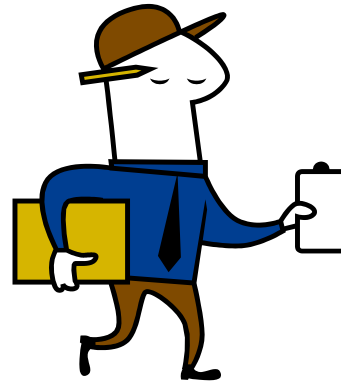


The importance of being on time ...



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Supported by: ORNL LDRD, DOE OASCR SciDAC TOPS-2 and BER



SciDAC

Scientific Discovery through Advanced Computing



Lots of focus on spatial accuracy, but time matters just as much ...

The Boston Globe

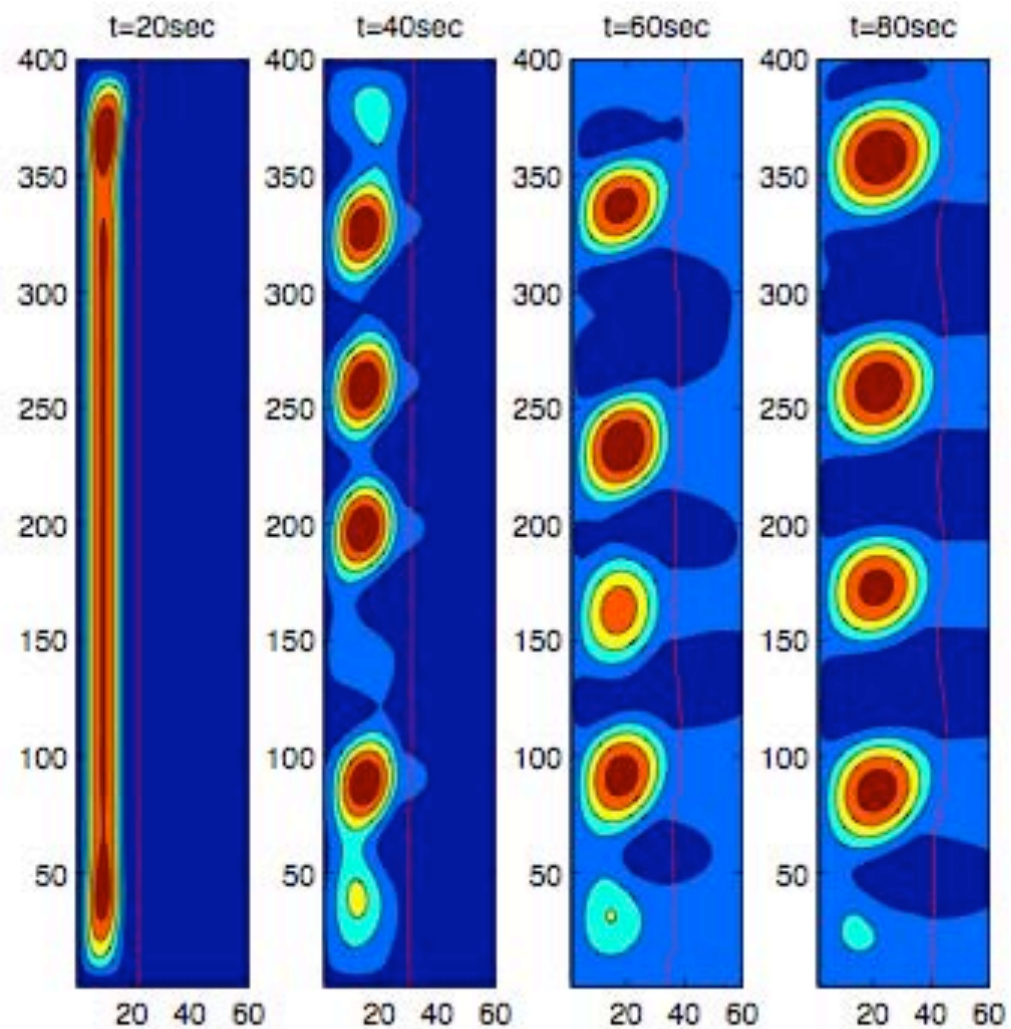
May 1, 2004. The way things turned out, the Sox and Rangers could have played for nearly an hour and 45 minutes before the rain began. Rangers officials said They were led to believe the storm would strike about 8:30 p.m., about 25 minutes after the scheduled start time. In fact, ...

