GRID REFINEMENT AND PARALLEL COMPUTING FOR MANTLE CONVECTION AND THERMOCHEMICAL CONVECTION

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Basic equations

$$\nabla \cdot \vec{v} = 0 \qquad (1)$$

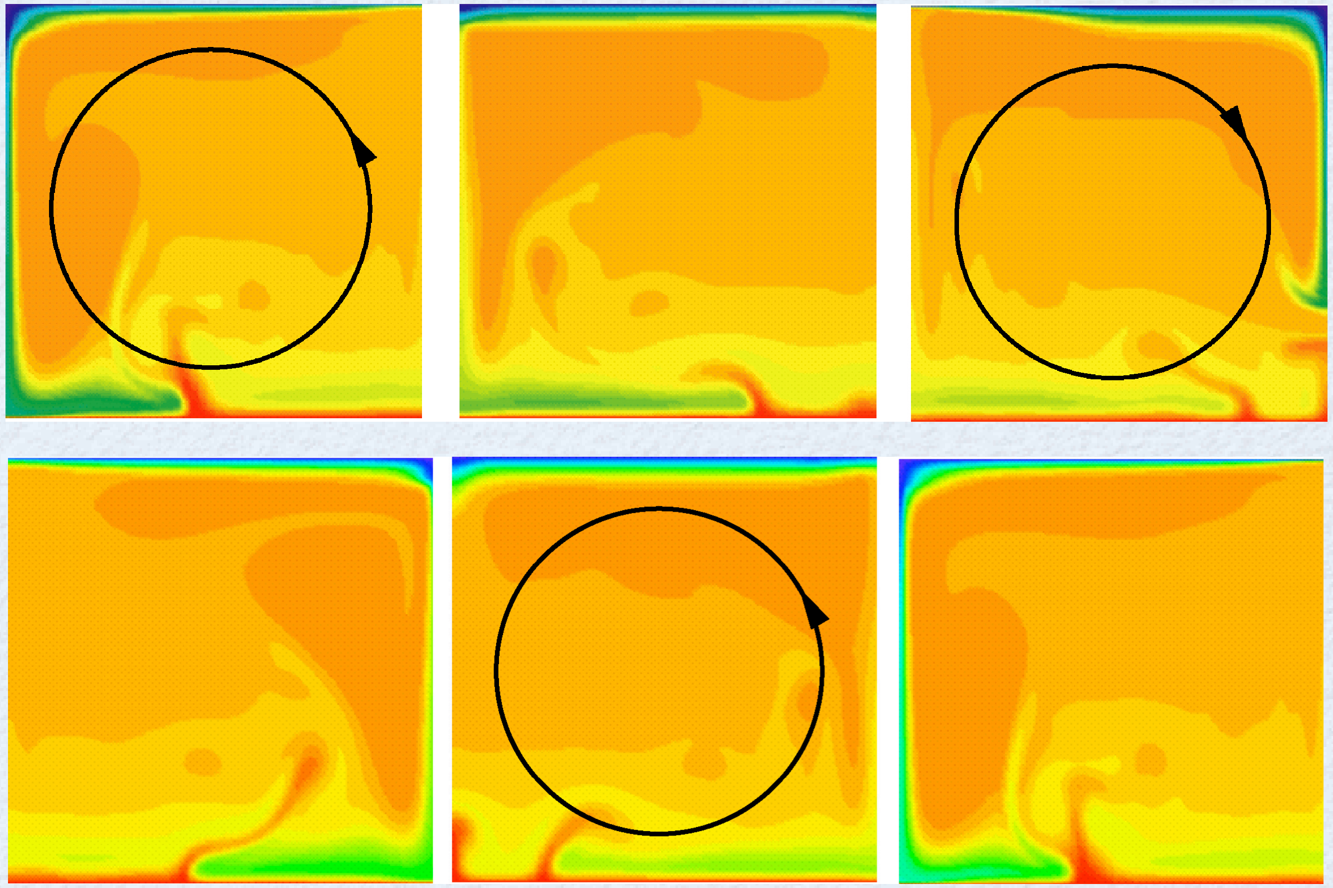
$$\nabla^2 \vec{v} - \vec{\nabla} p = -Ra.(T + BC)\hat{\vec{z}} \qquad (2)$$

$$\frac{\partial T}{\partial t} - \vec{v} \cdot \vec{\nabla} T = \nabla^2 T \qquad (3)$$

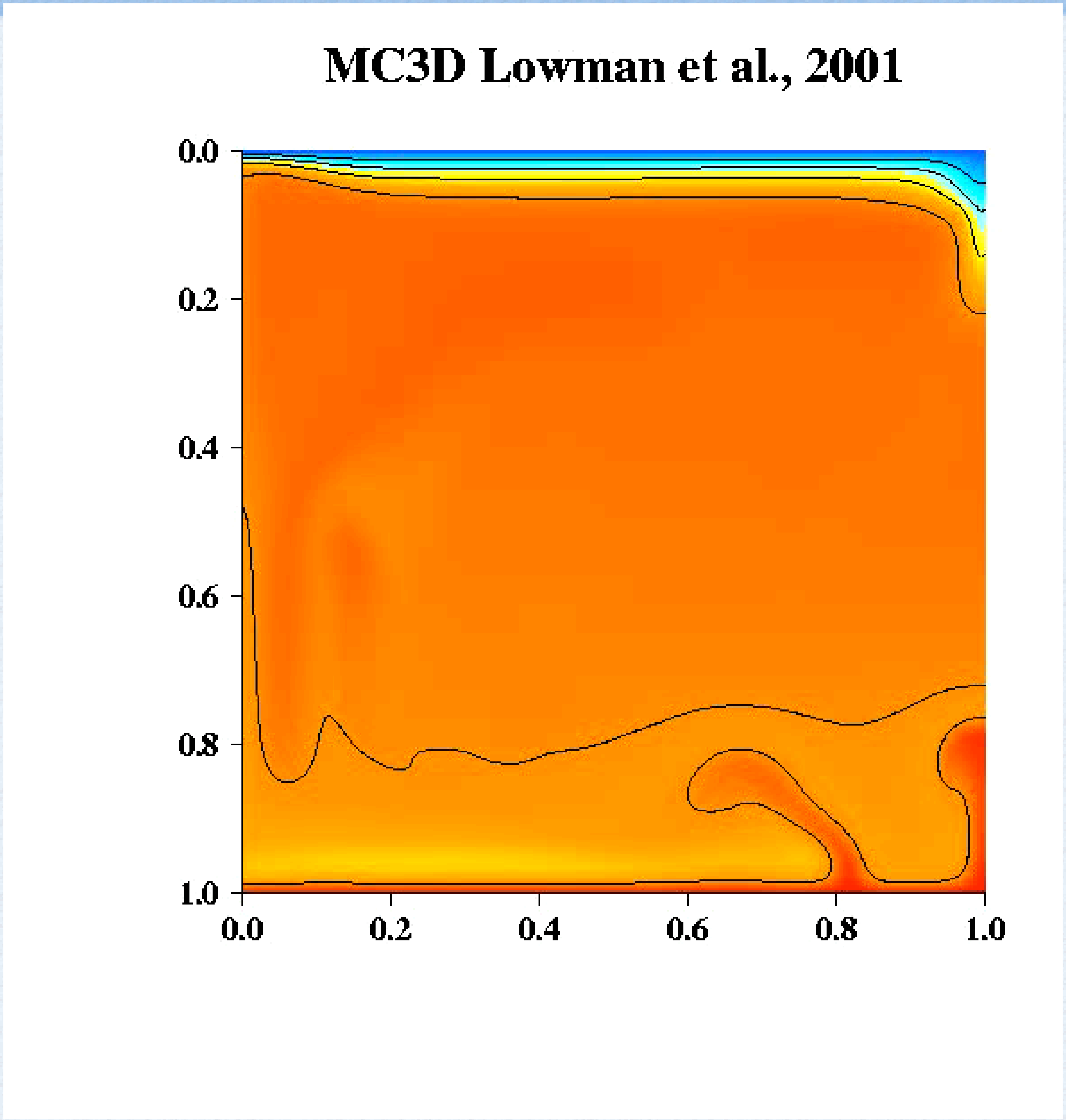
$$\frac{\partial C}{\partial t} - \vec{v} \cdot \vec{\nabla} C = \frac{1}{Le} \nabla^2 C \qquad (4)$$

Convection with Plates

- the six panels are equally-spaced snap shots in time
- colors indicate temperature (blue-cold, red-hot)
- blue material on the top behaves as a rigid plate.
- note the behavior of the orange 'eye' - that material is hotter (more buoyant) than the surrounding fluid.

