Possible projects of interest to the RAMS program

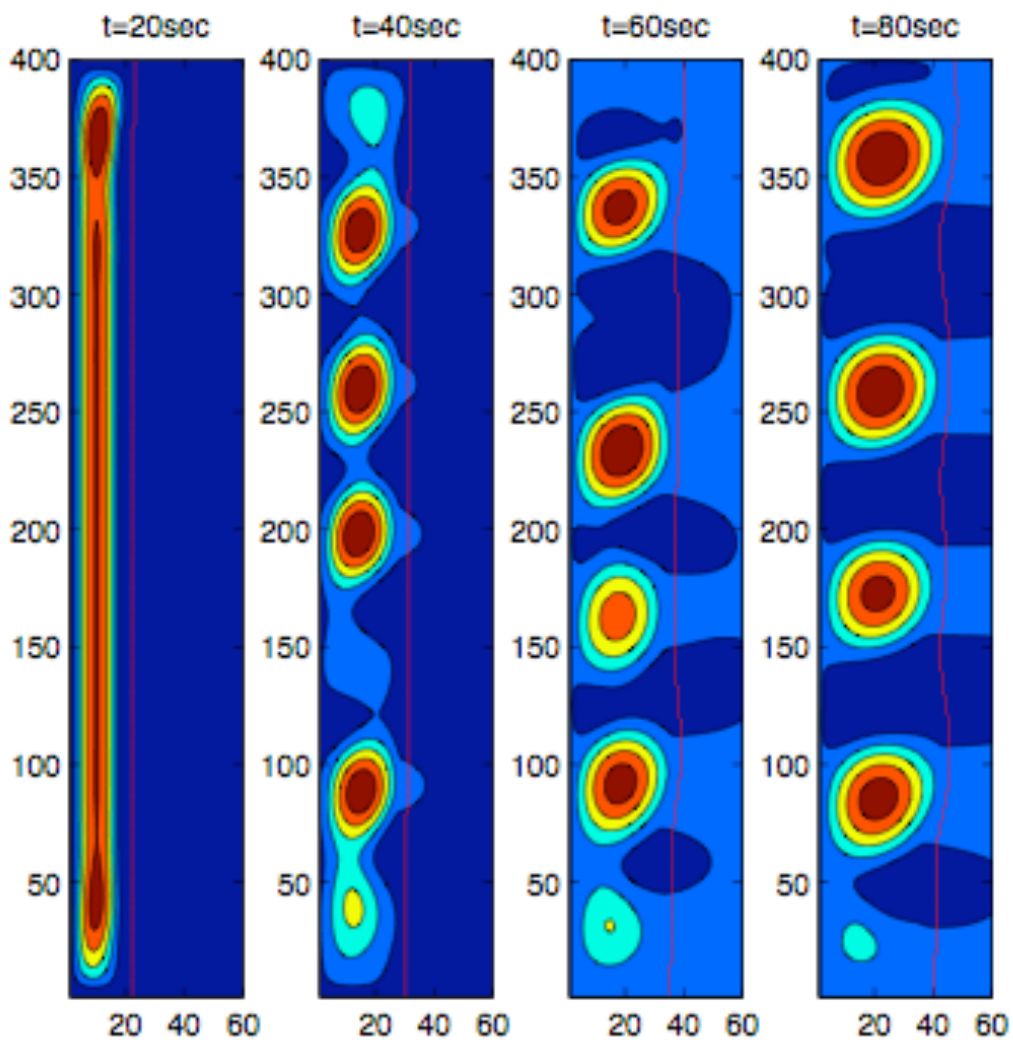
Kate Evans
Computational Earth Sciences
Oak Ridge National Laboratory

Convection and phase change simulation

- **Applications to materials science and technology**
- **Undesirable macrosegregation during the casting of metals**
- **Uneven and accelerated melting in polar ice fields**
- **Provides information for experiments and capturing observed behavior**