The Washington Post

Game 5 of Series Is Suspended Because of Rain, Oct 28, 2008. We obviously monitored the weather all day," Selig said after the game was suspended at about 11:10 p.m. "We were told about 7:45 [p.m.] that it would only be a tenth of an inch of rain between then and midnight or thereafter. . . . I had a nagging fear because **these forecasts have changed so much.**"



Benchmark: Melting of Pure Gallium



Contours:
Streamfunction,
Grid: 160x400

Fully implicit scheme:

Jacobian-Free Newton-Krylov Method, or JFNK

Goal: minimize the residual of the full nonlinear equations, $F(\mathbf{x})$, at new time level to a specified nonlinear tolerance

$$M\mathbf{x} - b = F(\mathbf{x}) = 0$$

M = continuous non-linear operator matrix

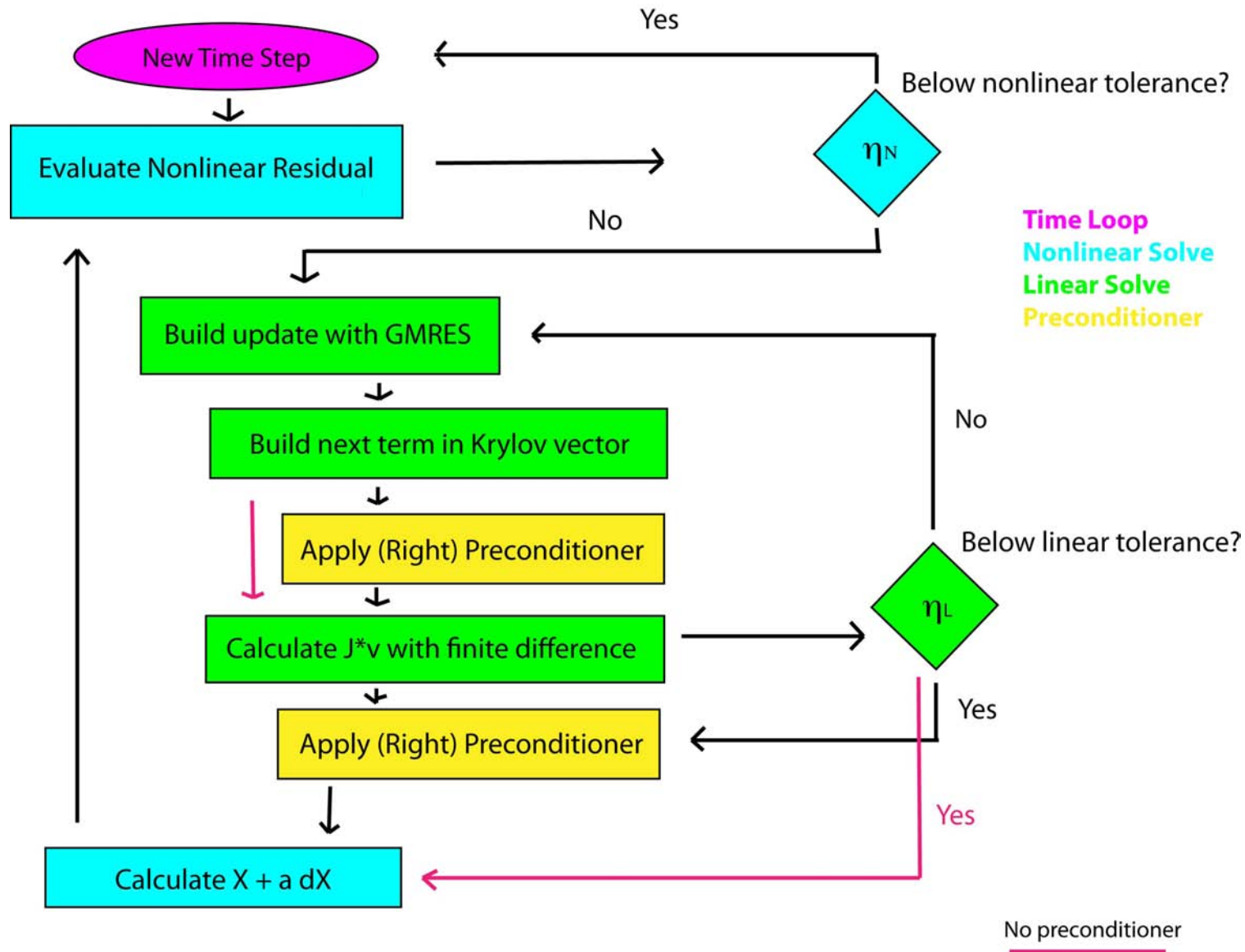
$$F(\mathbf{x}^k) = -J(\mathbf{x}^k)\delta\mathbf{x}$$