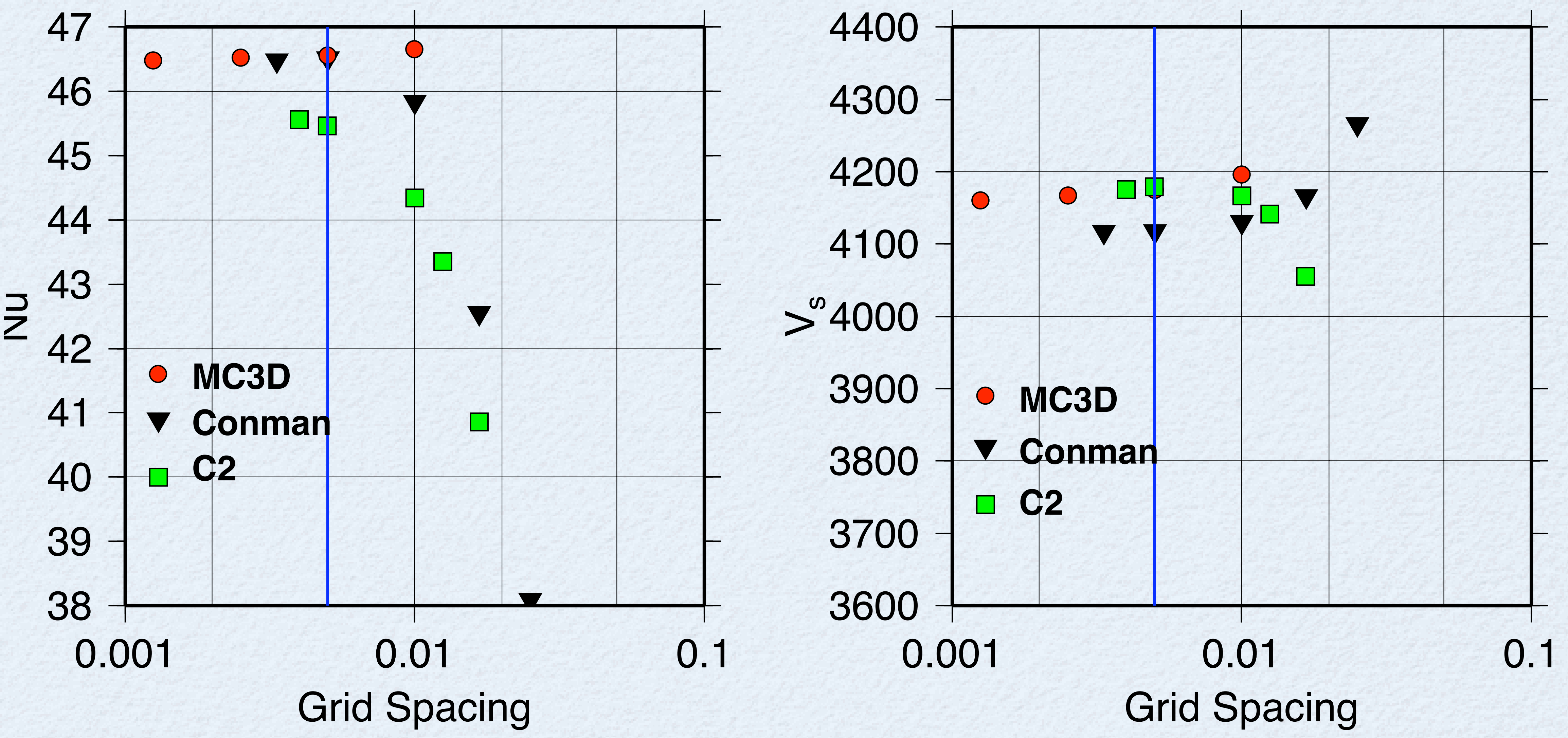


Problem of Interest

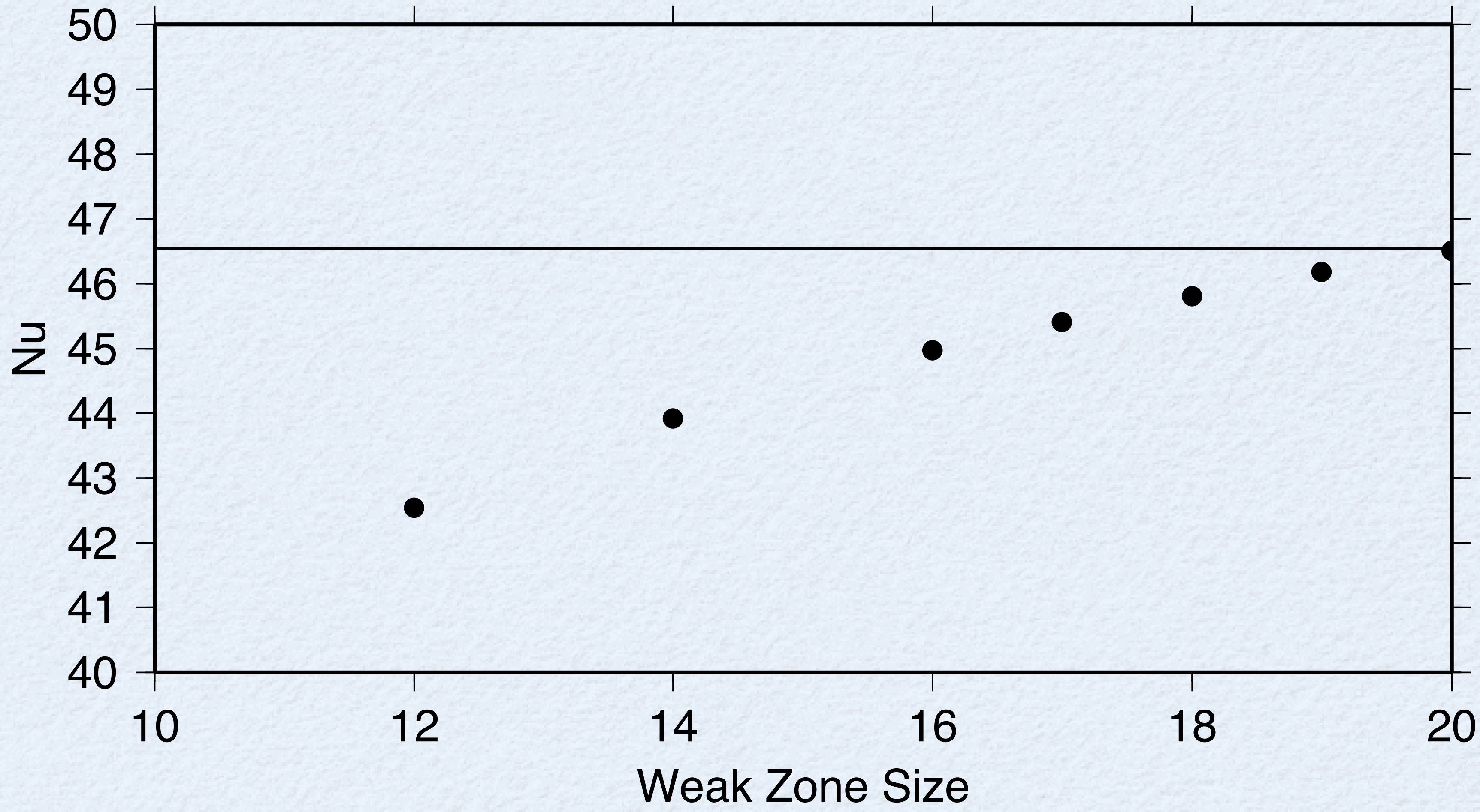


- variable rheology (T, P, strain-rate with yield stress, grain-size, water...)
- variable time-scales

2D, 1x1 Cartesian Box



Compare Plate Approaches



- different plate approaches in different codes
- no standardized problems (King et al., 1992)
- not clear what is the controlling physics

Thermochemical

- geochemistry - isolated reservoirs for billions of years
- ocean island basalts - some mix of these reservoirs

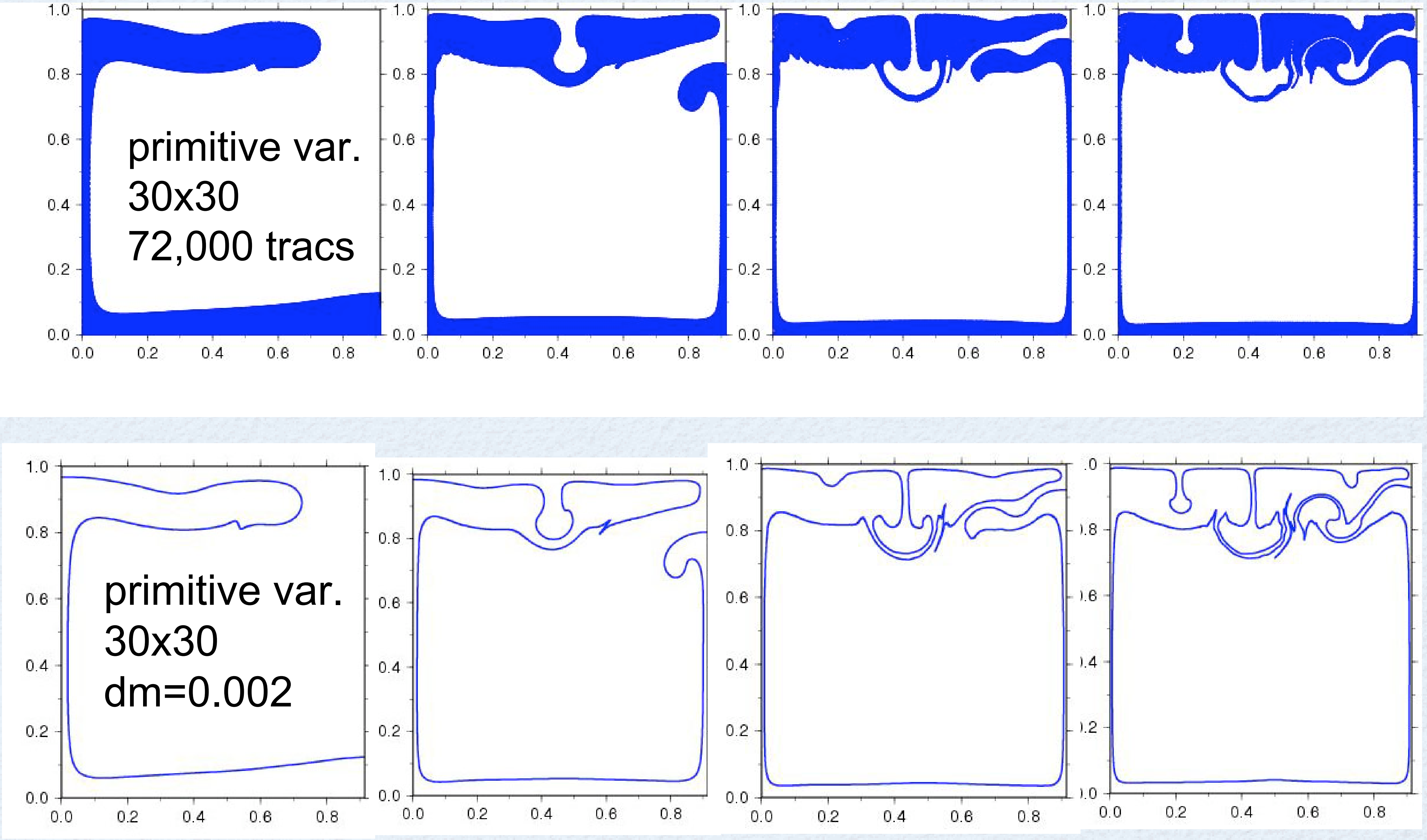
THERMO-CHEMICAL

- start with chemical buoyancy only (no diffusion)
- follow entrainment of compositional layer for long time periods
- three approaches (van Keken et al., 1997):
  - double diffusive with large Lewis number
  - tracers
  - marker chains