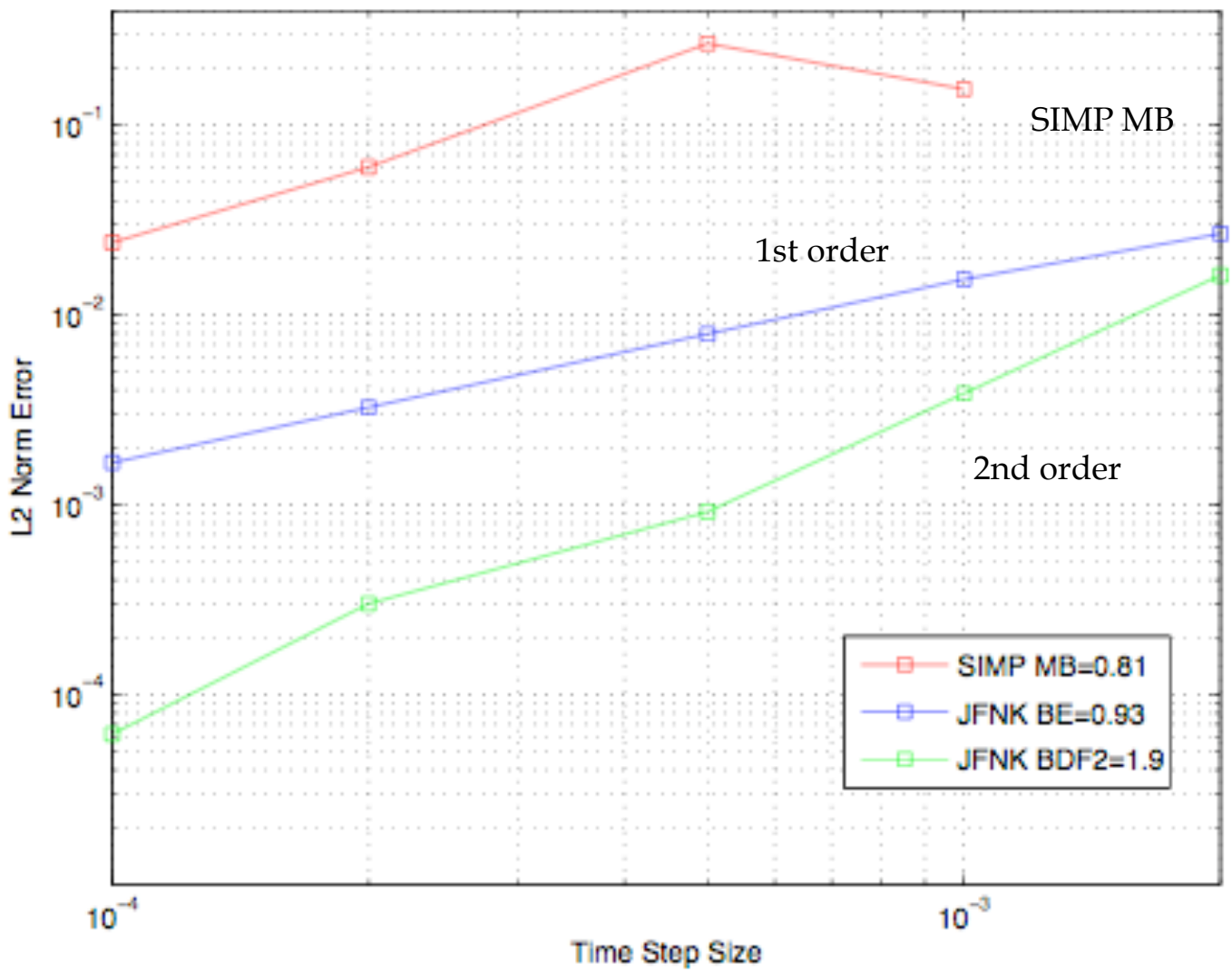
Past projects: Developing an algorithm to produce highly accurate simulations of phase interfaces and convective behavior

