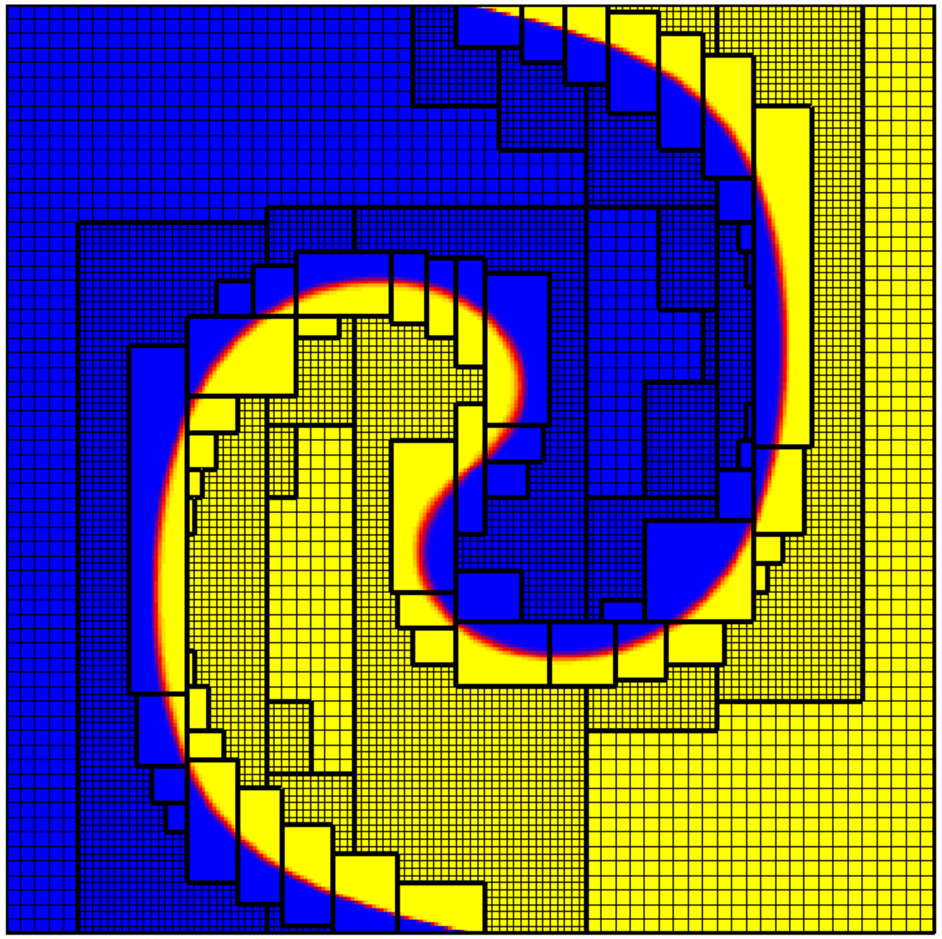


GeoClaw is a fully adaptive, second order finite volume scheme for logically Cartesian nested meshes.

GeoClaw (R. J. LeVeque, D. George, M. Berger) used to model recent landslide in Washington State

Berger-Oliger block-structured AMR





Almost exactly 30 years, Marsha Berger introduced block-structured AMR

M. Berger and J. Oliger, "Adaptive mesh refinement for hyperbolic partial differential equations", JCP Volume 53, March, 1984.

Block-structured AMR

- General purpose (freely available) block-structured codes
  - SAMRAI (Lawrence Livermore National Lab)
  - BoxLib (Lawrence Berkeley Lab)
  - Chombo (Lawrence Berkeley Lab)
  - AMRClaw (University of Washington/NYU)
  - AMROC (Ralf Deiterding, DLR, Germany)
  - PARAMESH (NASA/Goddard) (not technically "block-structured", but rather quadtree-based.)
- Most are large frameworks, with many developers
- Mostly C++ and Fortran libraries (no GUIs) that started life as research codes.

See my website for a list of many more application specific codes

Goal of patch-based AMR codes

- Make full use of existing solvers for Cartesian grids
- Operate locally on patches whenever possible
- Have the same order of accuracy as the single grid algorithm.
- Maintain conservation where appropriate
- Use local time stepping to maintain a constant CFL number across refinement levels,
- Fully couple solution between grids,
- Operate efficiently on latest hardware.

Goal is to do this without significant overhead associated with managing the grid hierarchy.

Why are AMR codes difficult to write?

- Heterogeneous data structures for storing hierarchy of grids,
- Dynamically creating and destroying grids,
- Need a "factory" paradigm to create user defined auxiliary data arrays (material properties, metric terms, bathymetry, etc) needed for each new grid,
- Communication between patches,
- Parallel load balancing and IO,
- Efficient implementation of multi-rate time stepping schemes,
- User interface for mixed type equations and solvers,
- Error estimation, tuning for efficient use of grids,
- ....

...and hard to use

- Time stepping methods beyond one-step, single stage methods, including multi-stage Runge-Kutta, IMEX, SSP, parallel-in-time, exponential integrators, HEVI, spectral deferred correction, …
- Accuracy of multi-rate schemes for PDEs with mixed elliptic/parabolic/hyperbolic terms.
- Elliptic and parabolic solvers (iterative? direct? Explicit? Implicit?)
- Refinement criteria?
- Higher order accuracy
- Complex physics
- Visualization
- Debugging and post-processing

AMR Skeptics?

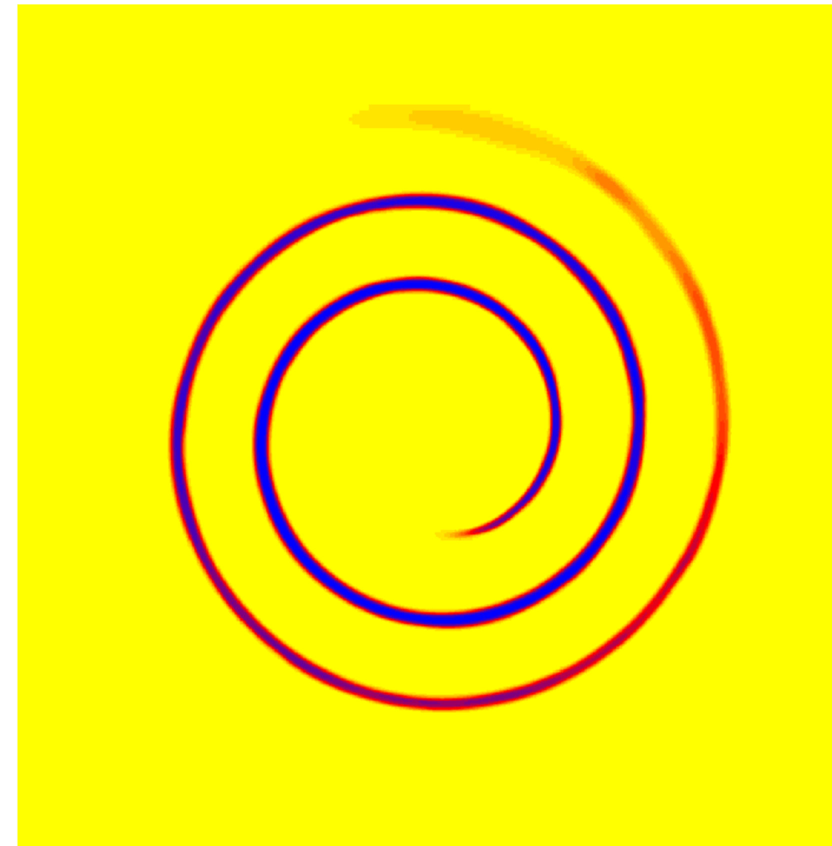
- Coarse/fine boundaries with abrupt resolution changes are regarded with suspicion,
- Lack of good refinement criteria dampens enthusiasm for trying out AMR,
- Not obvious how to extend sophisticated numerical algorithms and applications to the adaptive setting,
- Physics parameterizations

When multi-resolution grids are used …

- Multi-rate time stepping is not often used (it seems)
- The goals are often modest : "Do no harm!"
- One way coupling of regional, static grids