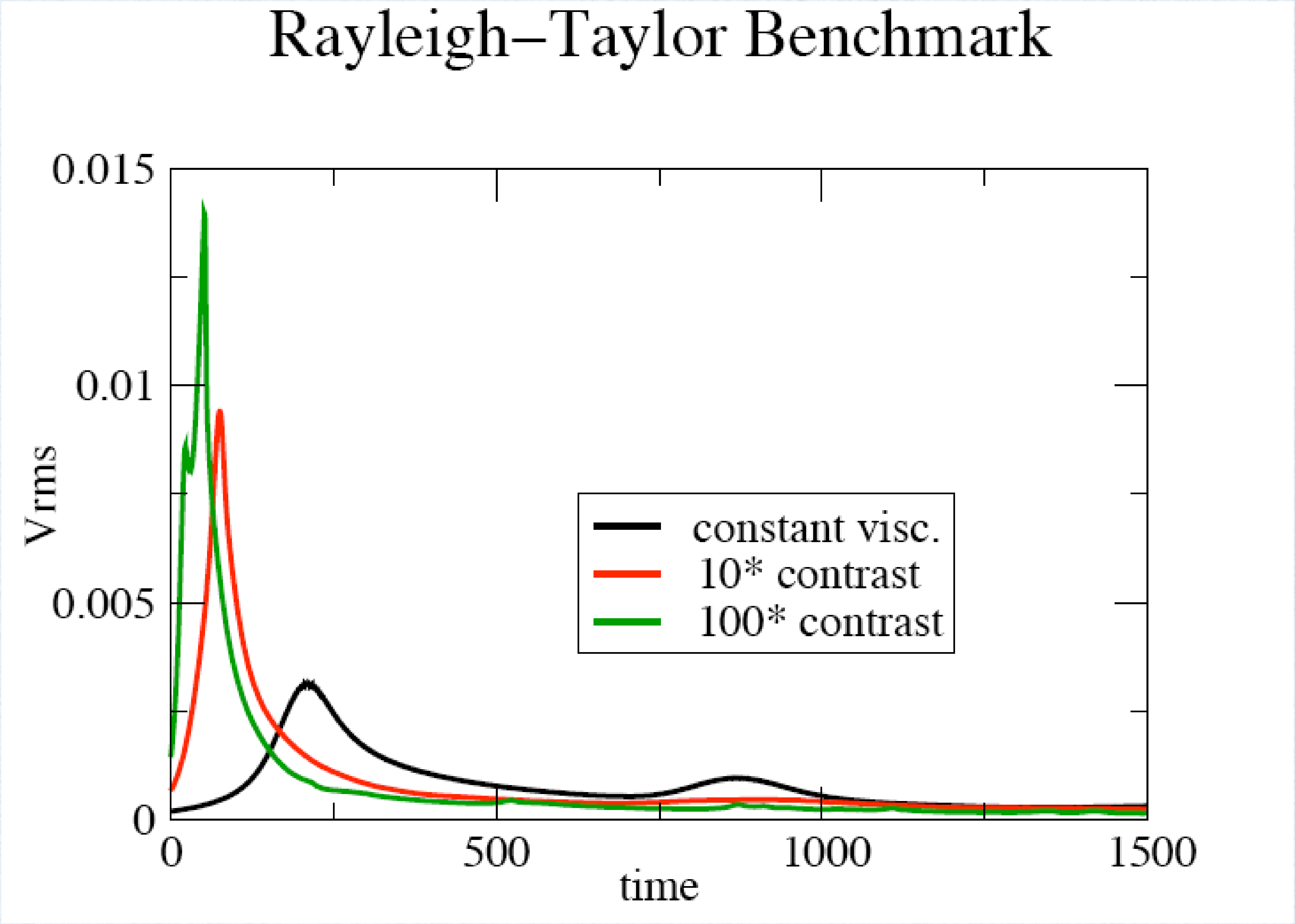
Computational Issues

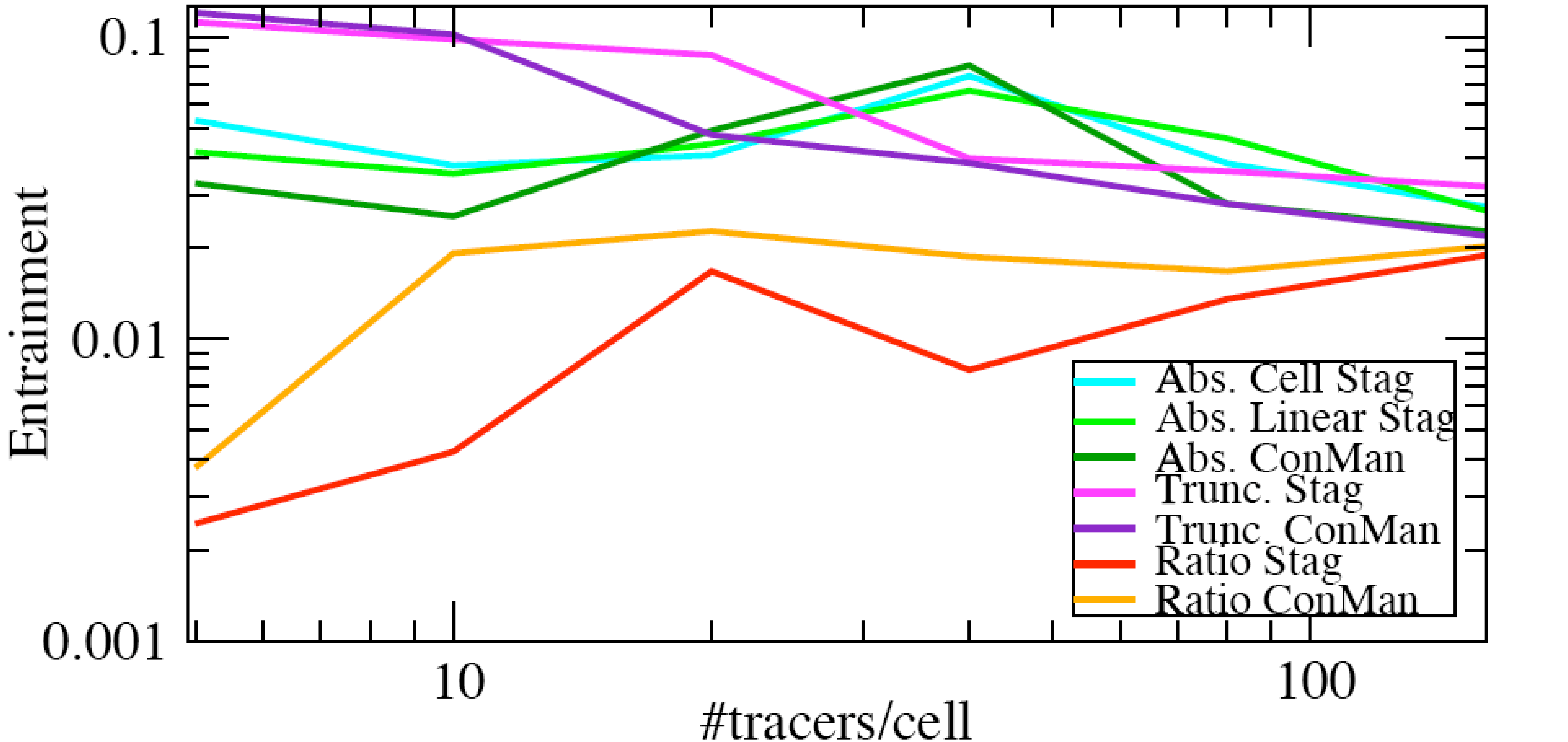
- double-diffusive: we understand the methods
- tracers: require large # of tracers per element depressing for 3D :(
- tracers: independent, easy to parallelize (except when tracers move from one domain to another) - equation - 4th order RK or similar