Benchmark: Melting of Pure Gallium

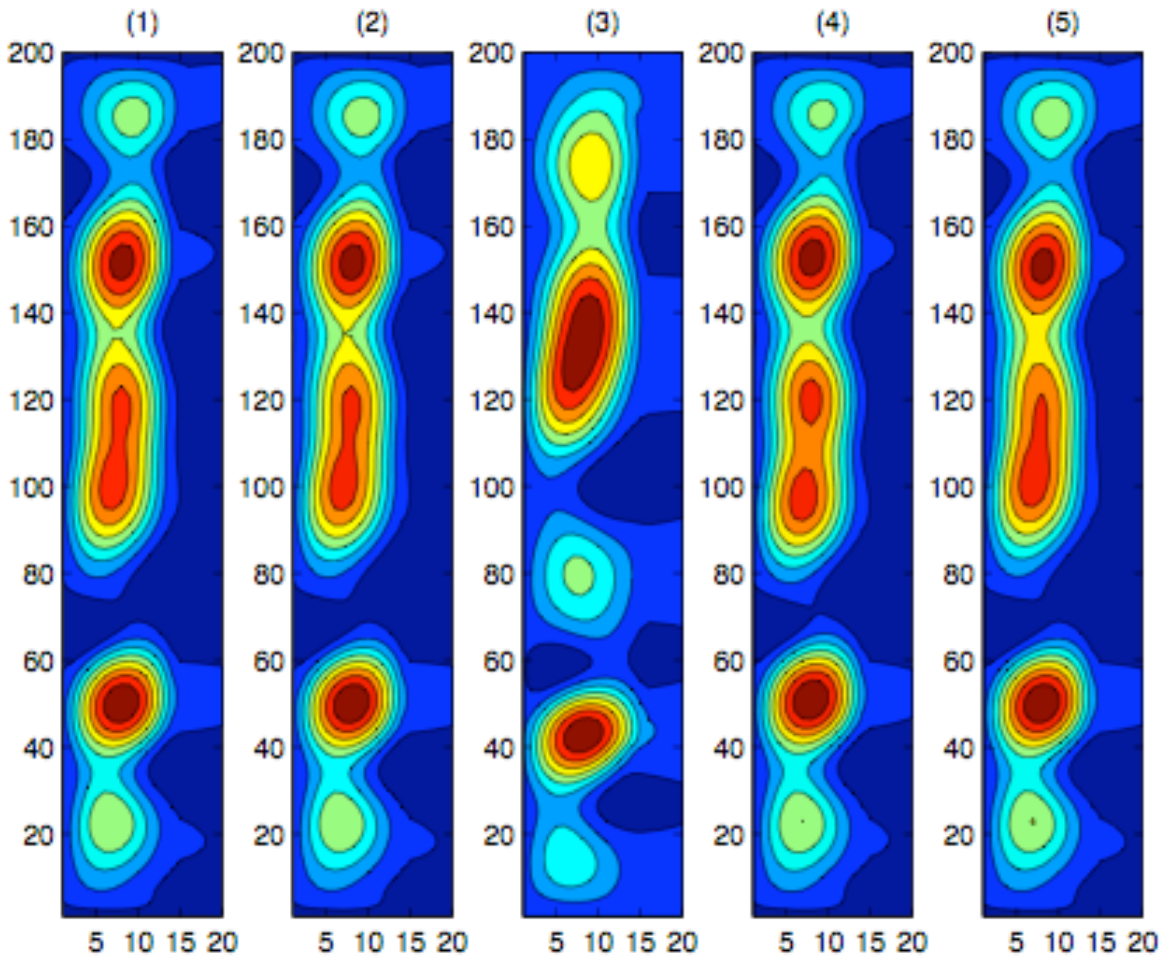


Contours:
Streamfunction,
Grid: 160x400

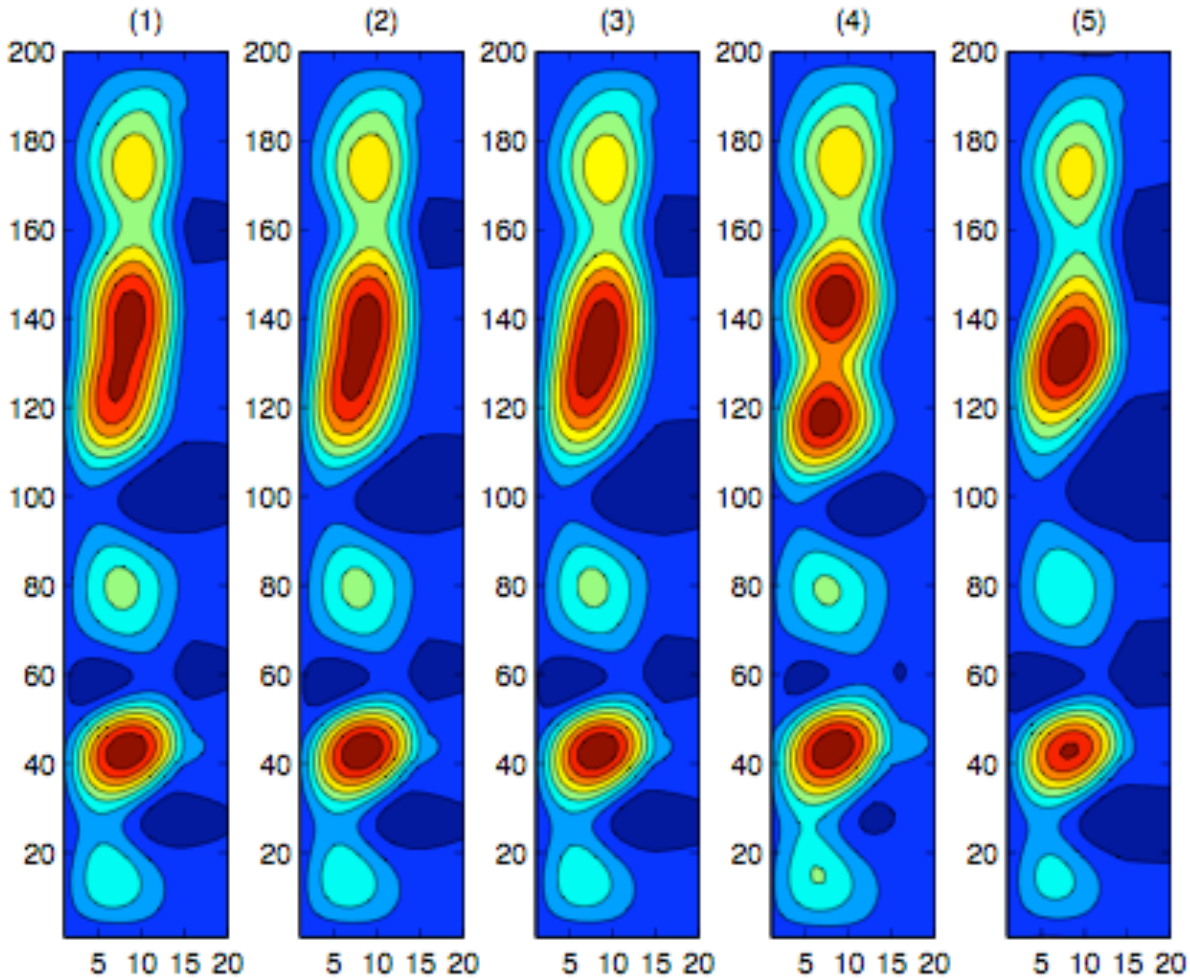