Tracer transport

64 x 64



1024 x 1024

Tracer transport of pollutants, volcanic ash

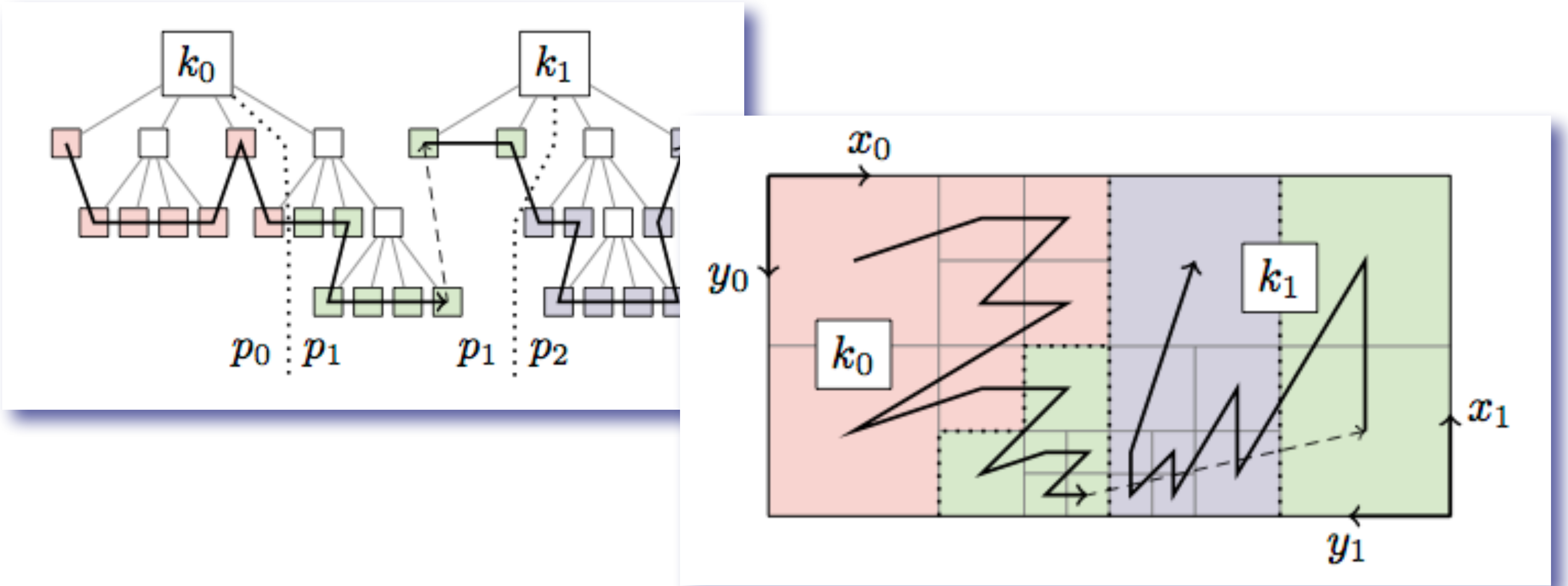
Behrens, J., Dethloff, K., Hiller, W., and Rinke, A. Evolution of small-scale filaments in an adaptive advection model for idealized tracer transport. Monthly Weather Review 128 (2000), 2976–2982.

AMR for the computational mathematician

- Support for grid management that is separate from the numerics, that is intuitive, with easily manageable data structures,
- Support for multi-rate time stepping with flexibility to include new time stepping schemes (MOL solvers, for example),
- Easy to add diagnostics for convergence studies,
- Natural code for iterating over arrays (*in Fortran?*),
- Flat data structures - little reliance on templates, and exotic object oriented data structures,
- Parallelism should happen automatically.
- Simple build system

Building your own code is reasonable if you start with…

p4est - dynamic grid management



p4est (Carsten Burstedde, Univ. of Bonn) is a highly scalable library for dynamically managing an octree of grids.

Carsten Burstedde, Lucas C. Wilcox, and Omar Ghattas, "p4est: Scalable Algorithms for Parallel Adaptive Mesh Refinement on Forests of Octrees", SISC (2011)

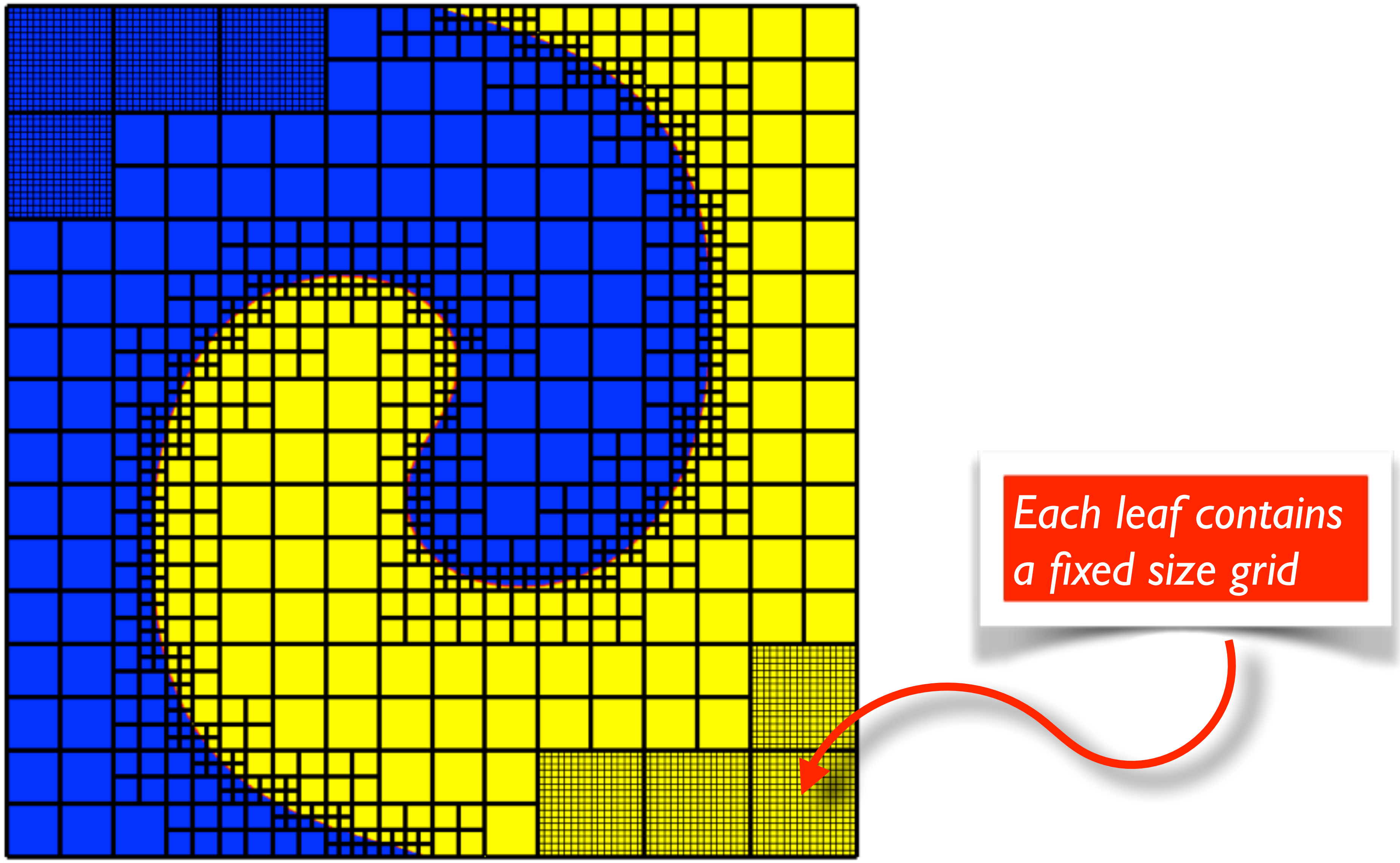
Add solvers

- Wave propagation algorithm - Clawpack (R. J. LeVeque) - second order finite volume scheme for hyperbolic conservation laws.
  - assumes logically Cartesian smooth or piecewise smooth meshes,
  - suitable mapped Euclidean and non-Euclidean grids
  - Available in well tested Clawpack (www.clawpack.org)

- Runge-Kutta Chebyshev solvers for explicit diffusion problems (reaction diffusion)

- Flexibility in user choosing their own solver.