Rayleigh Taylor Instability



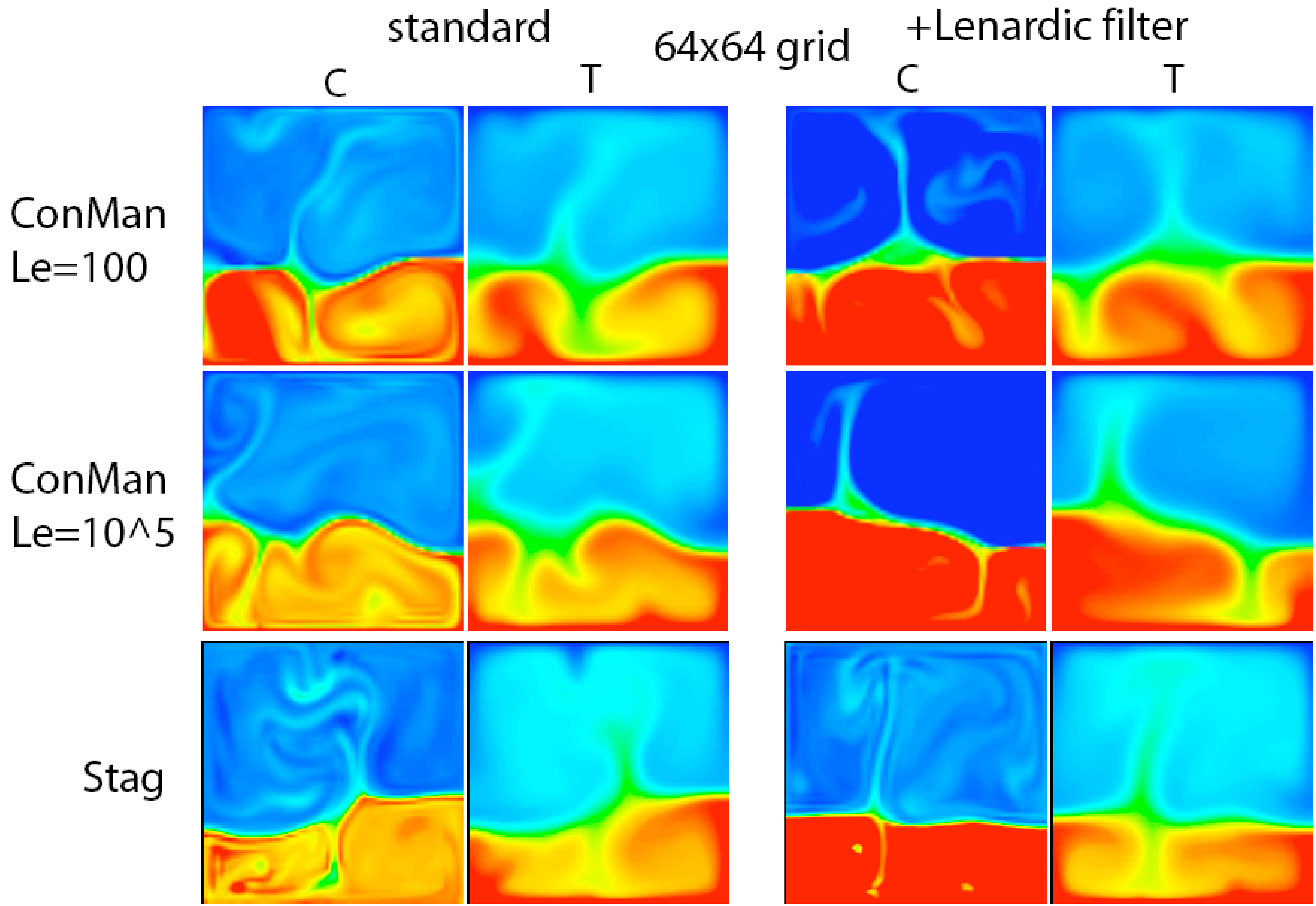
van Keken et al., 1997

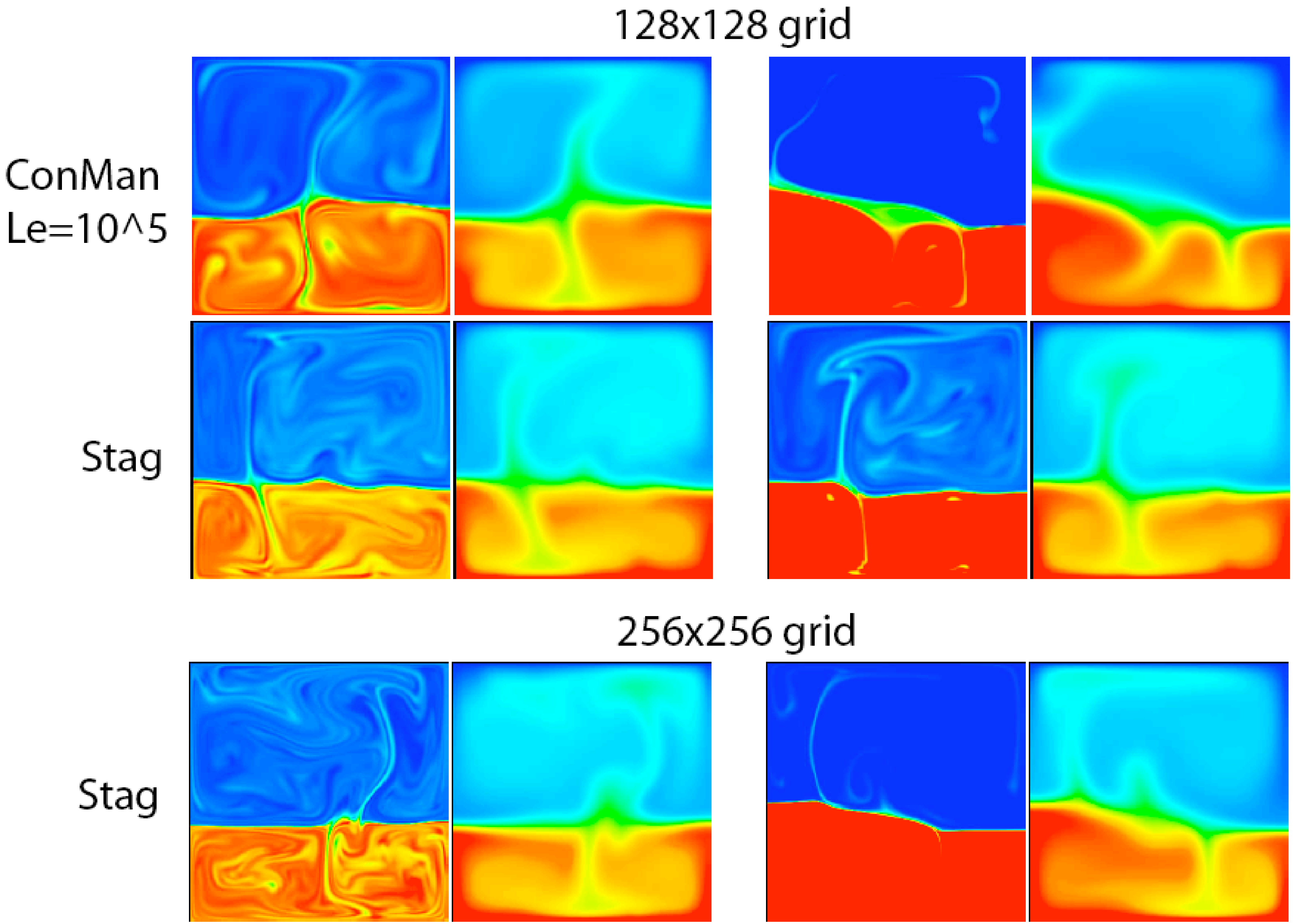

Rayleigh–Taylor Benchmark
0.015
0.01
0.005
0
Vrms
0
500
1000
1500
time
constant visc.
10* contrast
100* contrast

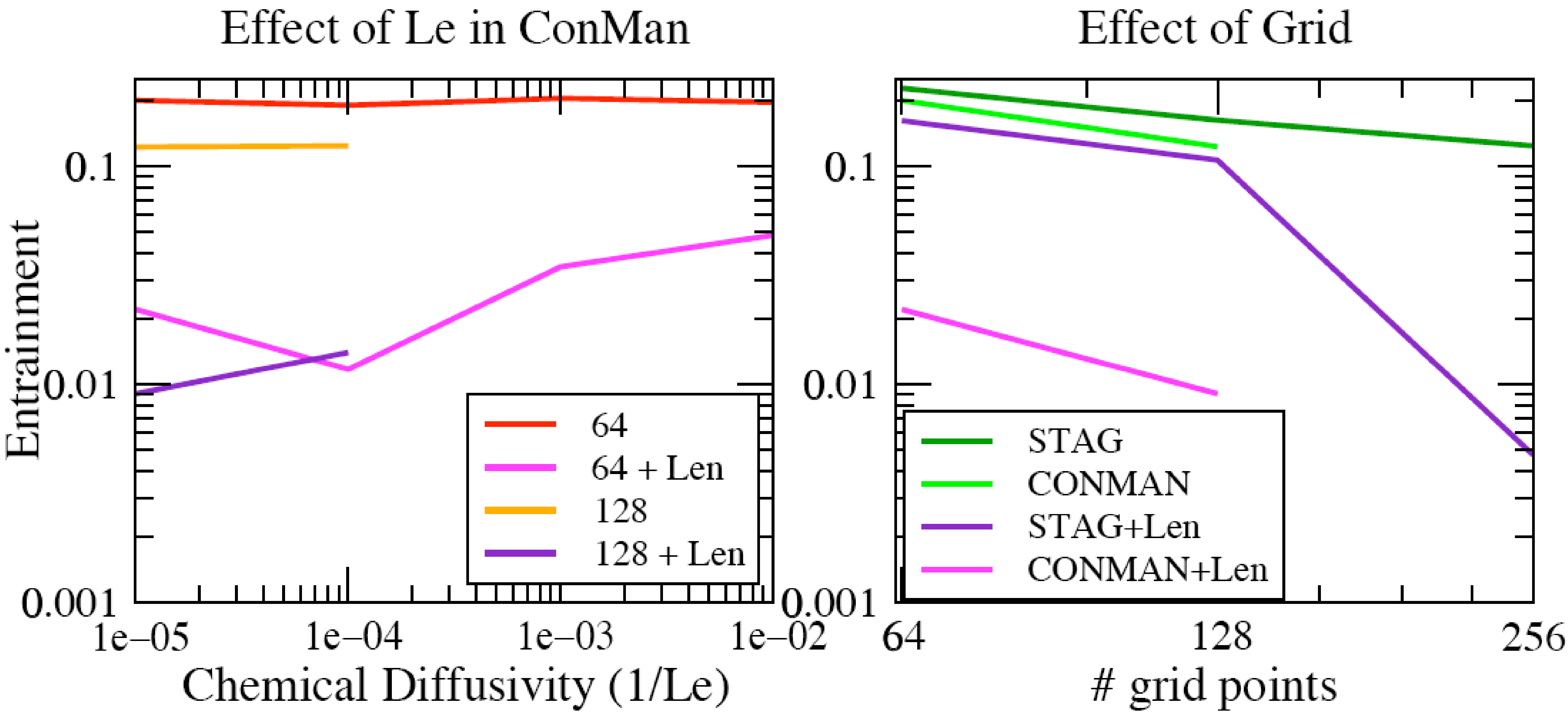


0.1
0.01
0.001
Entrainment
10
100
#tracers/cell
Abs. Cell Stag
Abs. Linear Stag
Abs. ConMan
Trunc. Stag
Trunc. ConMan
Ratio Stag
Ratio ConMan

Grid-based advection




128x128 grid
ConMan
Le=10^5
Stag
256x256 grid
Stag

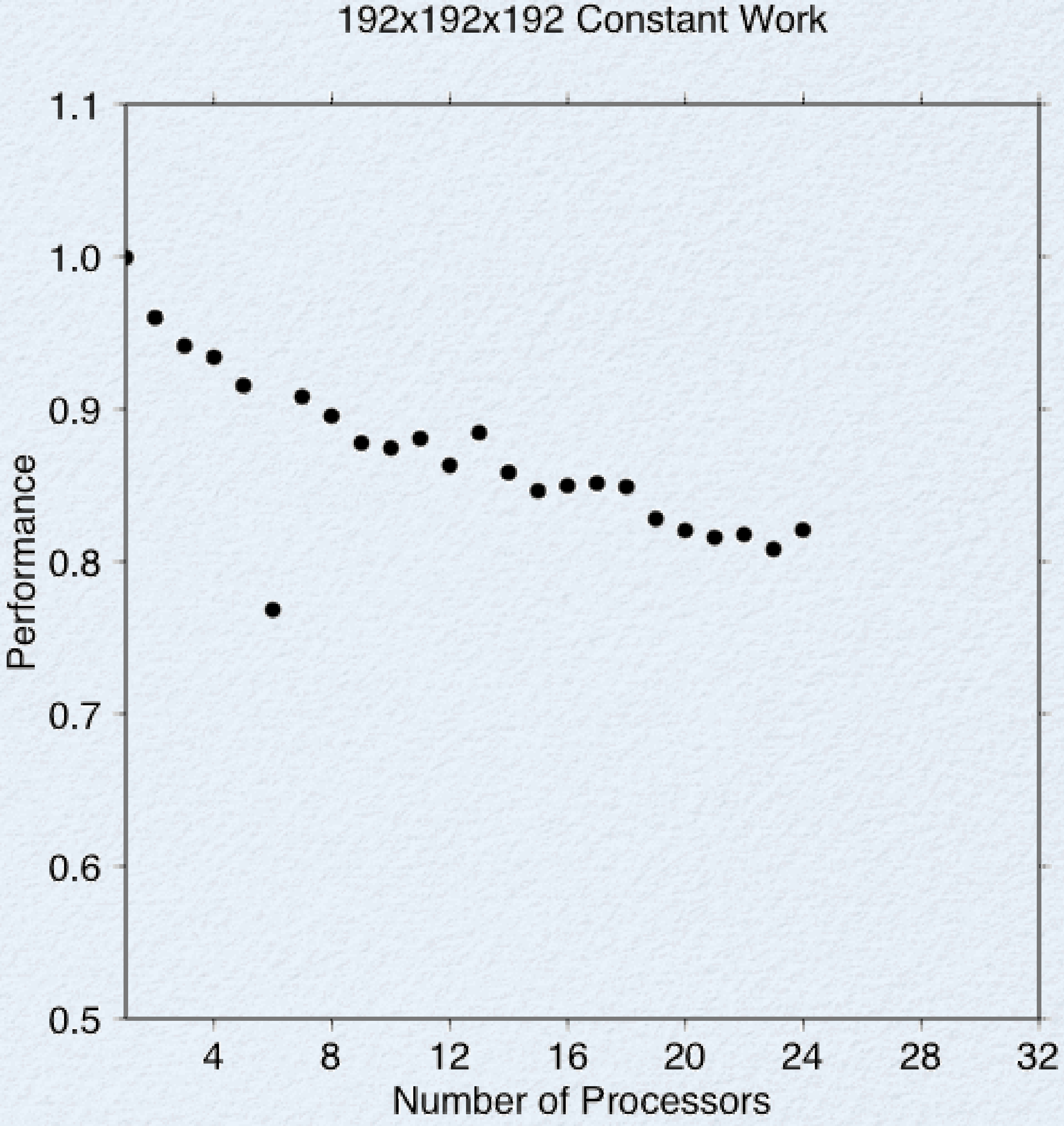

Effect of Le in ConMan
Entrainment
0.1
0.01
0.001
1e−05
1e−04
1e−03
1e−02
Chemical Diffusivity (1/Le)
64
64 + Len
128
128 + Len
Effect of Grid
0.1
0.01
0.001
64
128
256
grid points
STAG
CONMAN
STAG+Len
CONMAN+Len

Take Home Message

- Optimal choice depends on
  - Solution method for Stokes equation
  - Geometry of domain
  - Mixing geometry
- Evaluation of accuracy, efficiency, applicability
  - Van Keken et al., JGR, 1997
  - Tackley and King, G-cubed, 2003
  - Schmalzl and Loddoch, G-cubed, 2003
    - approximate ‘diffusive’ marker sheet technique in 3D