Time step convergence study of Gallium melting simulations at early times, 80x200 grid



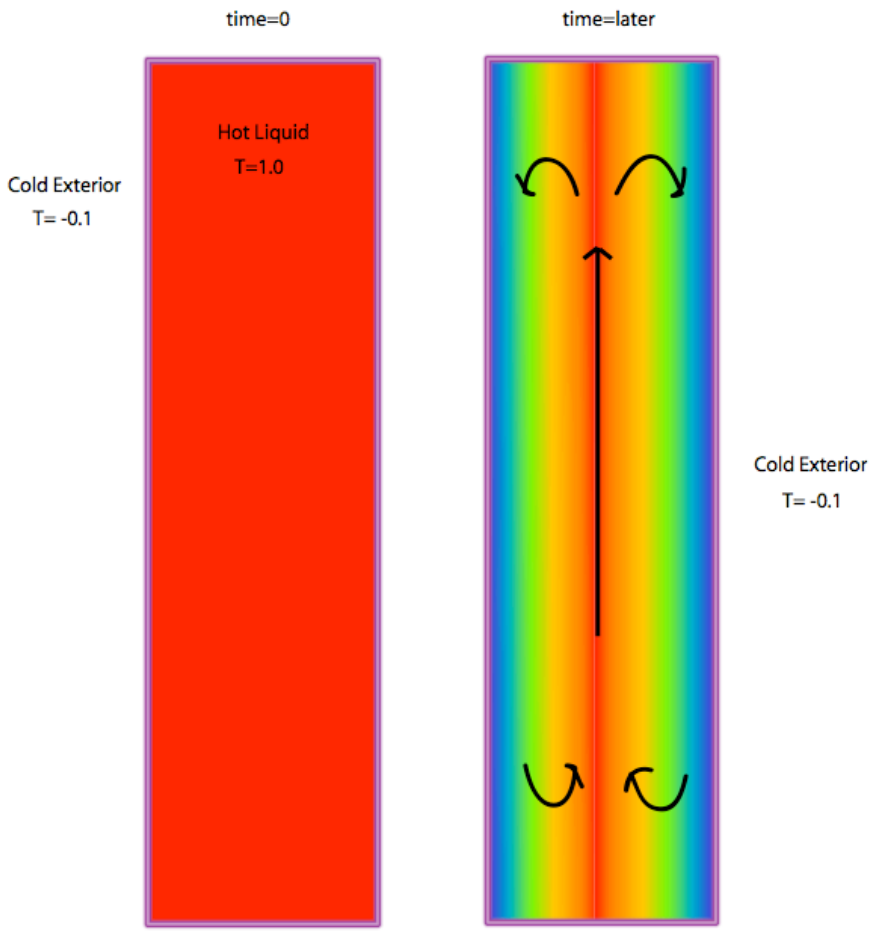
Streamfunction contours at 44s for a range of solution algorithms