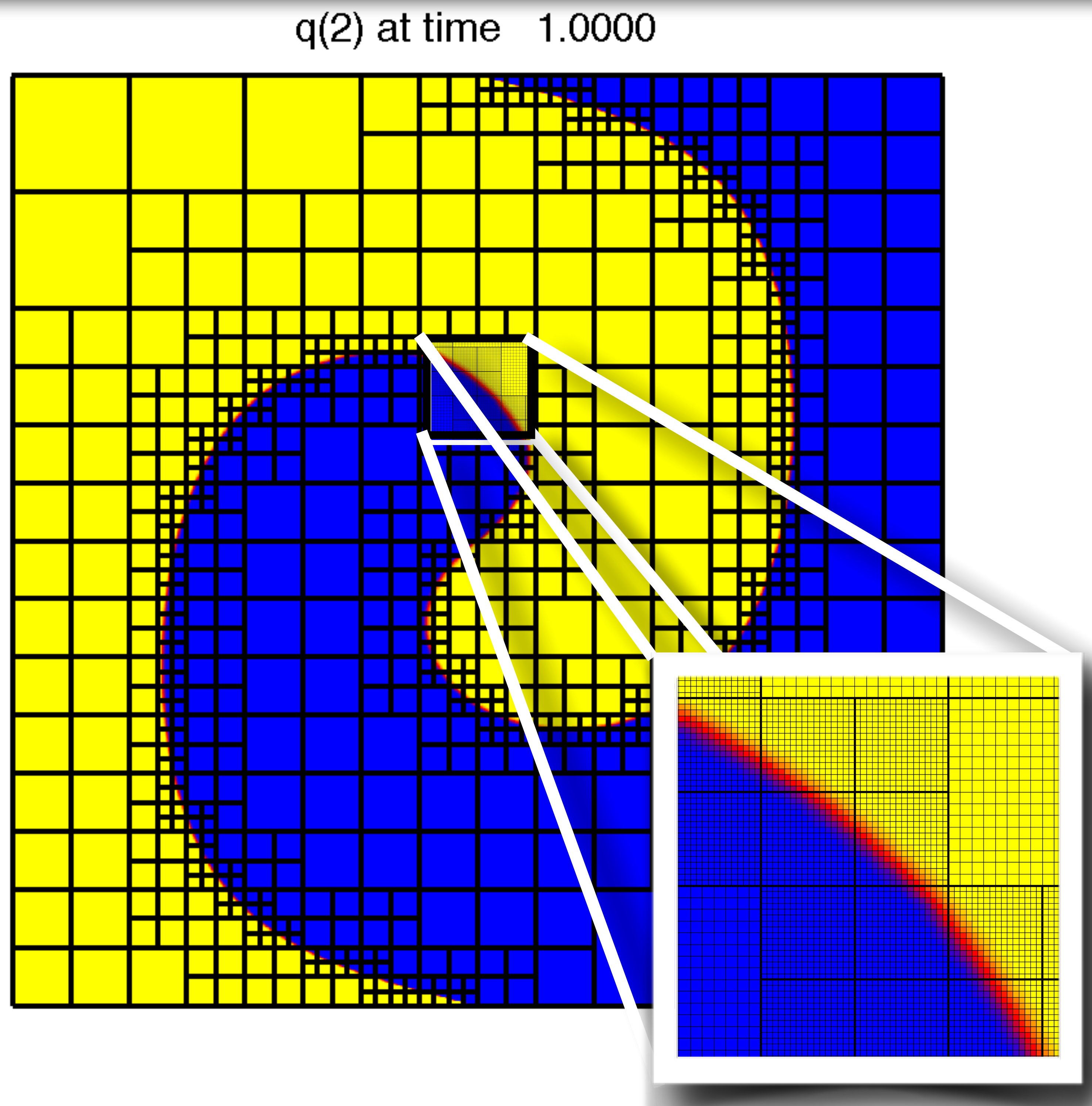
AMR using ForestClaw



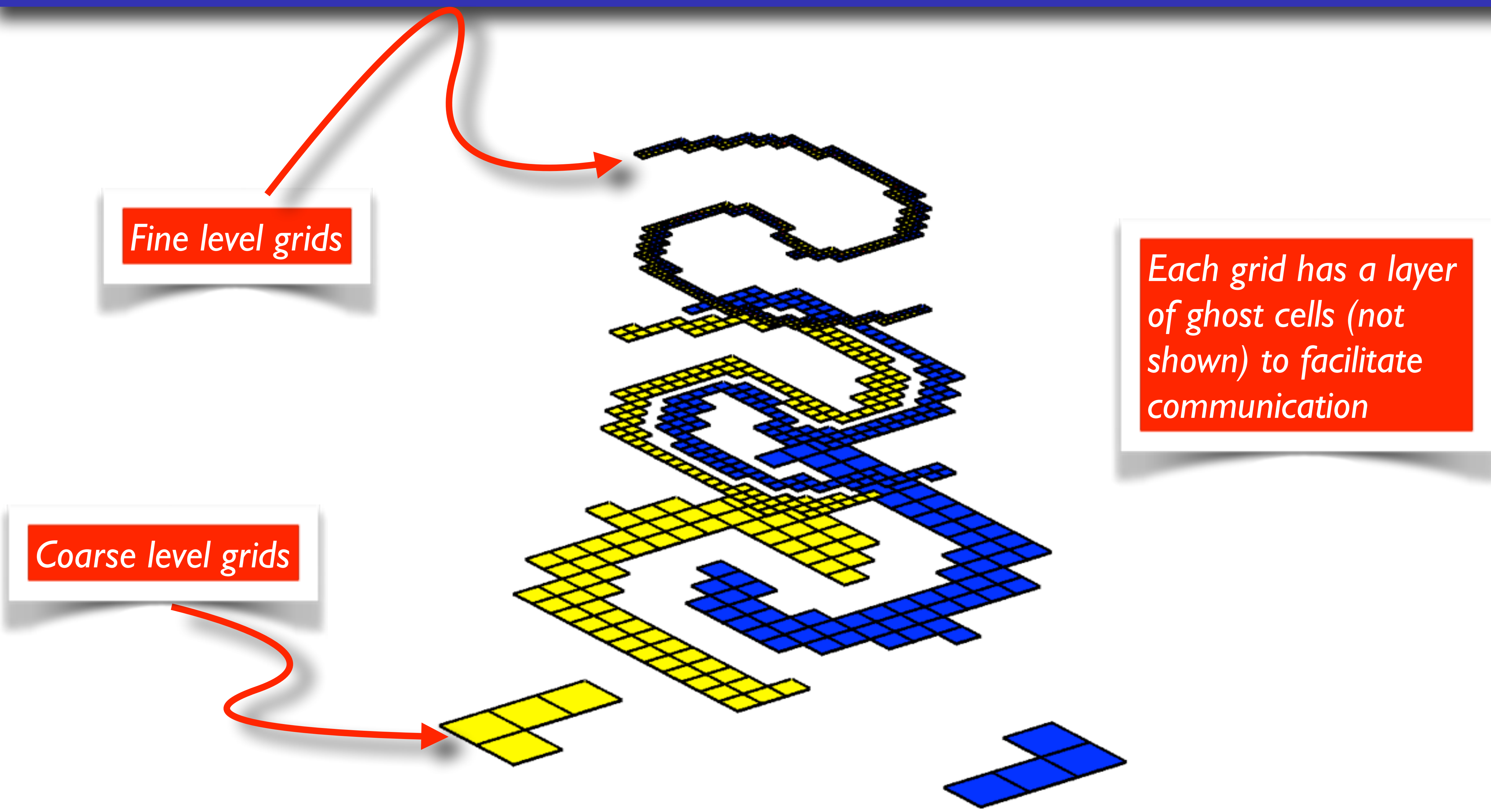
Local grid refinement based on subdividing quadrants of the computational domain.

ForestClaw (D. Calhoun, C. Burstedde)