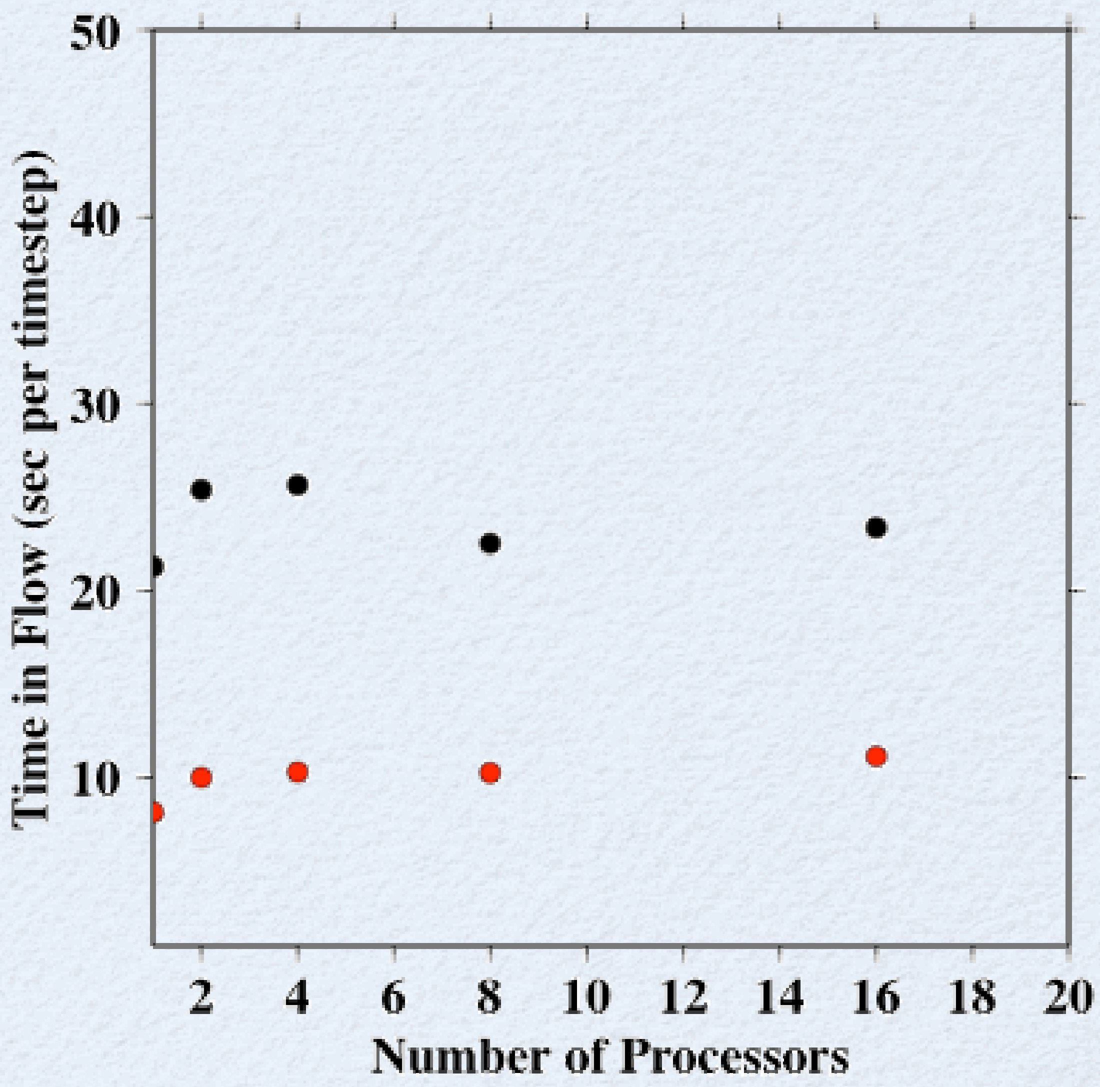
MC3D 3D Cartesian

- MC3D: hybrid spectral/ finite-difference code
- extensively tested and benchmarked
- enforces plate-like behavior by integrating tractions on the base of the plate
- developed at Los Alamos in the late 1980's for Cray/Vector architecture
- parallelized (MPI) to run on clusters (1999)

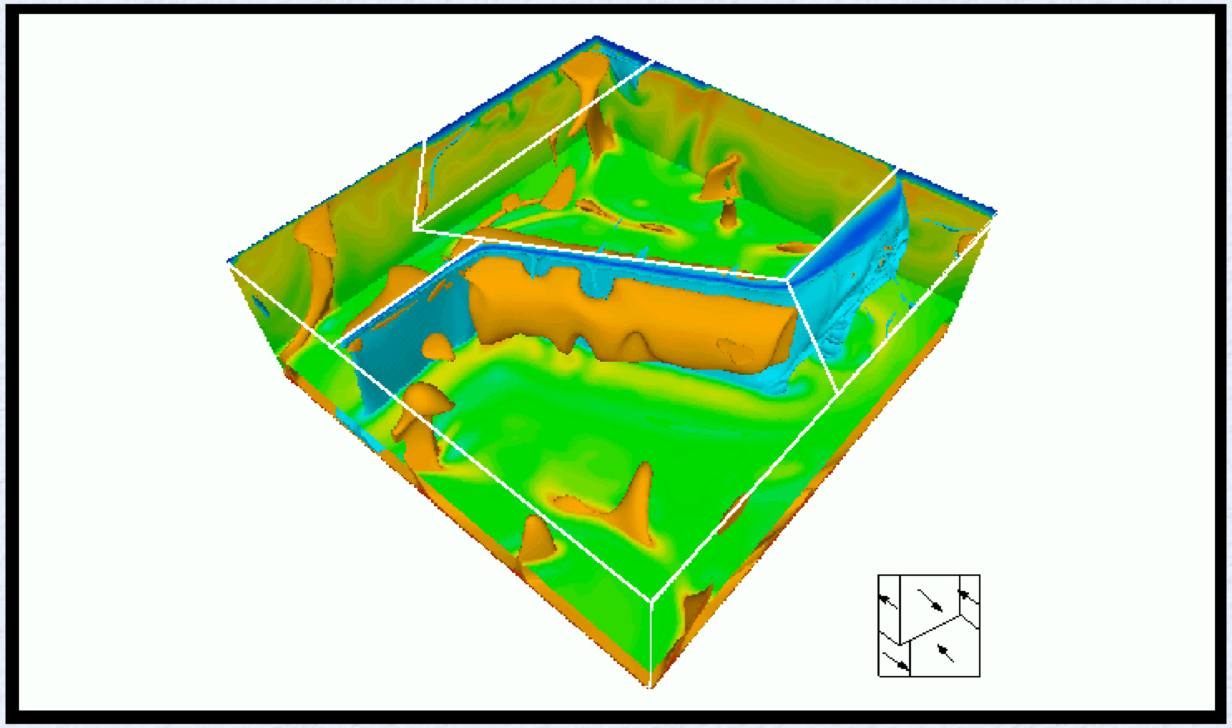


MC3D

- FLOW: Solve the equations of motion (2D ffts in horizontal direction, series of ODEs in vertical direction)
- domain decomposition by blocks in ix-iy space
- HEATFLO: Solve the energy equation (3D finite difference with a series of diffusion tensor correction terms)
- domain decomposition by layers in iz space