Same comparison, at 48s



Next: Apply JFNK-MG-SIMPLE to a double solidification front



RAMS 2008: Katherine Roddy Linear Stability Analysis of Ice Water Convection

Project: Develop a theory to identify possible regions of enhanced ice melting and test with simulation

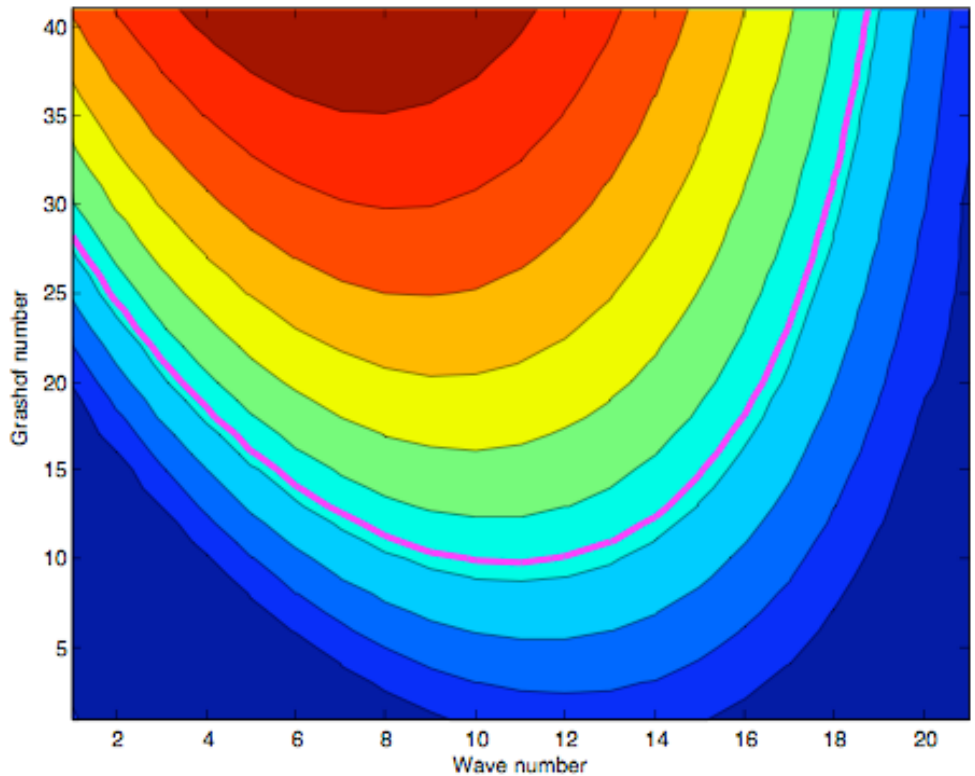
- **Uneven and accelerated melting in polar ice fields**
- **Field operations are difficult and expensive**
- **Provides information for experiments and capturing observed behavior**
- **Serve as subgrid scale model to large climate sea and land ice models**

Preliminary Results: Saltwater

- **Conduction regime, primary shear flow**
- **Perturbation to bifurcation:**
  - **Critical Rayleigh number**
  - **Critical wavenumber**
- **Convection regime, secondary flows**

Stable below a critical Grashof Number for a given wavenumber (the pink line)