AMR using ForestClaw



AMR using ForestClaw

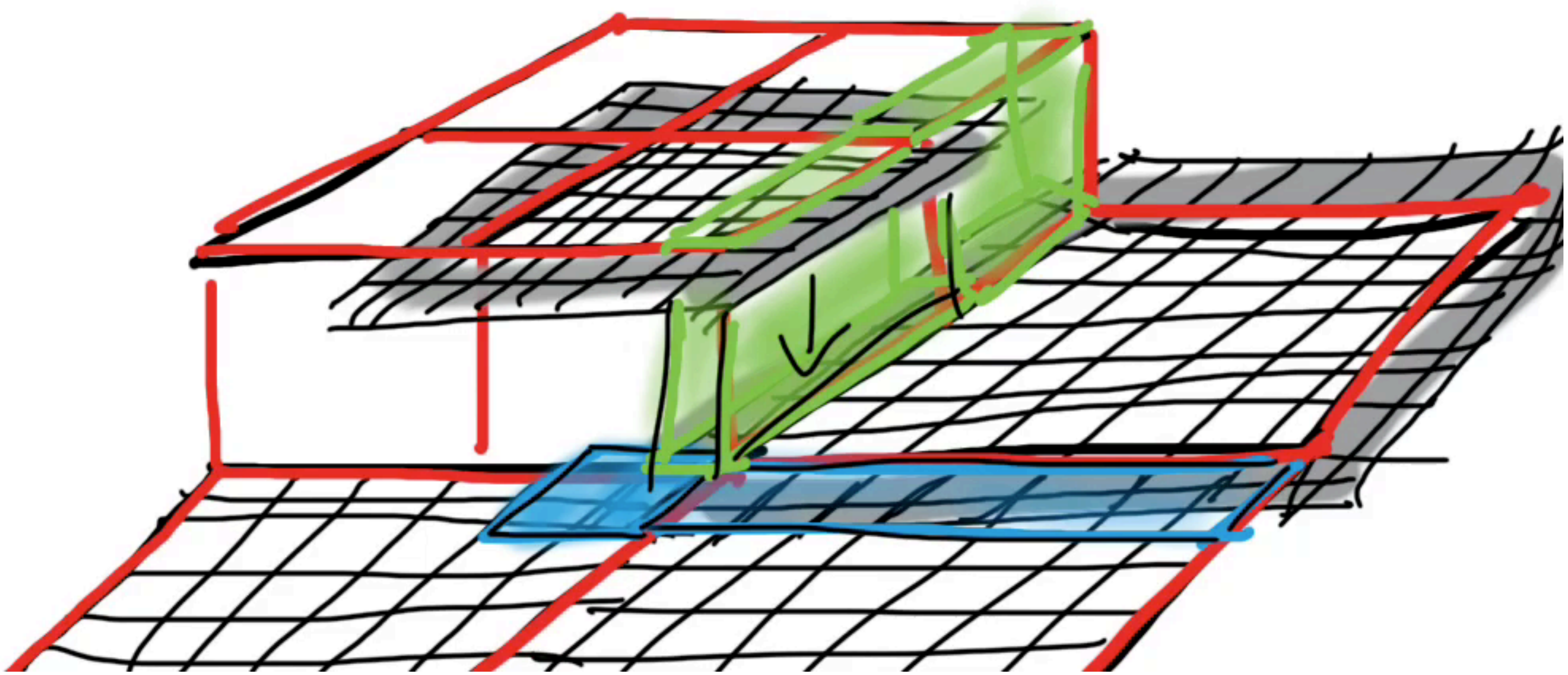


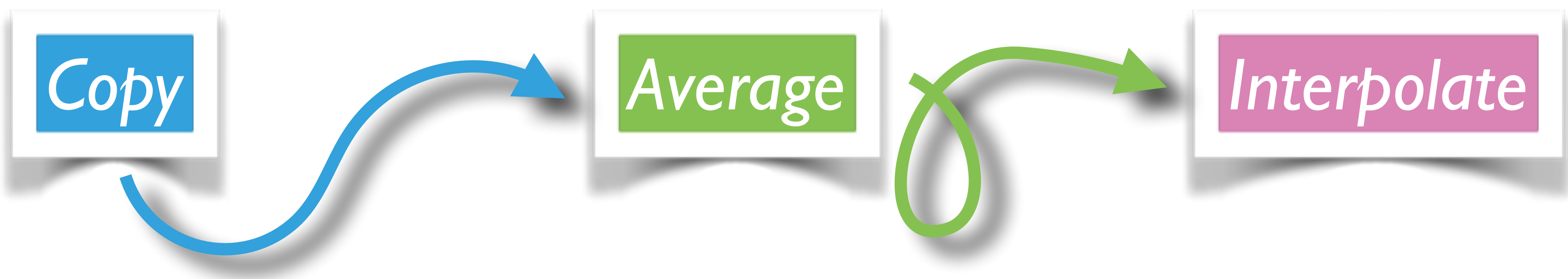
Quadtree based refinement

Details

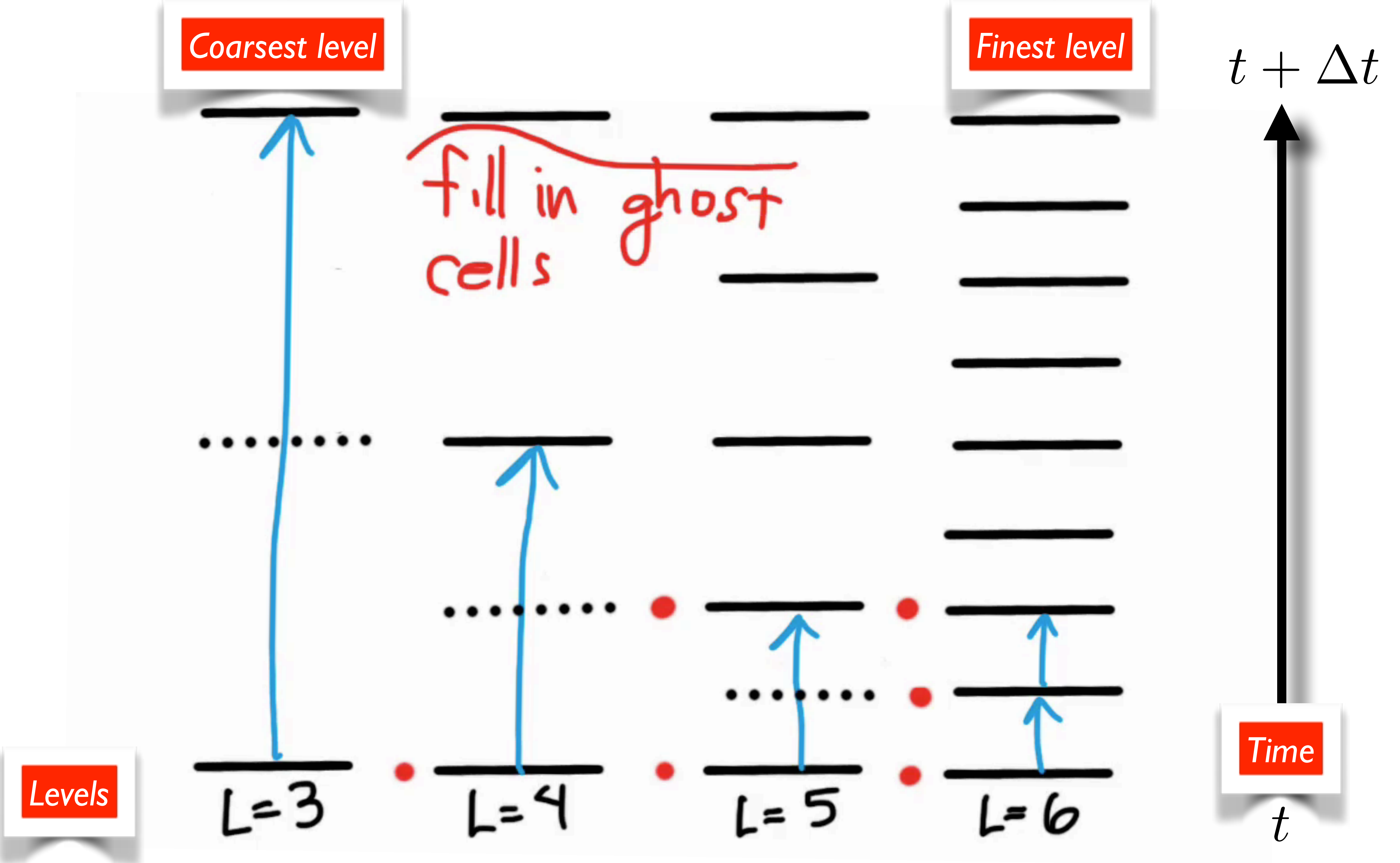
- Ghost cell exchanges
- Multi-rate time stepping
- Parallel communication

How are ghost cells filled?