Take the 1st order Taylor series approximation

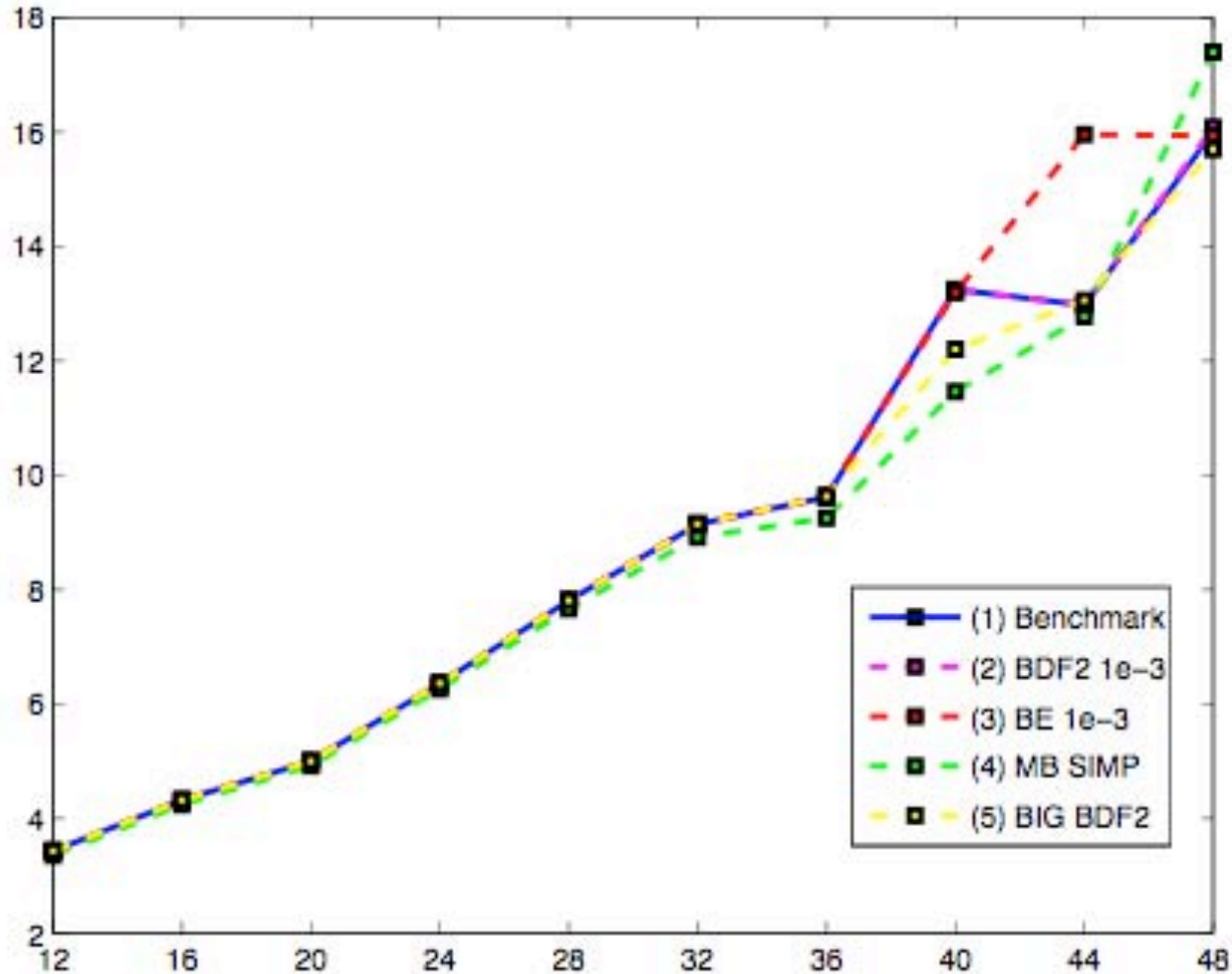
$$\mathbf{x}^{k+1} = \mathbf{x}^k + \delta\mathbf{x}$$