Grashof #

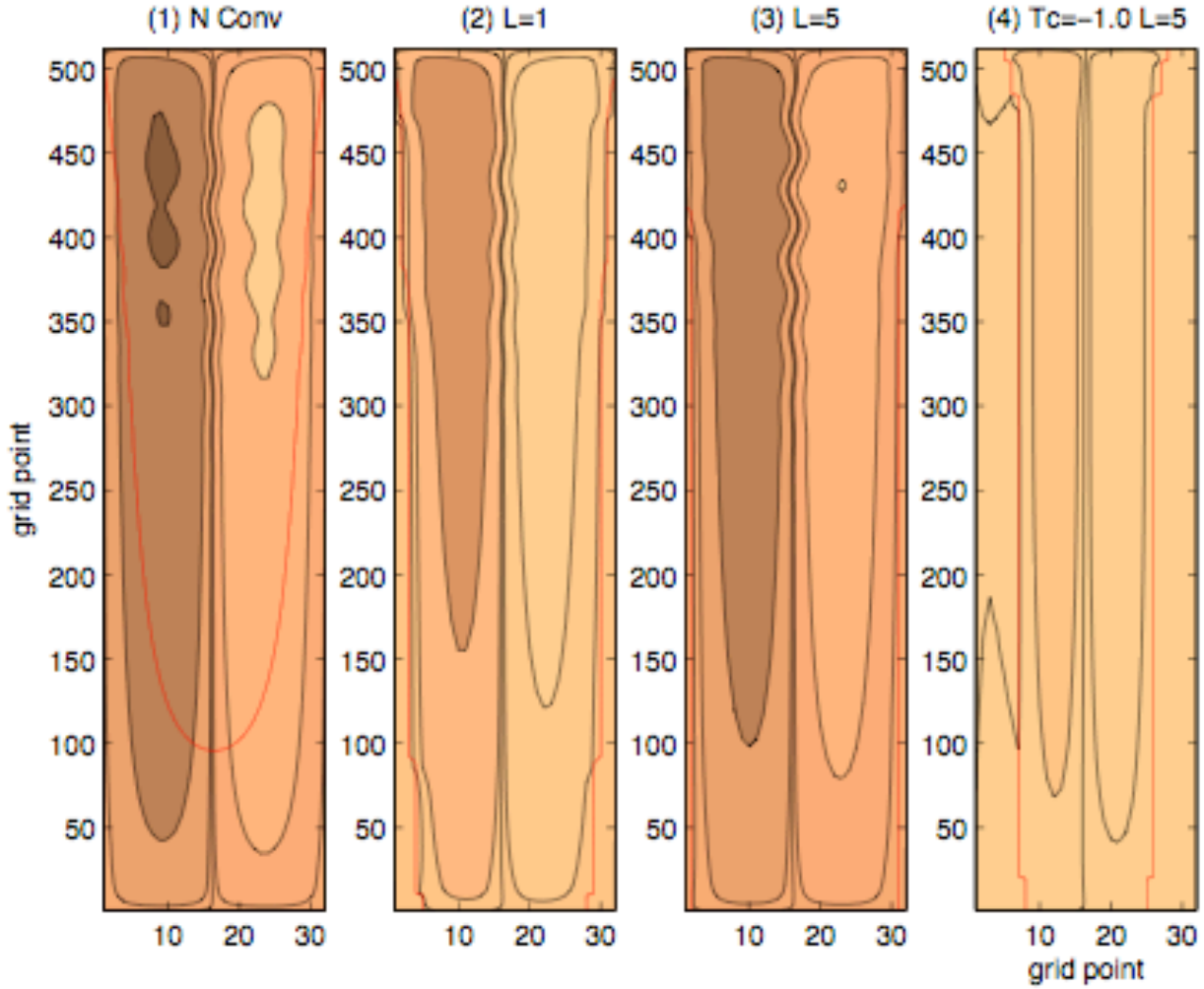


Wave #

Solidification can influence the onset of multiple cellular structure.