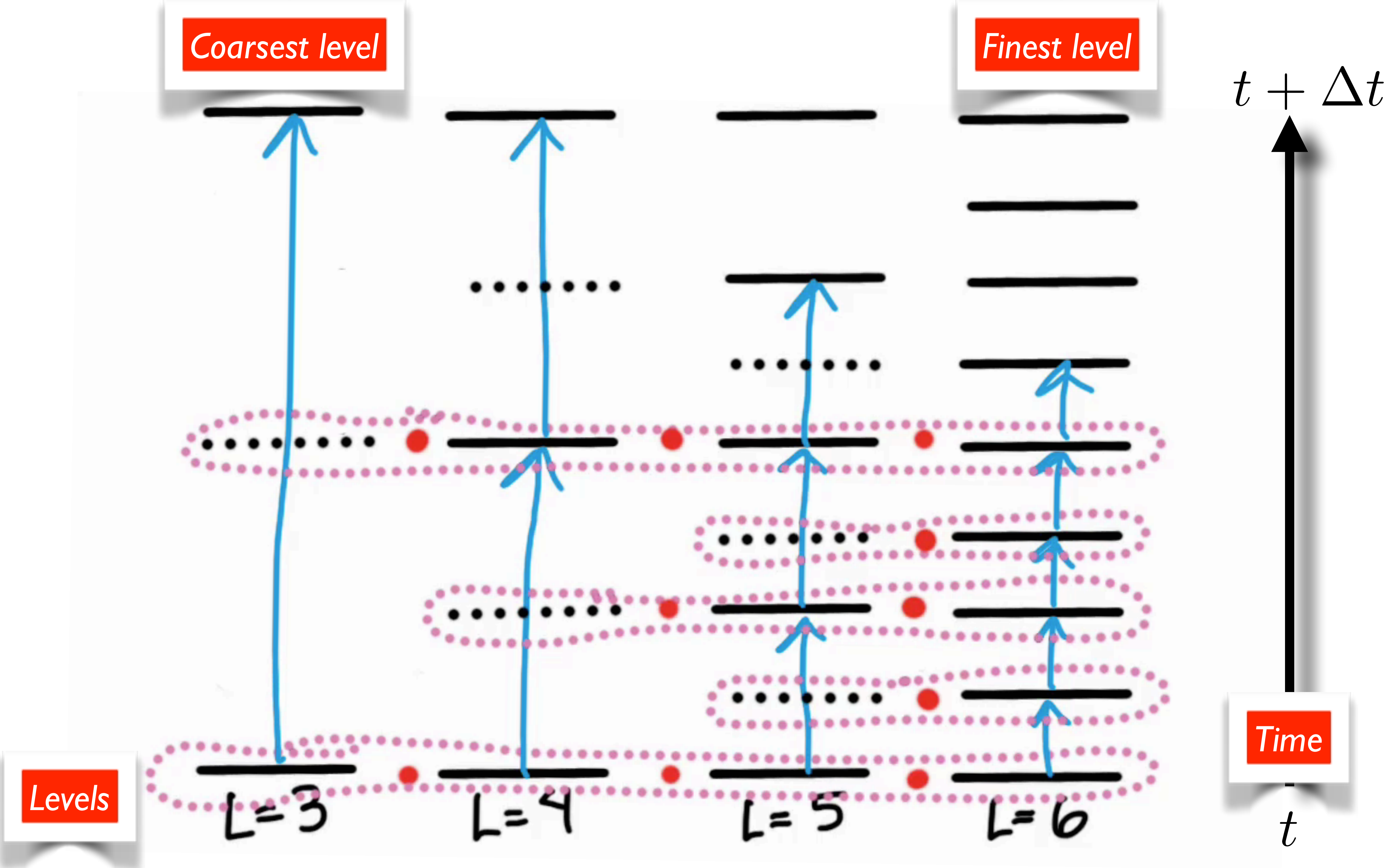




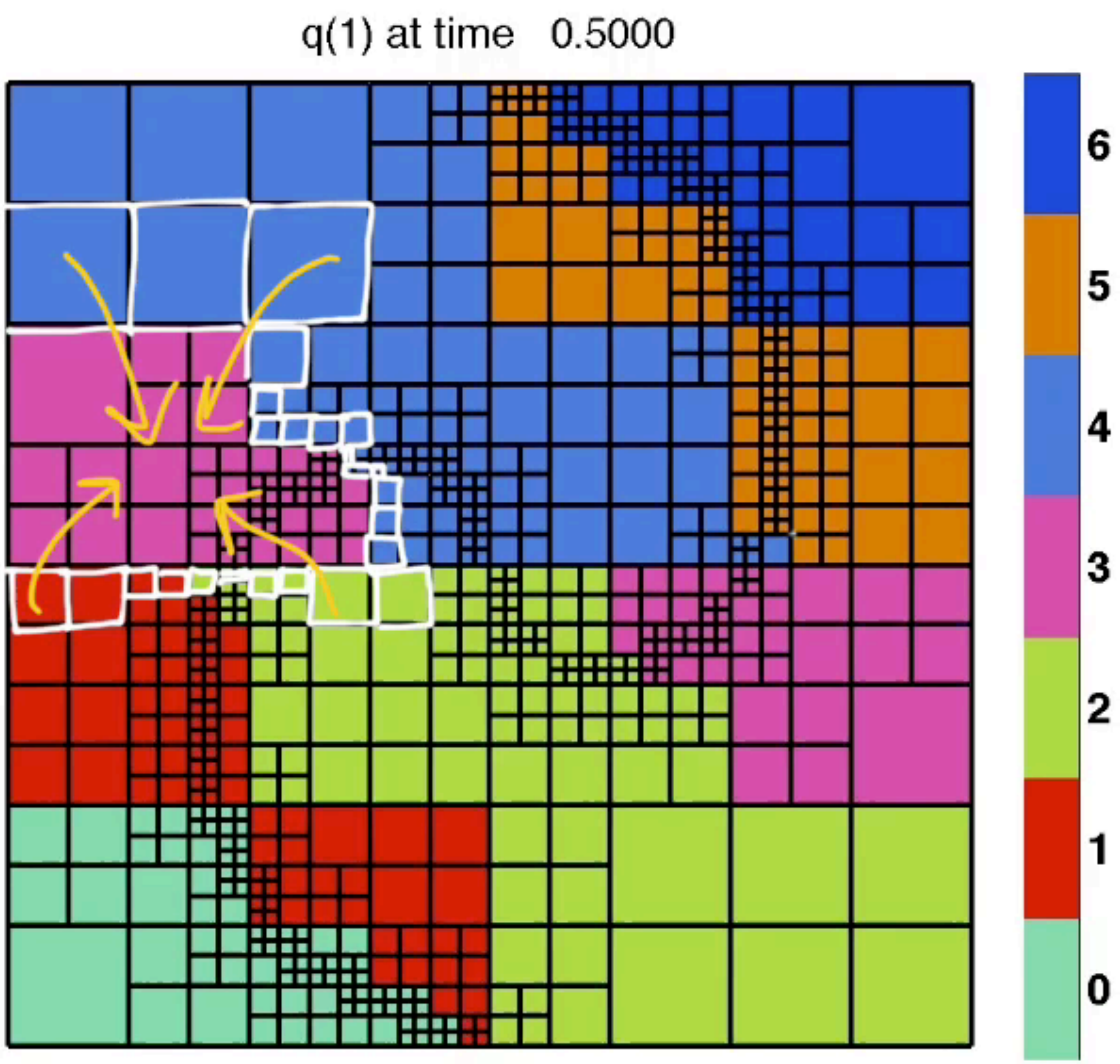
Multi-rate time stepping



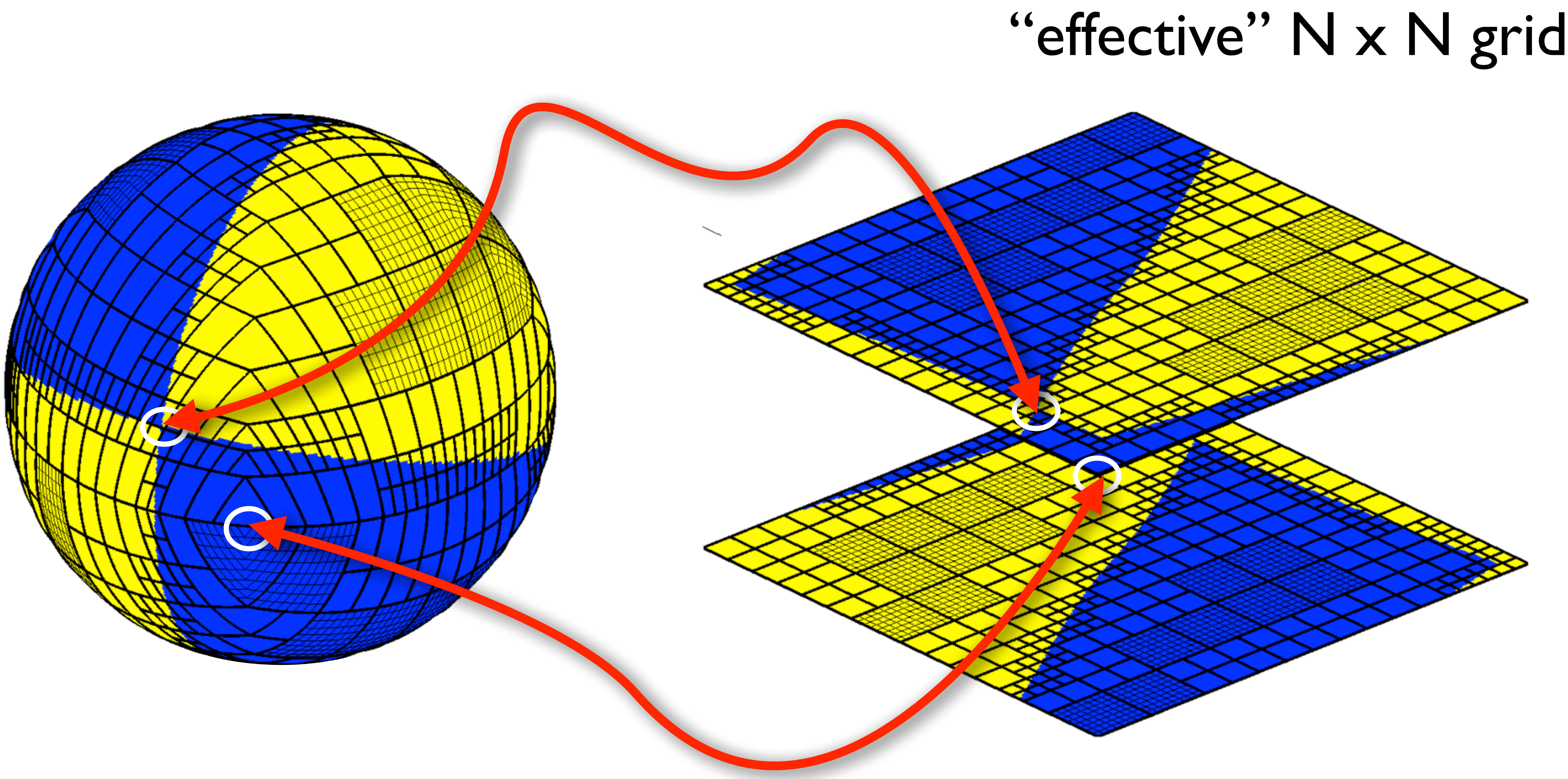
Multi-rate time stepping



Parallel patch exchange