Generate a good update to test for convergence at iteration k

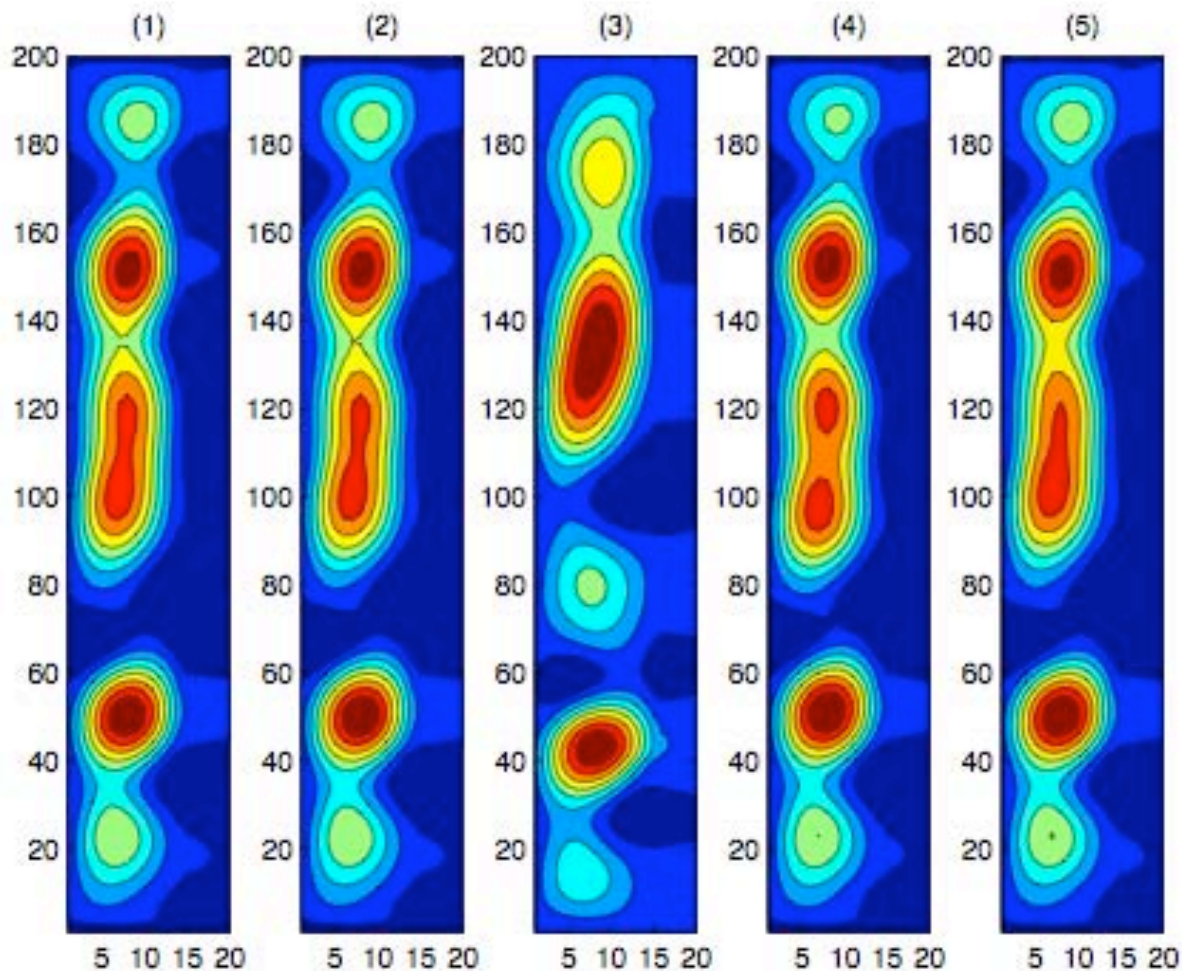
Fully Implicit JFNK Algorithm