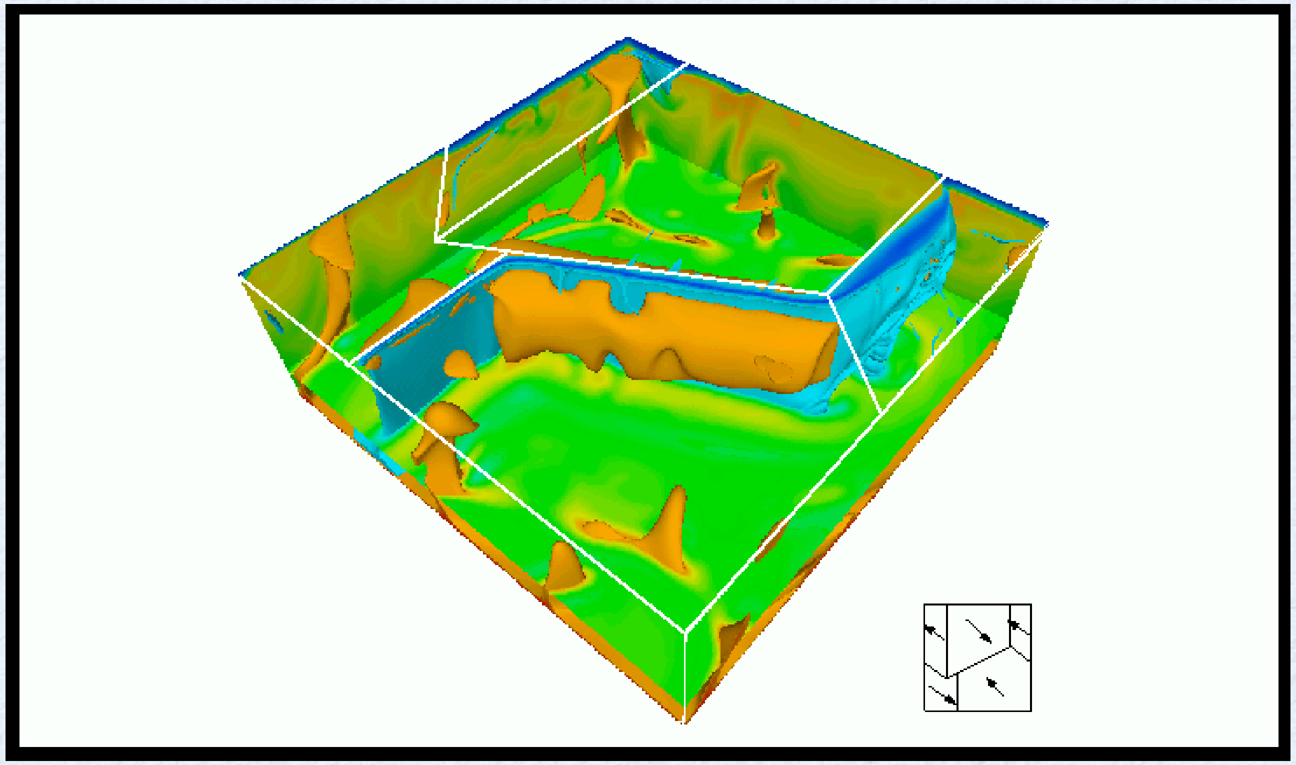


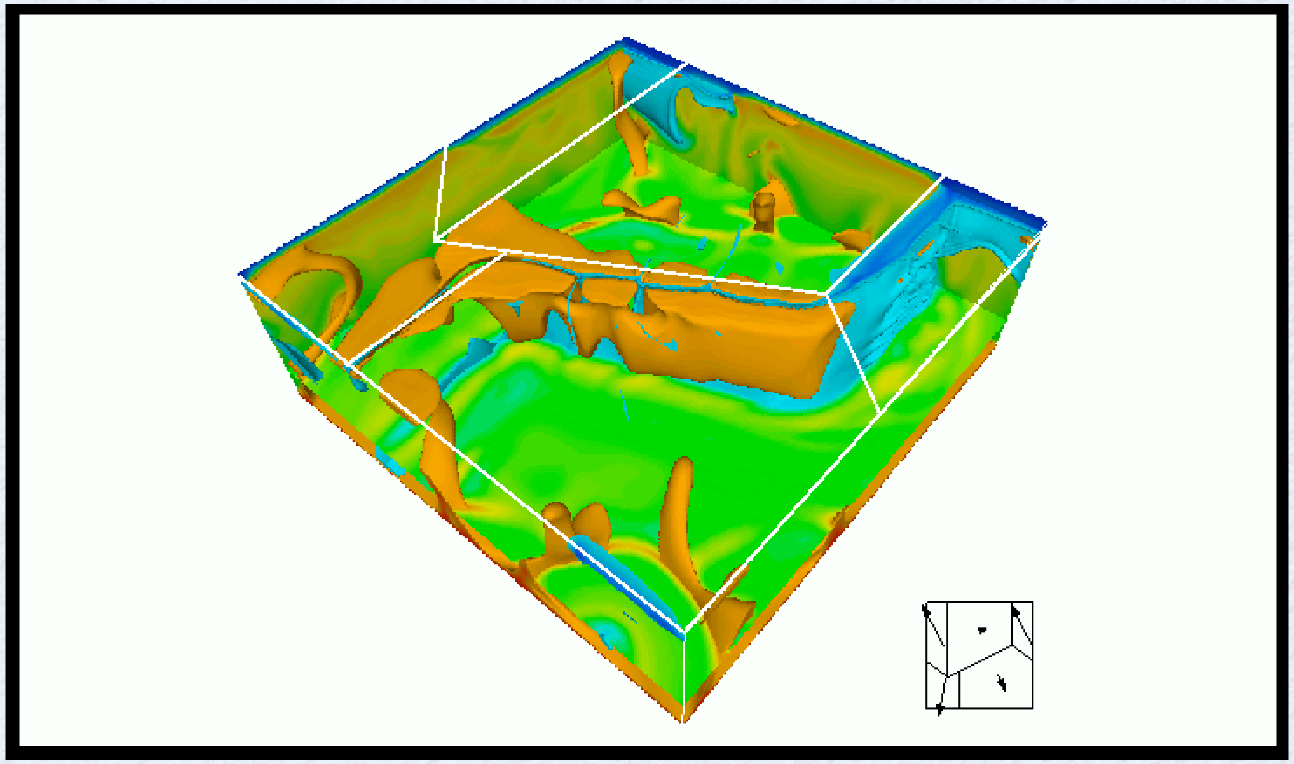
3D Problem, Computation, Visualization, Storage



- 3D 3x3x1 box with four mobile plates
- 324x324x128 node grid
- isosurfaces represent constant temperature
- I want to work ‘interactively’ with data (vary the value of the isosurface, change the view angle, …)