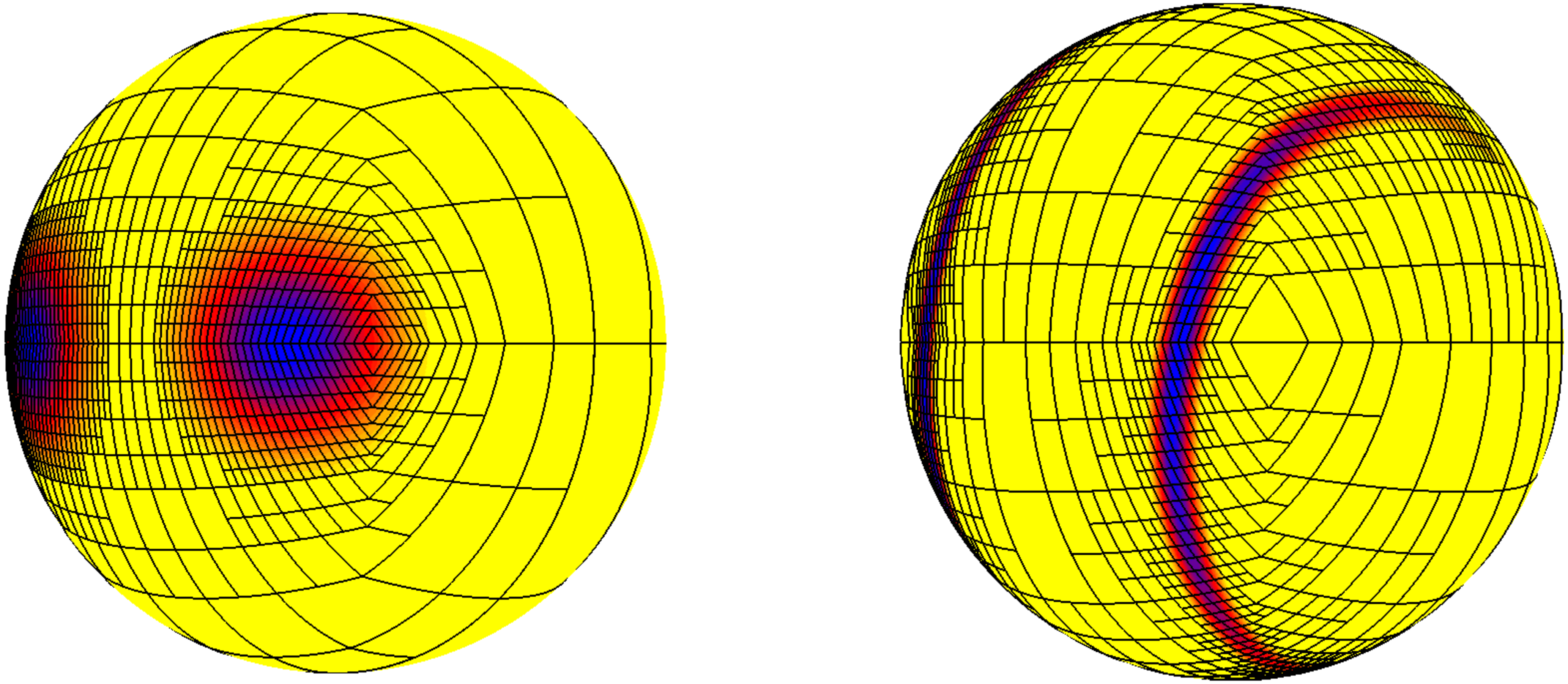
Multiblock sphere grid



D. Calhoun, C. Helzel and R. J. LeVeque, "Logically rectangular grids and finite volume methods for PDEs in circular and spherical domains", *SIAM Review*, 2008.