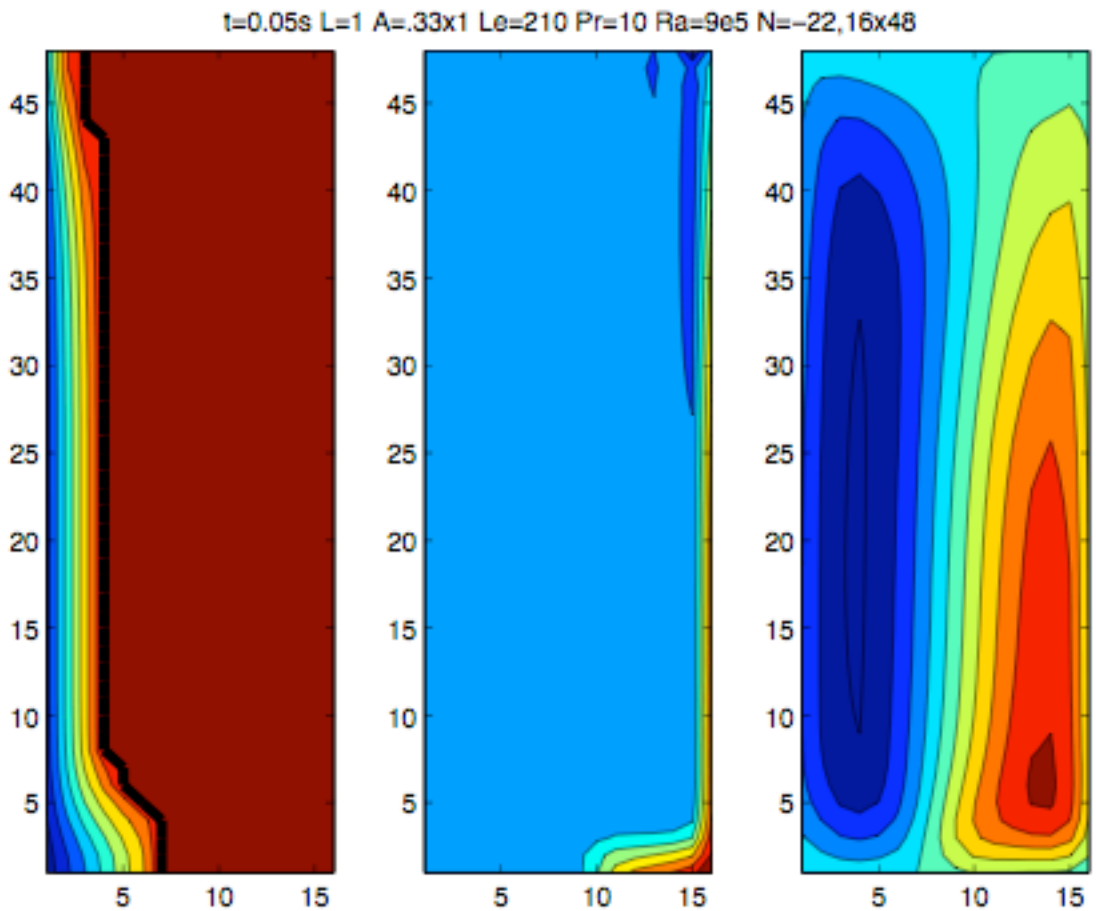
- Thermodynamic properties affects shape of melted region and local shear flow, which determines onset and persistence of multicellular convection
  - Parameters such as latent heat and exterior temperature
  - Phase front must move more slowly than time scale for multicellular growth
- High aspect ratio cavity with latent heat release along cell edges encourages multiple convection cells to form

Simulation of double convection: Comparison of simulations, time=0.12s

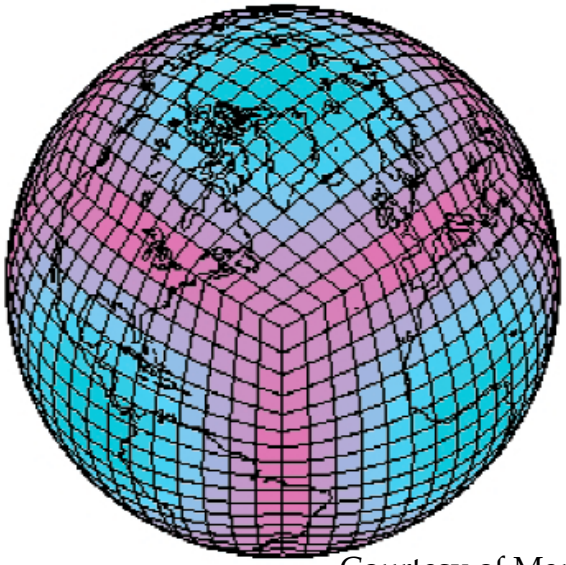


More of these simulations need to be performed to assess Simulation. Parallelism is needed.

Simulation of water with solidification and an 'inert' solute source (salt). Does theory predict onset of multiple celled convection?