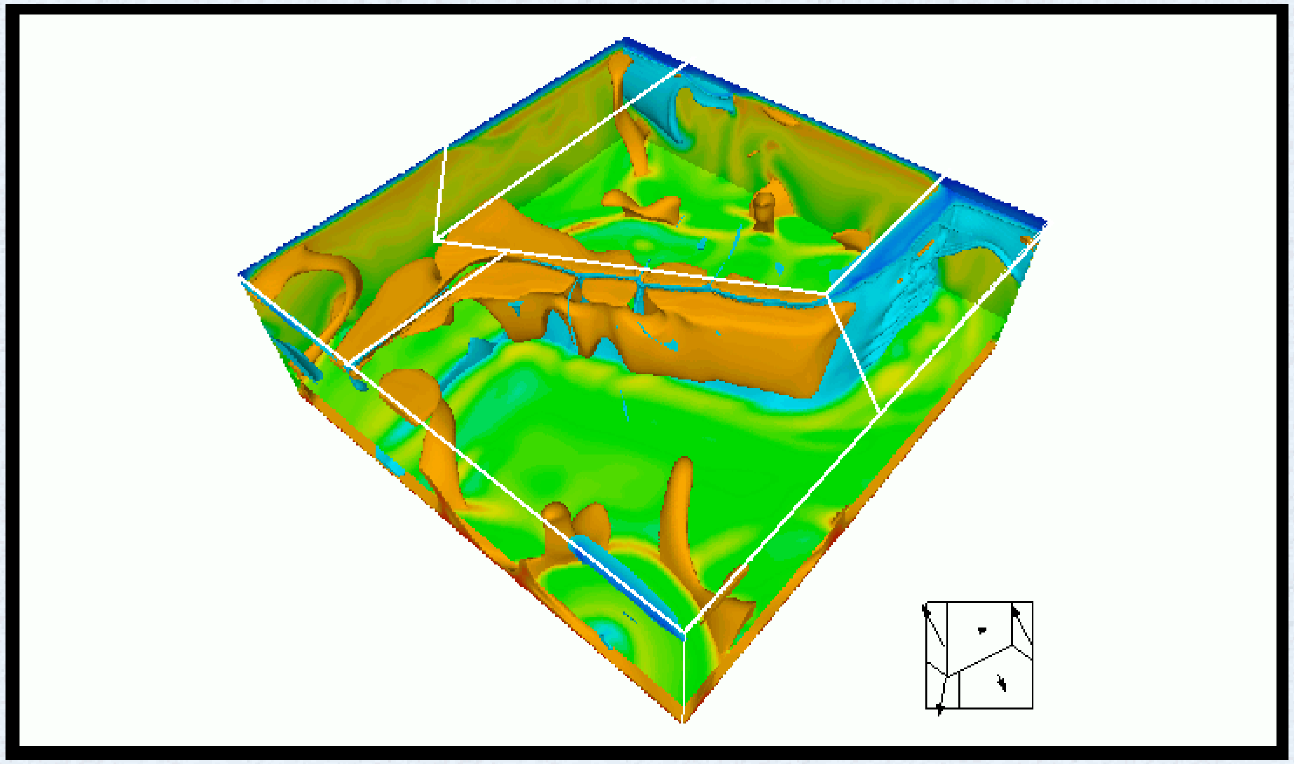
Successive Snapshots

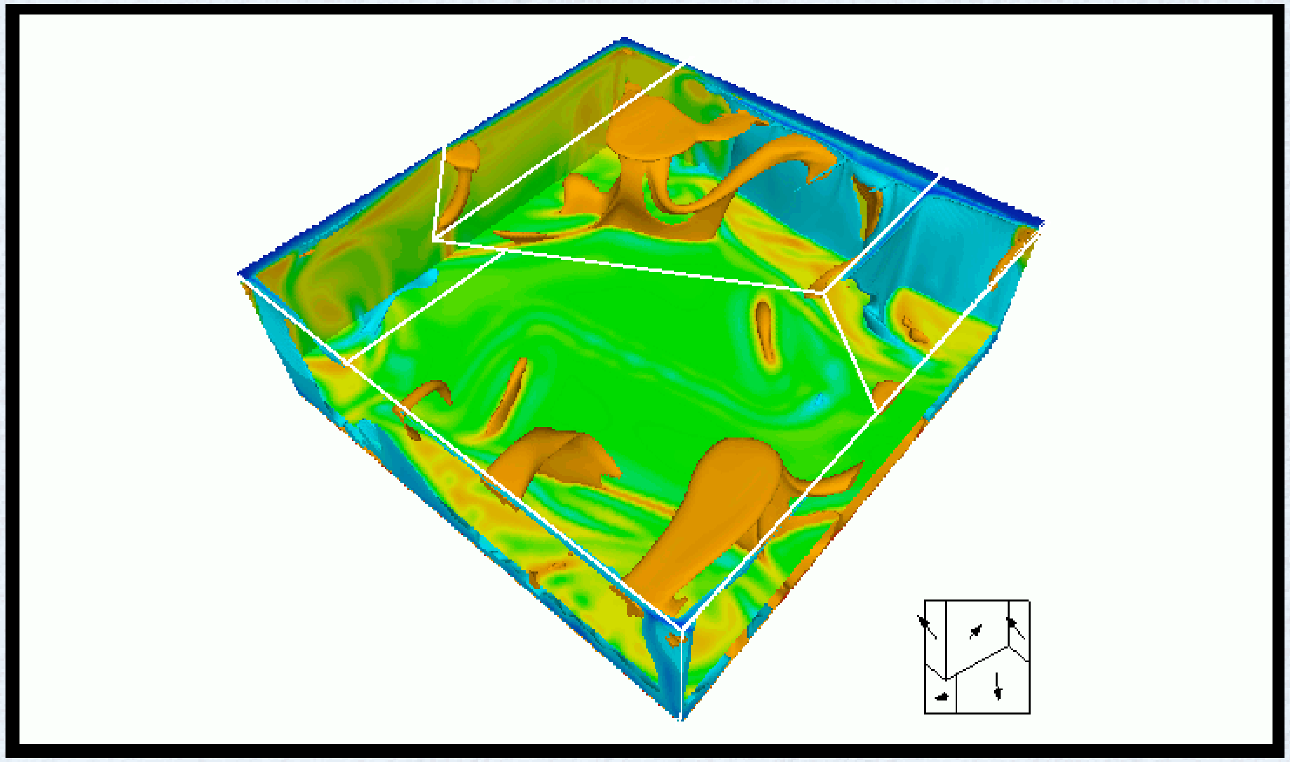




5 Myr model time

Successive snapshots

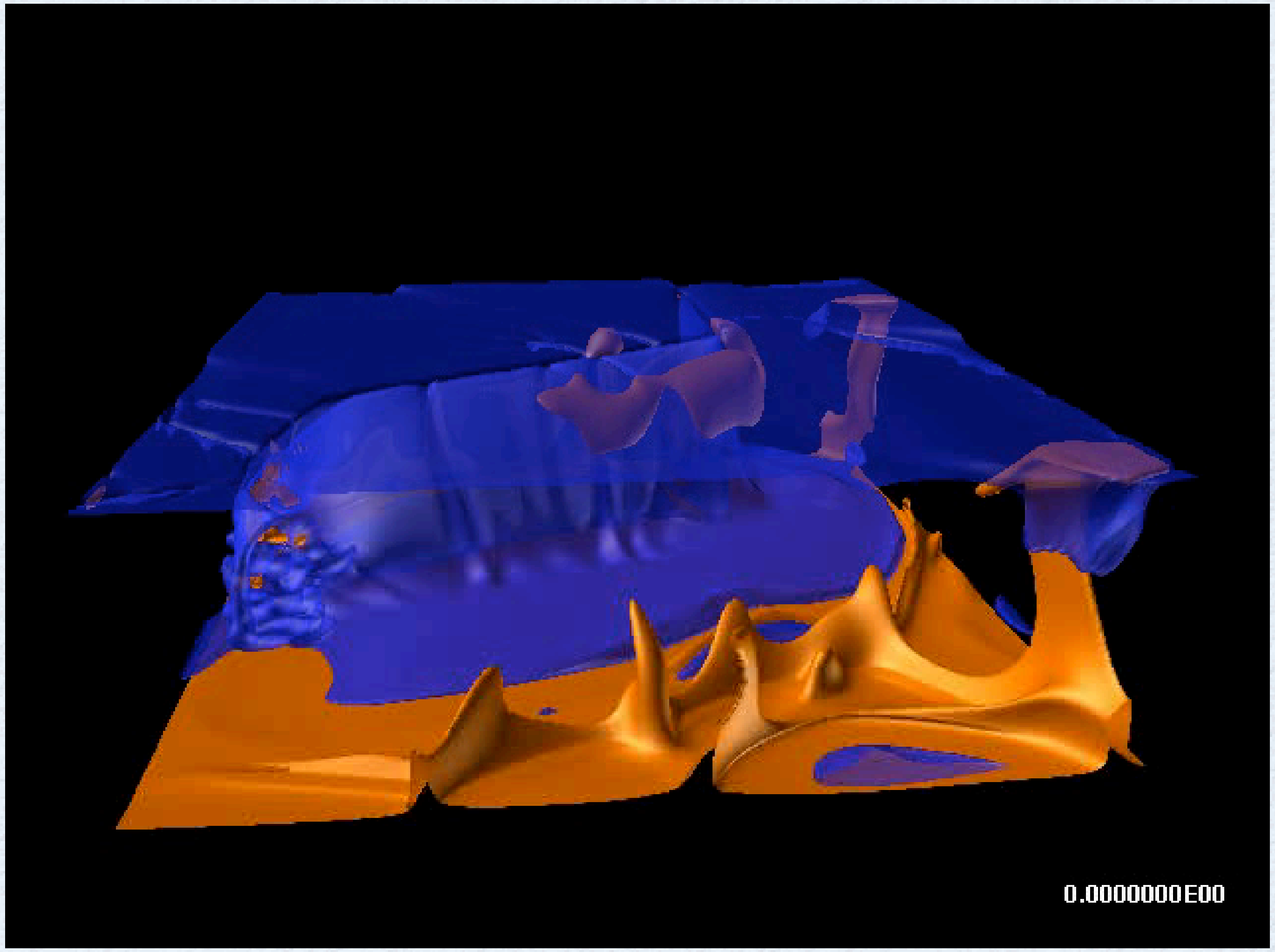




also 5 Myr model time

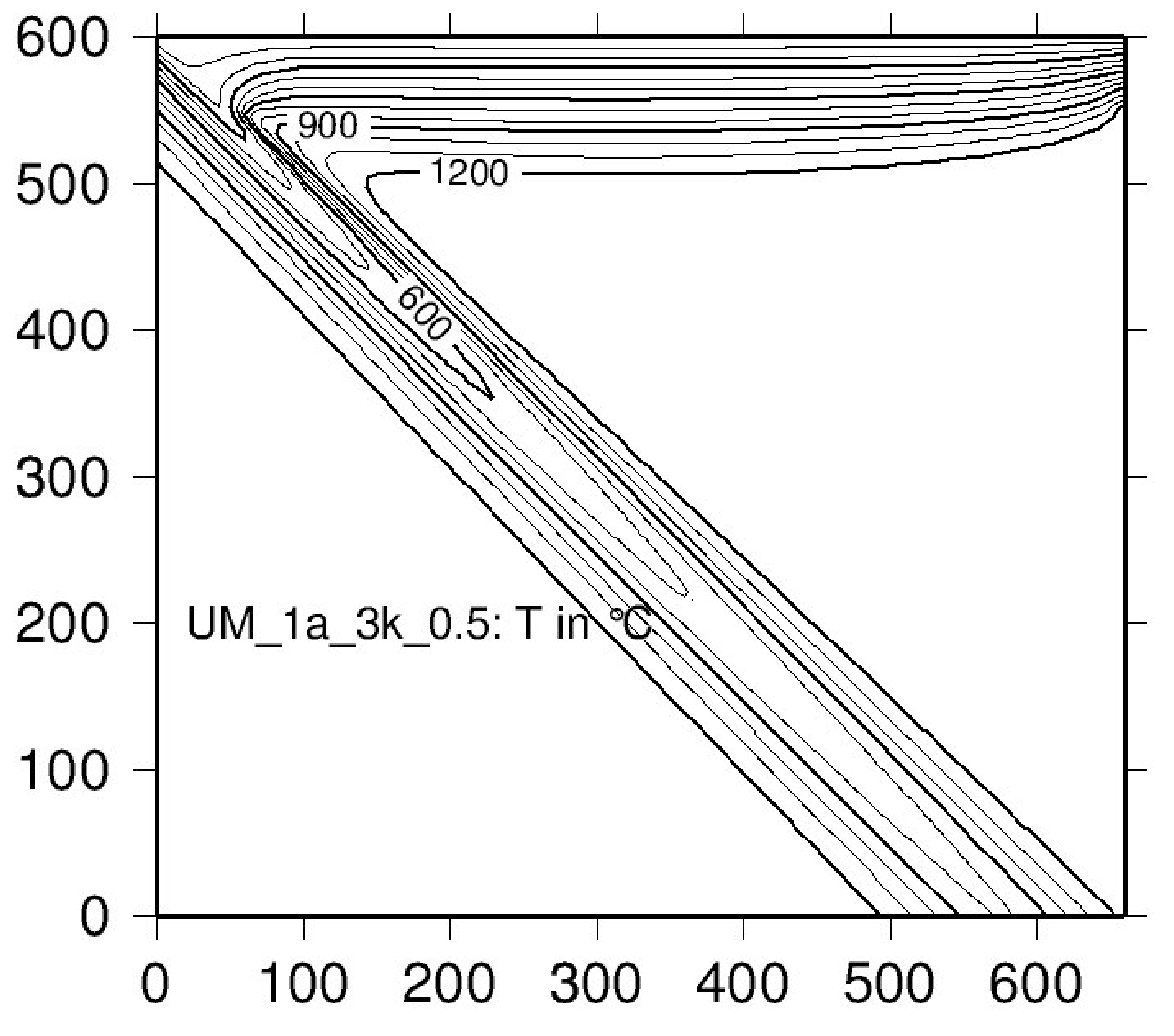
ANIMATION

- The animation here is the compilation of approximately 600 hours (wall clock) on 8-32 processors of IBM SP2
- >50 million unknowns (each step)
- It required almost 50 GB of storage (for the raw binary)
- This is about 1/4 of the size grid we would like to be using



circa 2000

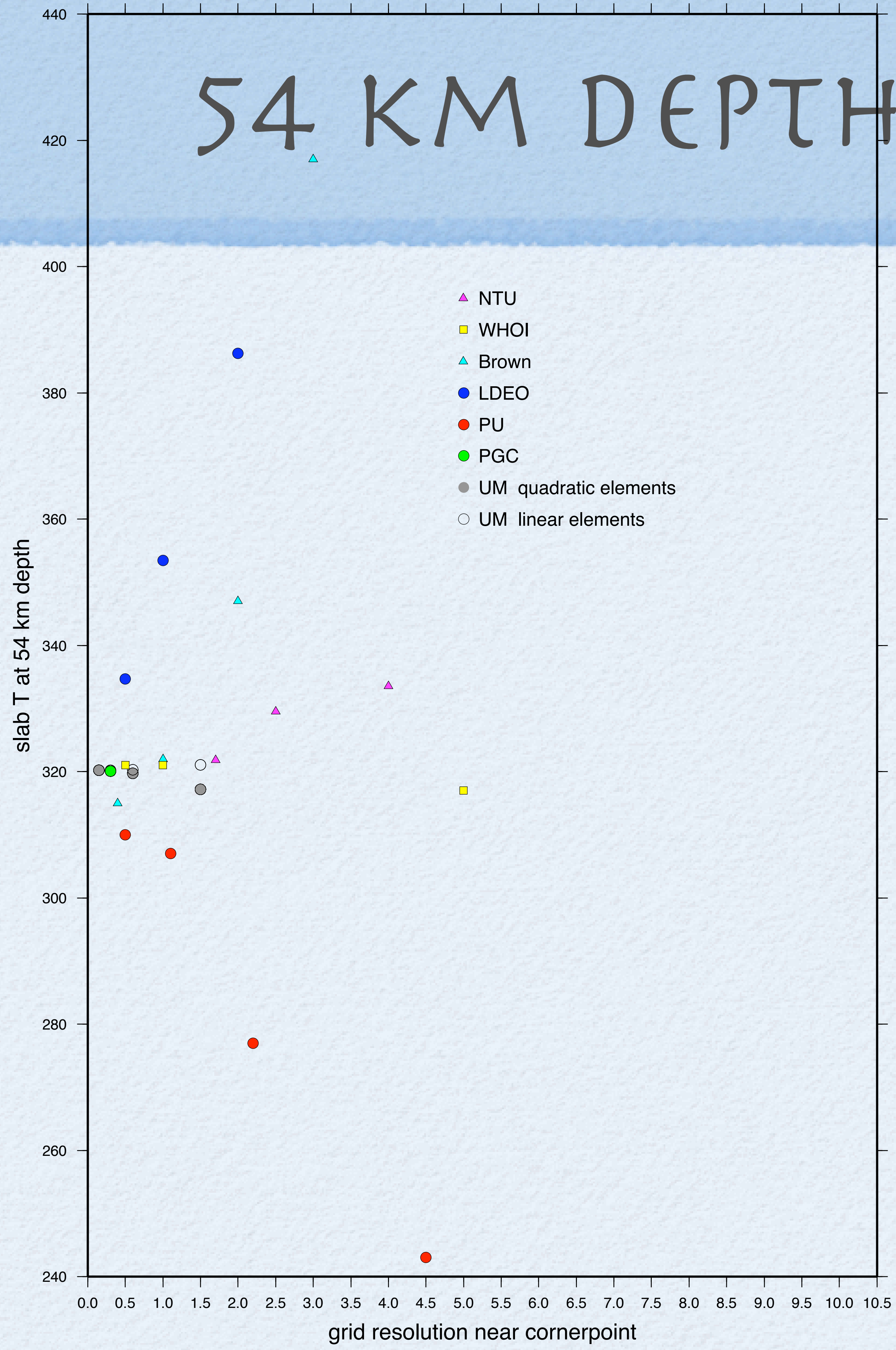
Subduction Grids



Start with kinematic (corner flow solution), only test advection/ diffusion

2002 AA Meeting

54 km depth along slab



deceptively hard problem:

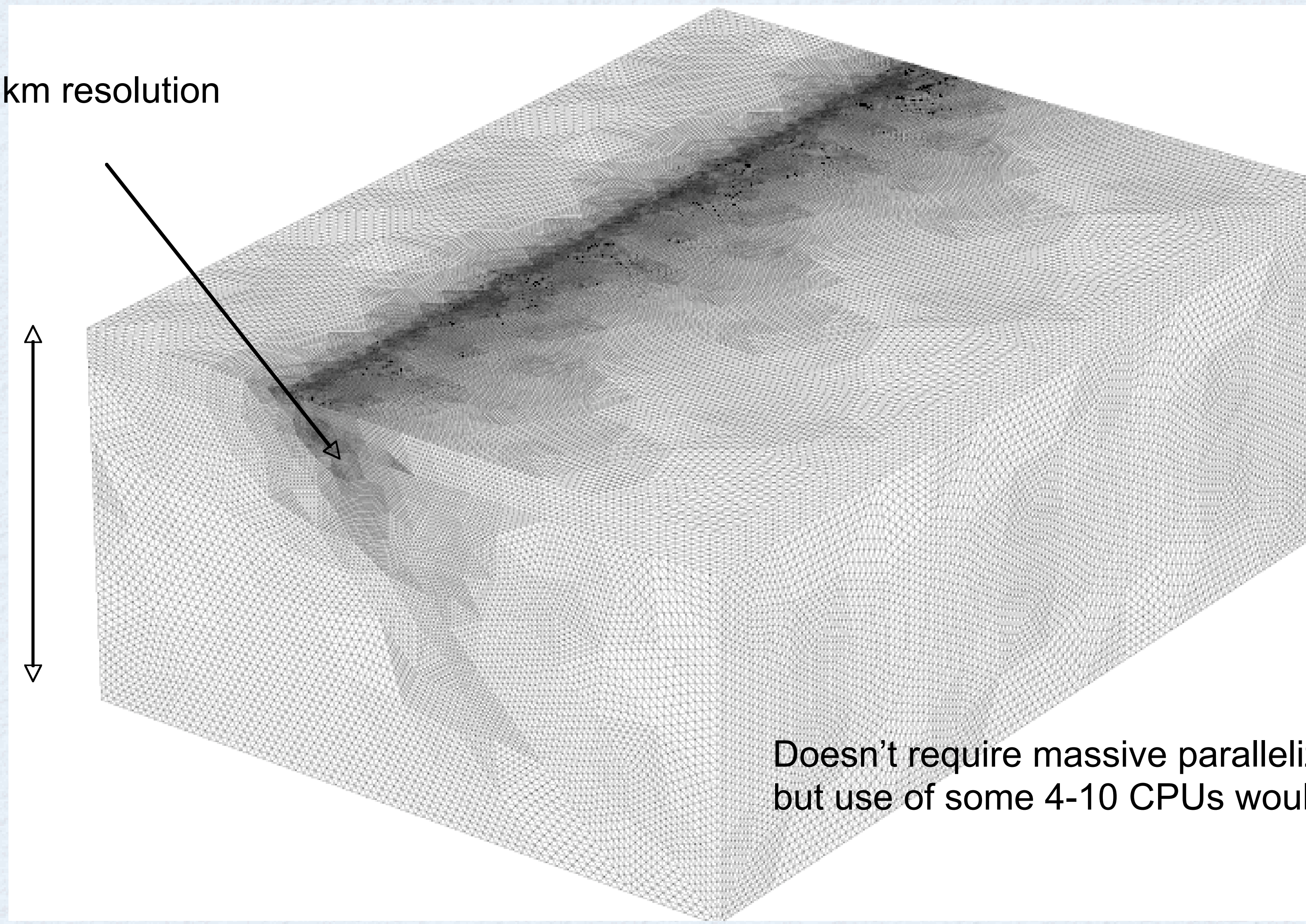
1) singularity in pressure

2) what is the right BC for the seismogenic zone?

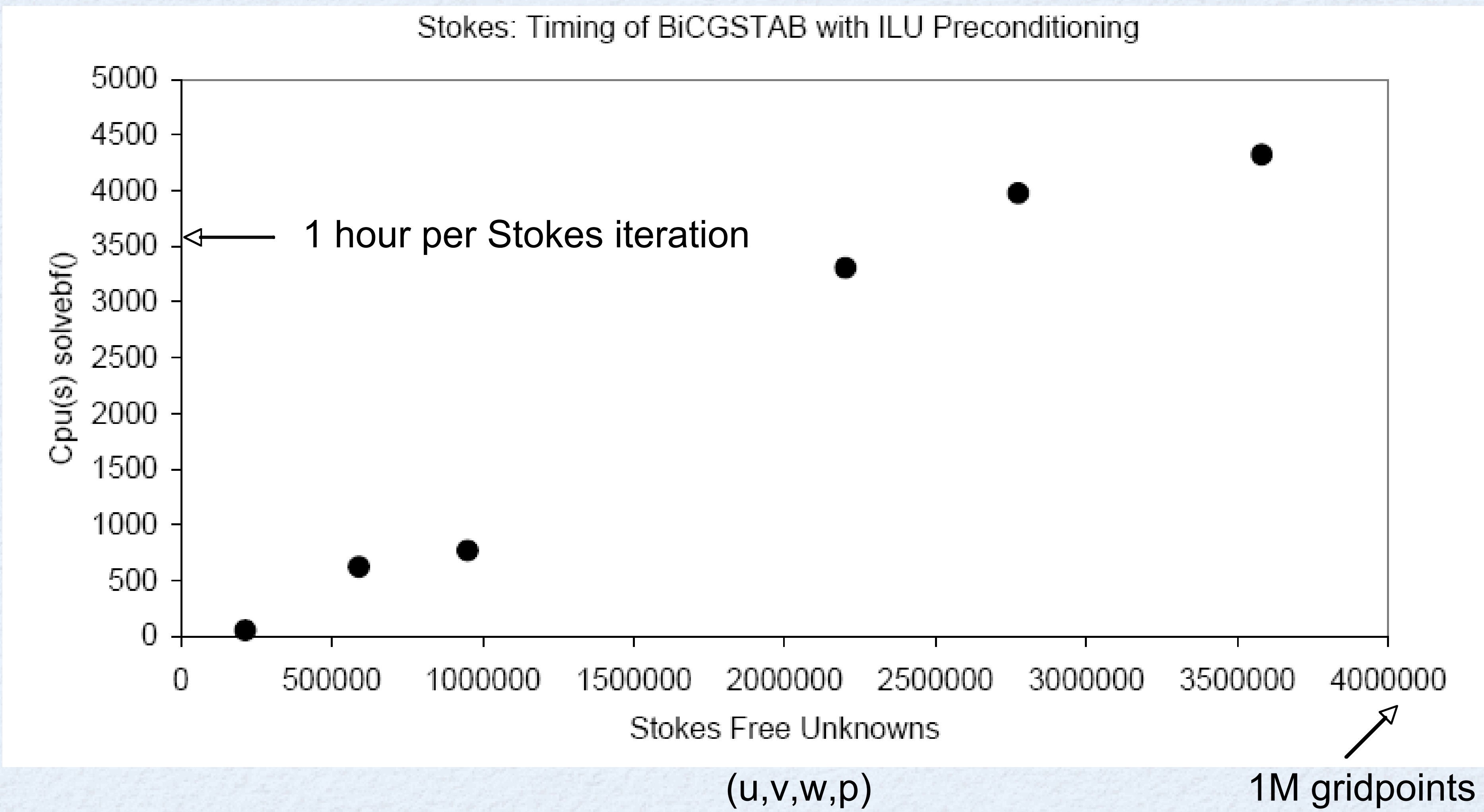
Sepran Finite Element Approach www.sepran.nl

- Sepran FEM (www.sepran.nl)
  - semi-commercial code ($3k one time fee, source provided)
  - in use by several US and European groups
- Penalty function formulation (2D)
  - primitive variables & (quadratic) Crouzeix-Raviart elements
  - direct solution method
  - not suited for iterative techniques (but please tell us otherwise!)
    - very high condition number of matrix
- Alternative: iterative solution (2D + 3D)
  - linear or quadratic Taylor-Hood elements
  - ILU preconditioning with BiCGstab
  - slower but allows for parallelization

Subduction Grid



Doesn't require massive parallelization,
but use of some 4-10 CPUs would be nice.



Stokes: Timing of BiCGSTAB with ILU Preconditioning
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
Cpu(s) solvebf()
1 hour per Stokes iteration
0
500000
1000000
1500000
2000000
2500000
3000000
3500000
4000000
Stokes Free Unknowns
(u,v,w,p)
1M gridpoints

Solver challenges

- BiCGstab + ILU/bjacobi
  - stable
  - fairly slow, CPU time scales as $N^{5/4}$
  - can multigrid be employed in preconditioning or in mesh design?
- GMRES and other Petsc solvers
  - not as efficient or stable as BiCGstab with Taylor-Hood element for Stokes equation (in my=*Peter* experience)

Preliminary (up to 4 CPUs) Results

Approaches:

1) native Sepran parallelization (using MPI)

2) Petsc + Sepran element routines

very similar results (but first doesn't require programming)

Building of system

scales linearly with #elements/ #unknowns

parallelizes efficiently

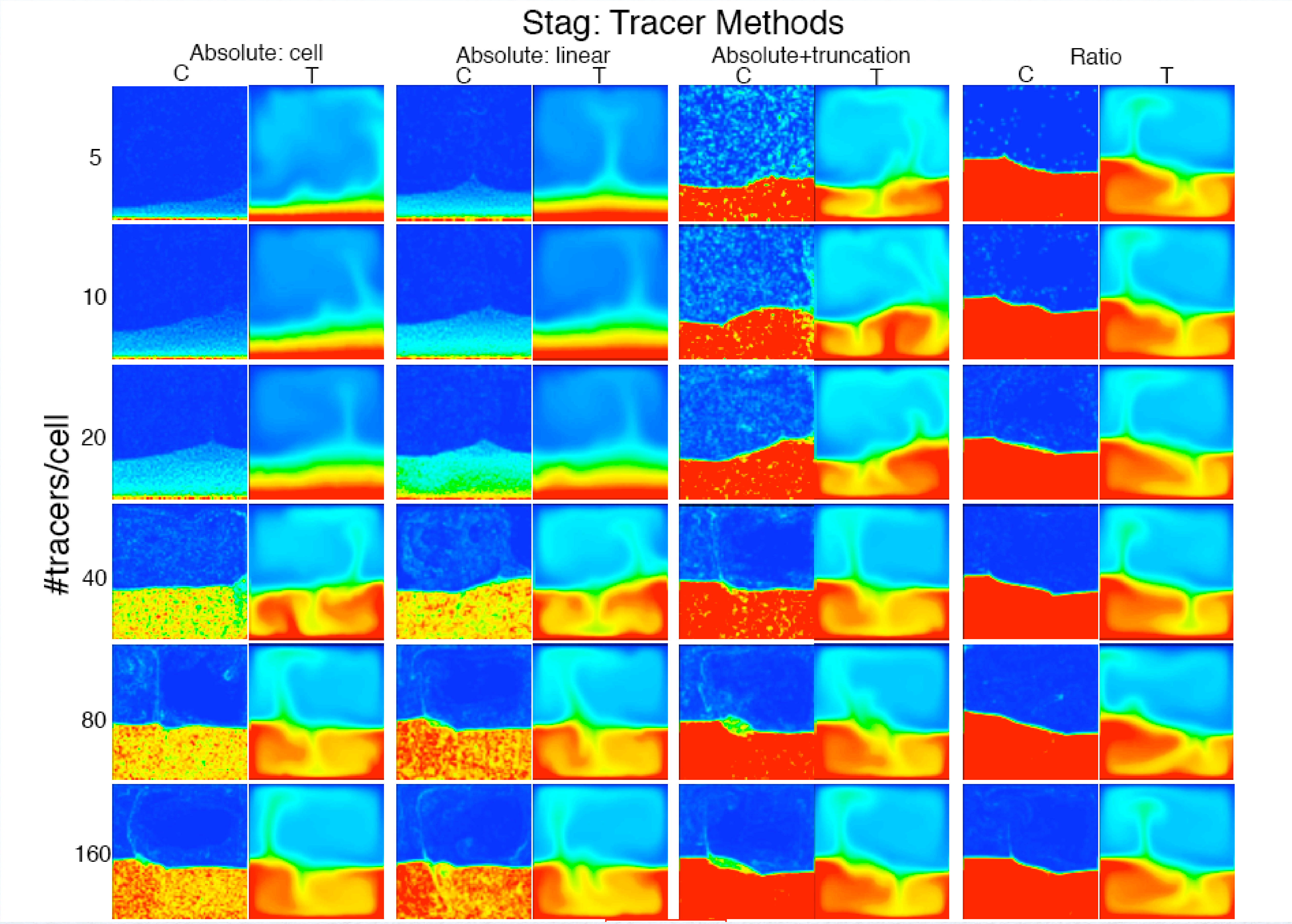
Solution of system (BiCGstab + bjacobi)

becomes dominant step for larger grids

scales non-linearly with #unknowns

relative poor parallelization in 2D; better in 3D

Critical step to be improved upon


Stag: Tracer Methods
Absolute: cell
Absolute: linear
Absolute+truncation
Ratio
C
T
#tracers/cell
5
10
20
40
80
160