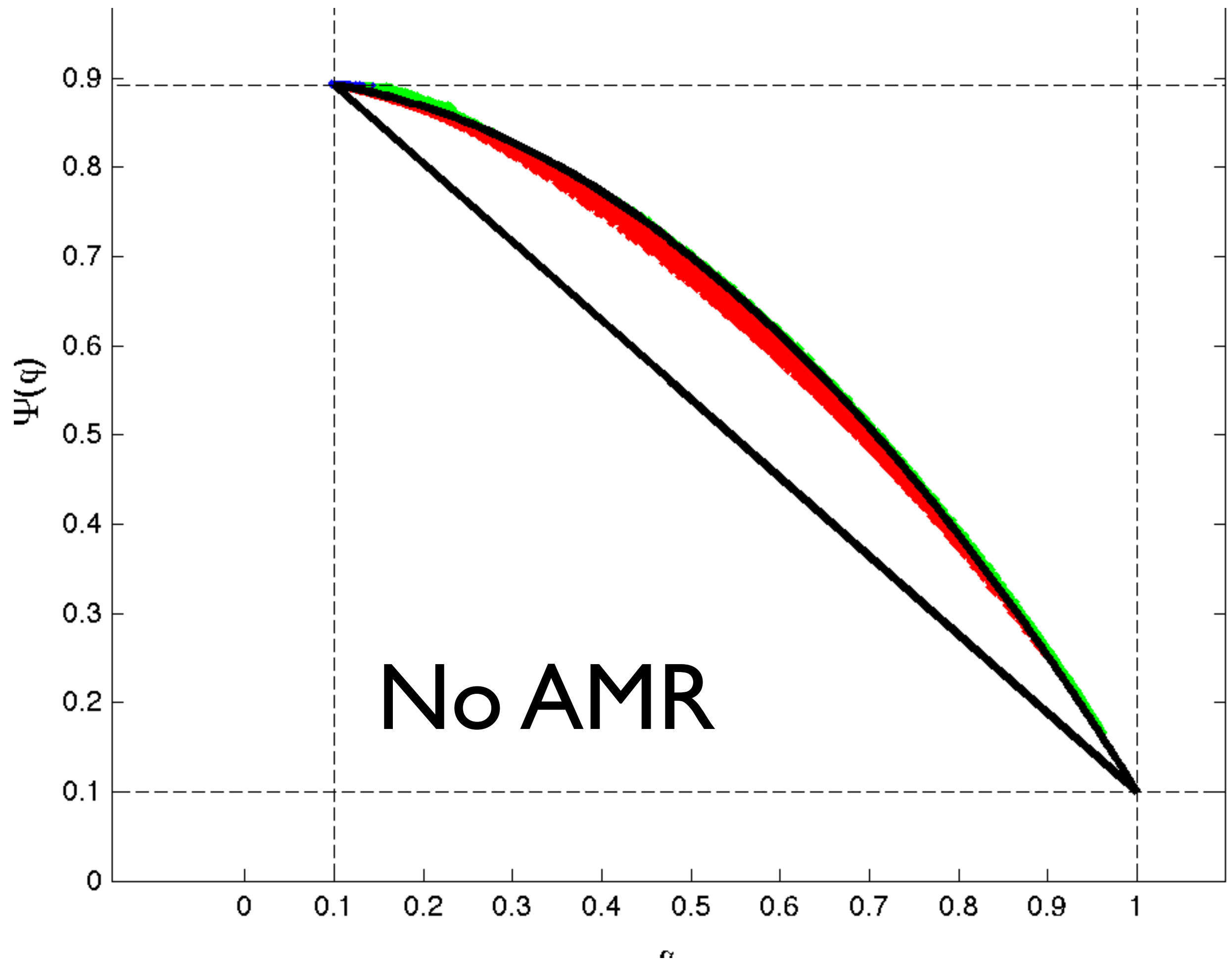
Mixing diagnostic

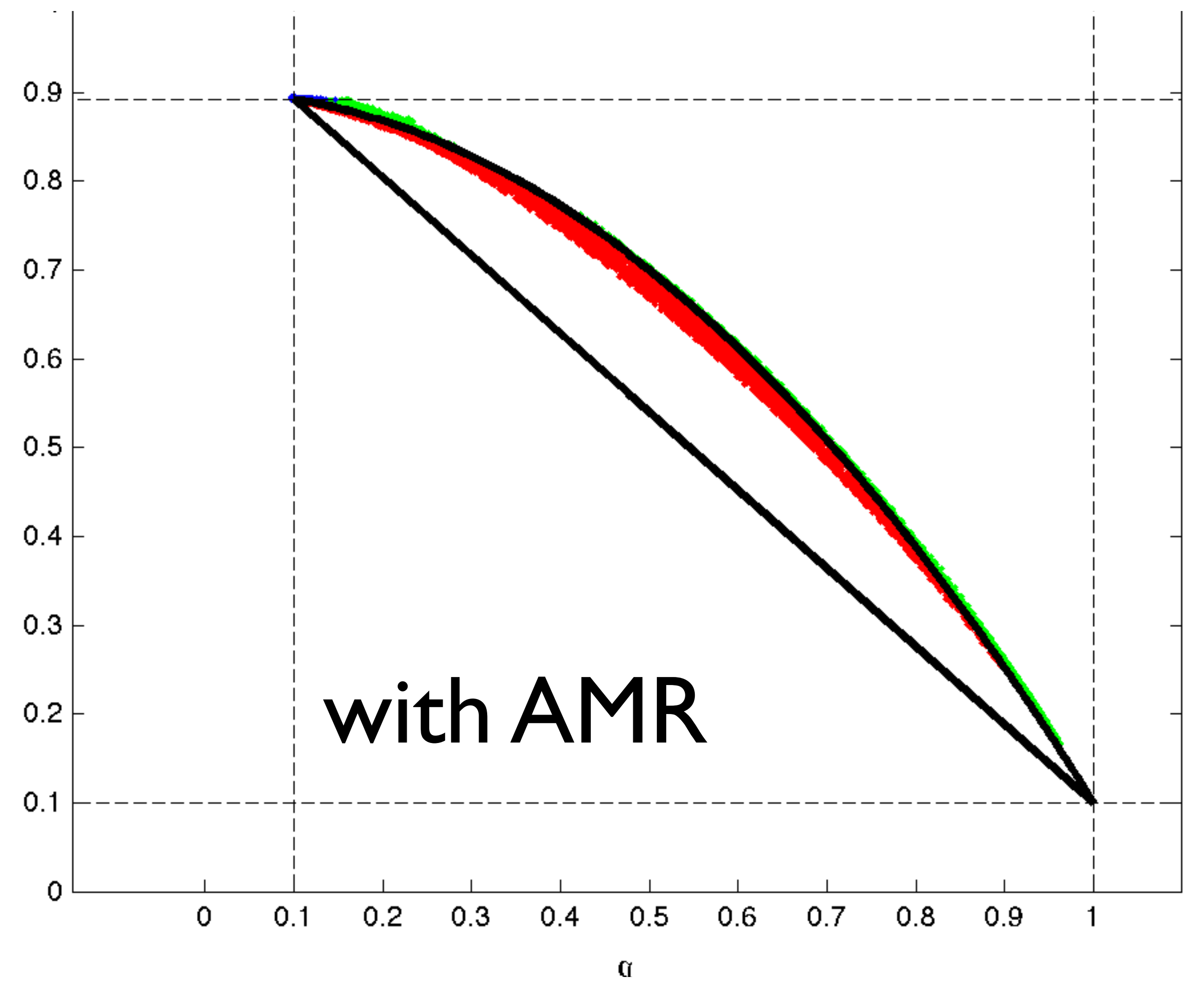
Preservation of functional relationship between tracers.



Lauritzen, P. H., Skamarock, W. C., Prather, M. J., and and, M. A. T. A standard test case suite for two-dimensional linear transport on the sphere. Geoscientific Model Development 5 (2012), 887–901.

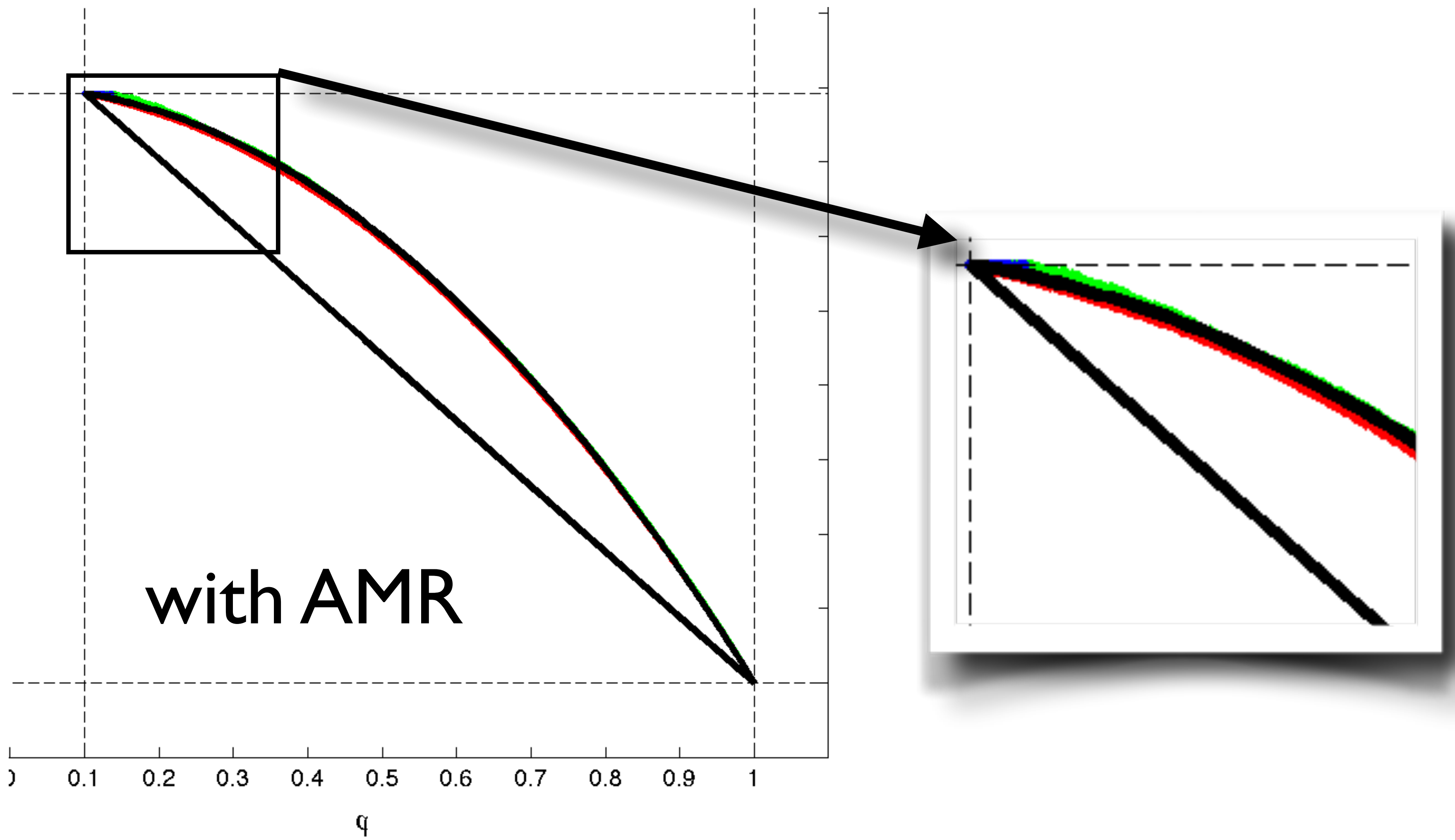
Mixing diagnostics (256 x 256)