CAM-HOMME: Spectral Element Cubed Sphere Dynamic Core



Courtesy of Mark Taylor

.86 <- Aspect Ratio -> 1.0

Benefits of Spectral Elements:

- Combines benefits of spectral transform and finite element methods
- Superior Scalability: runs on >80,000 cores. Communication needed only at element edges
- Robust Mesh refinement: either increase the number of elements or order of spectral degree

Benefits of Cubed Sphere:

- Avoids high aspect ratio elements near the pole
- Regular latitude/longitude grid on each cube face
- No mapping singularities from grid to cube

Oak Ridge National Laboratory

Fully Implicit solution method option is being implemented in CAM:HOMME

- **Benefit: Large time steps**
  - **Additional capability: Crucial for steady state calculations, parallel in time methods, and parameter sensitivity studies**
  - **Superior accuracy: captures all nonlinear interactions at the time scale resolved**
- **Efficient solution methods and larger time steps outweigh iterative costs**

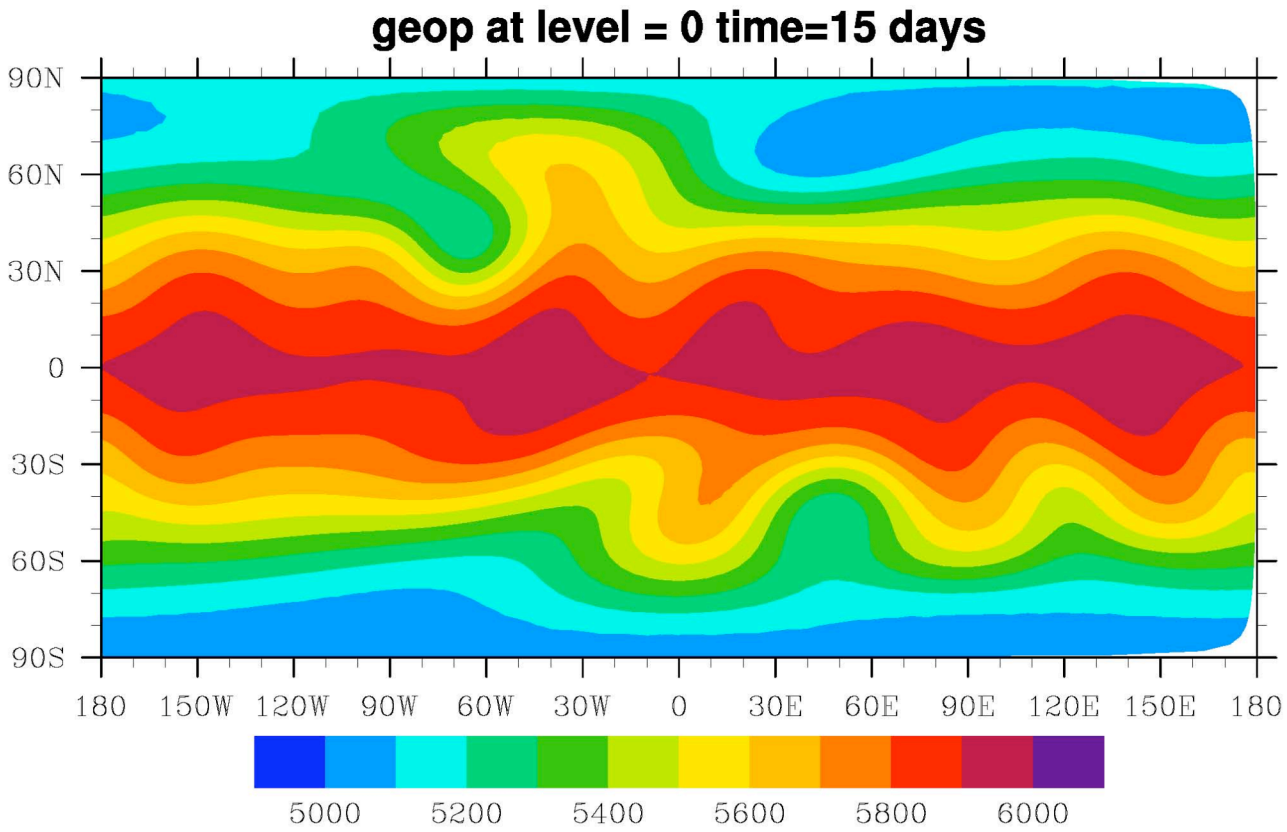
Example: Steady State Test Case with Shallow water equations on coarse grid

Method (4x8x8)	Time Step Size	Wall Clock time
Leapfrog	4 min=240s	28s
BDF2*	1 day=86400s	3.6s

•Efficiency gains from a work-in-progress preconditioner are expected

OAK RIDGE National Laboratory

Simulation of more realistic atmospheric flow: 15 day simulation of flow over a mountain feature



Questions?

Courtesy: Ivo Sandor