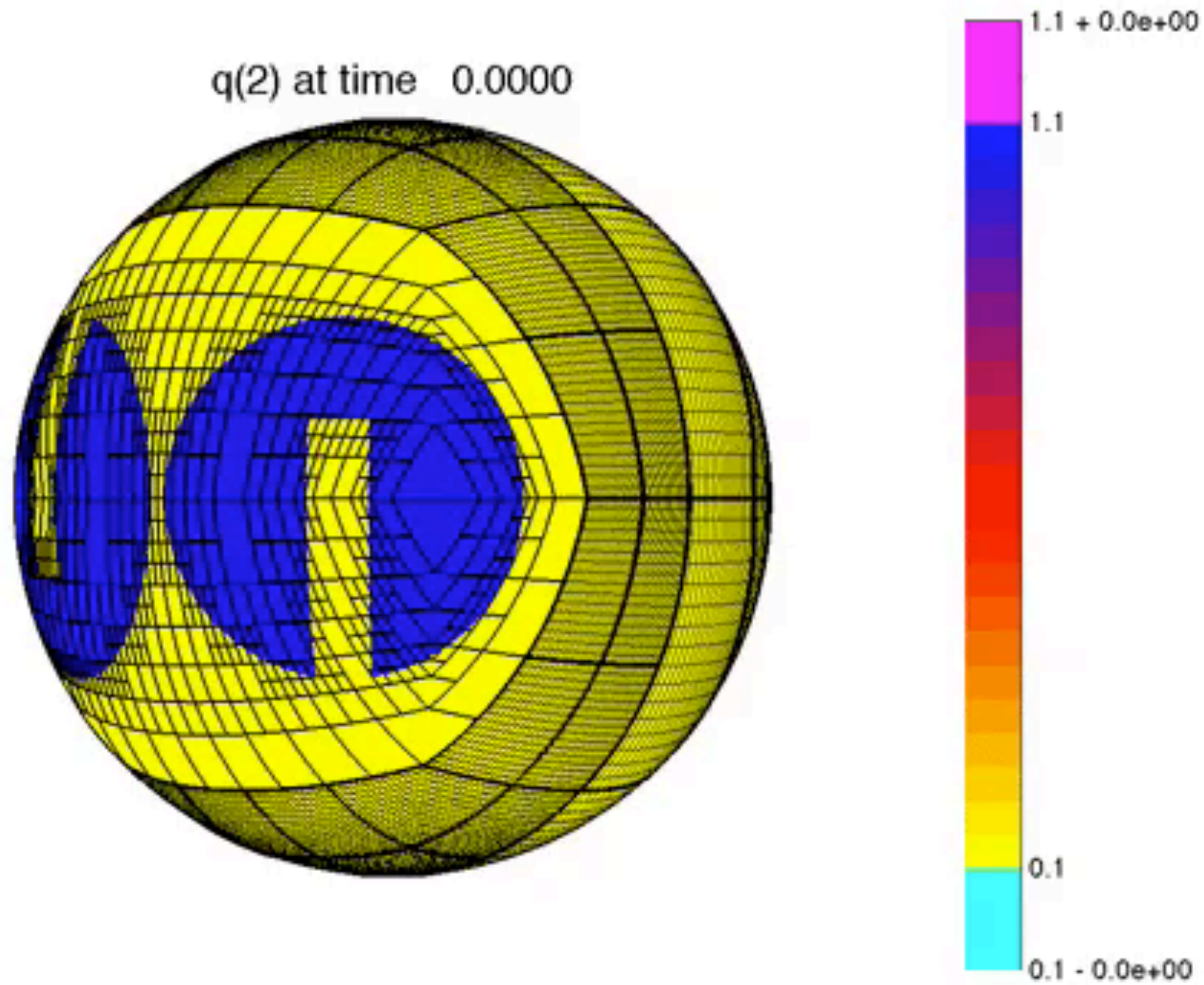
	Diagnostic	Fraction	Diagnostic	Fraction
Real mixing (r)	5.45E-04	0.7565	1.68E-04	0.7709
Range preserving mixing (g)	1.49E-04	0.2070	4.2E-05	0.1925
Under and over shoots (b)	2.63E-05	0.0365	7.98E-06	0.0366

Mixing diagnostic (1024 x 512)



	Diagnostic	Fraction
Real mixing (r)	1.5586E-05	0.6543
Range preserving unmixing (g)	6.9279E-06	0.2908
Under and over shoots (b)	1.3079E-06	0.0549

NCAR Tracer Transport Benchmark



Lauritzen, P. H., Ullrich, P. A., Jablonowski, C., Bosler, P. A., Calhoun, D., Con- ley, A. J., Enomoto, T., Dong, L., Dubey, S., Guba, O., Hansen, A. B., Kaas, E., Kent, J., Lamarque, J.-F., Prather, M. J., Reinert, D., Shashkin, V. V., Skamarock, W. C., Sorensen, B., Taylor, M. A., and Tolstykh, M. A. A standard test case suite for two-dimensional linear transport on the sphere: results from a collection of state-of-the-art schemes. Geoscientific Model Development 7 (2014), 105–145.

Parallel performance - swirl example

strategy				wall clock time	
mesh	remesh	partition	time step	$P = 16$	$P = 256$
uniform	none	by count	global	3961.	256.
AMR	every step	by count	global	252.	54.6
AMR	every 4	by count	global	178.	39.7
AMR	every step	by count	subcycle	99.9	17.3
AMR	every 4	by count	subcycle	87.2	14.0
AMR	every step	by weight	subcycle	95.7	18.2
AMR	every 4	by weight	subcycle	84.4	14.2

Factor of ~40 speedup for 16 processors, and close to 20 on 256 processors

C. Burstedde and D. Calhoun and K. Mandli and A. R. Terrel, ForestClaw: Hybrid forest-of-octrees AMR for hyperbolic conservation laws'', Proceedings of ParCo 2013, September 10-13, 2013, Technical University of Munich, Munich, Germany. (2013)

Goals and motivation

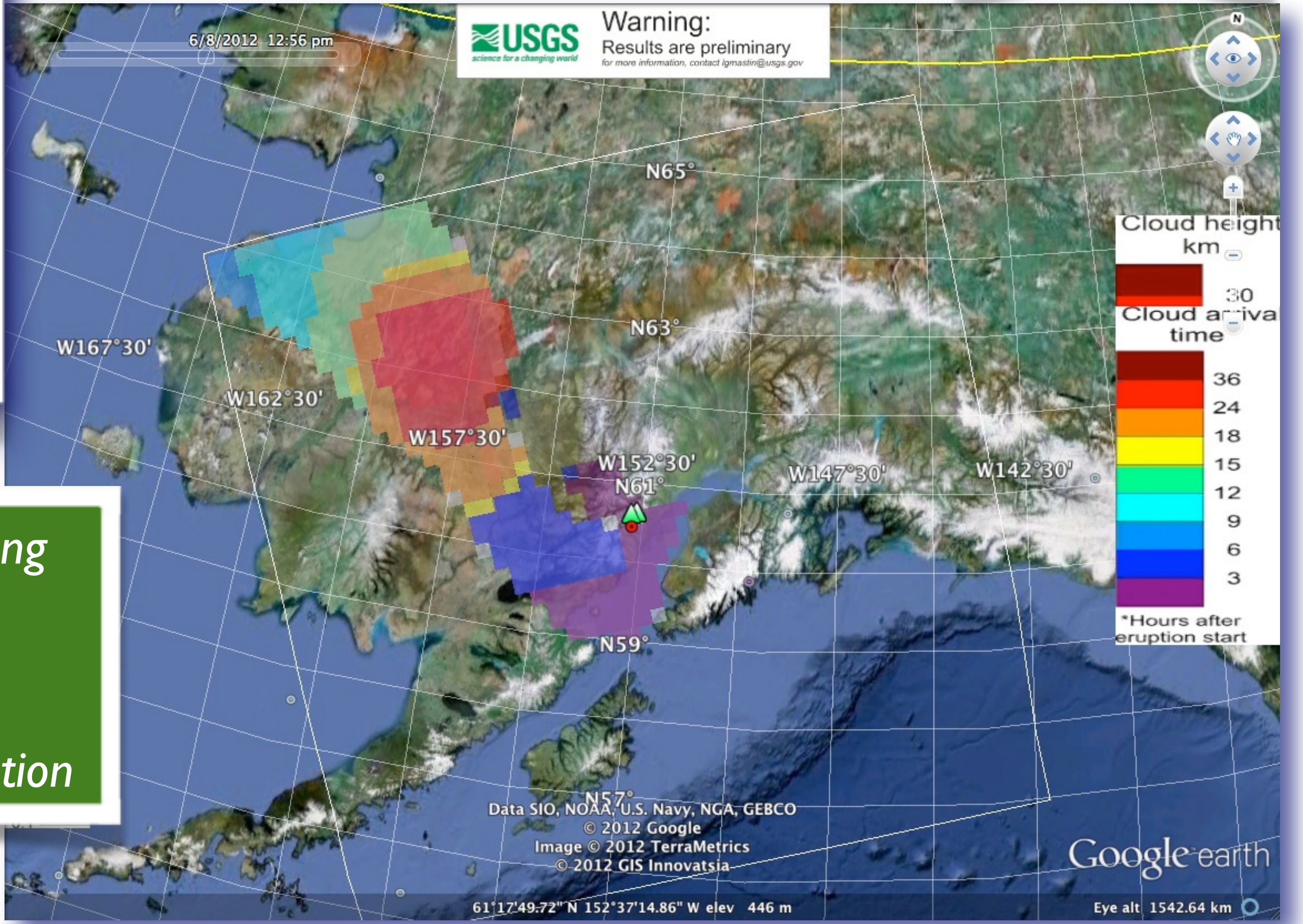
- Develop framework for general multi-rate time stepping schemes (work with D. Ketcheson)
- Improve parallel efficiency
- Handle general mapped multi-block case

Work towards full 3d simulations, with a stop along the way at 2.5d (refinement in horizontal only) for modeling ash cloud transport.

see **http://www.forestclaw.org**

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)