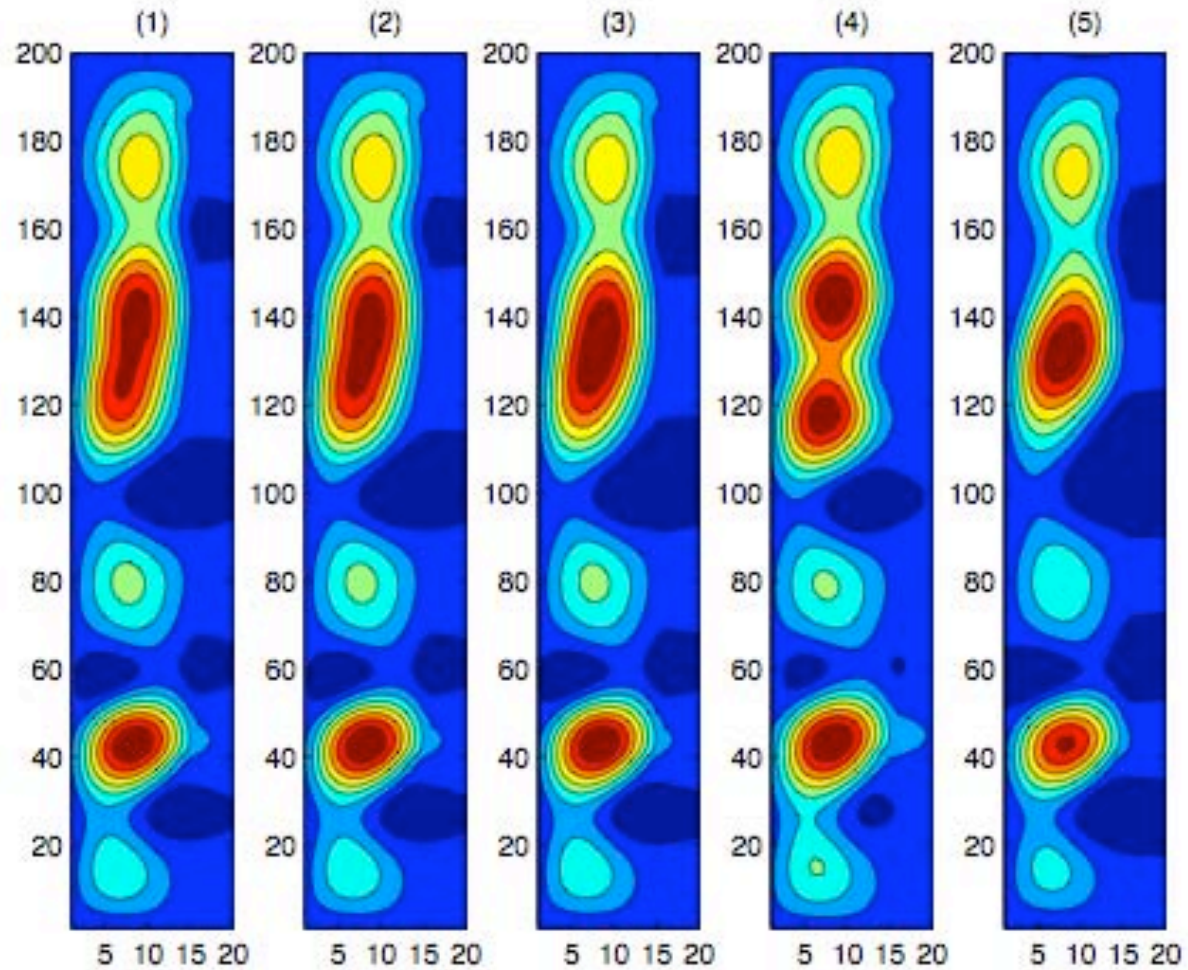
Maximum vorticity vs. time to 44s



Streamfunction contours at 44s for a range of solution algorithms



Same comparison, at 48s

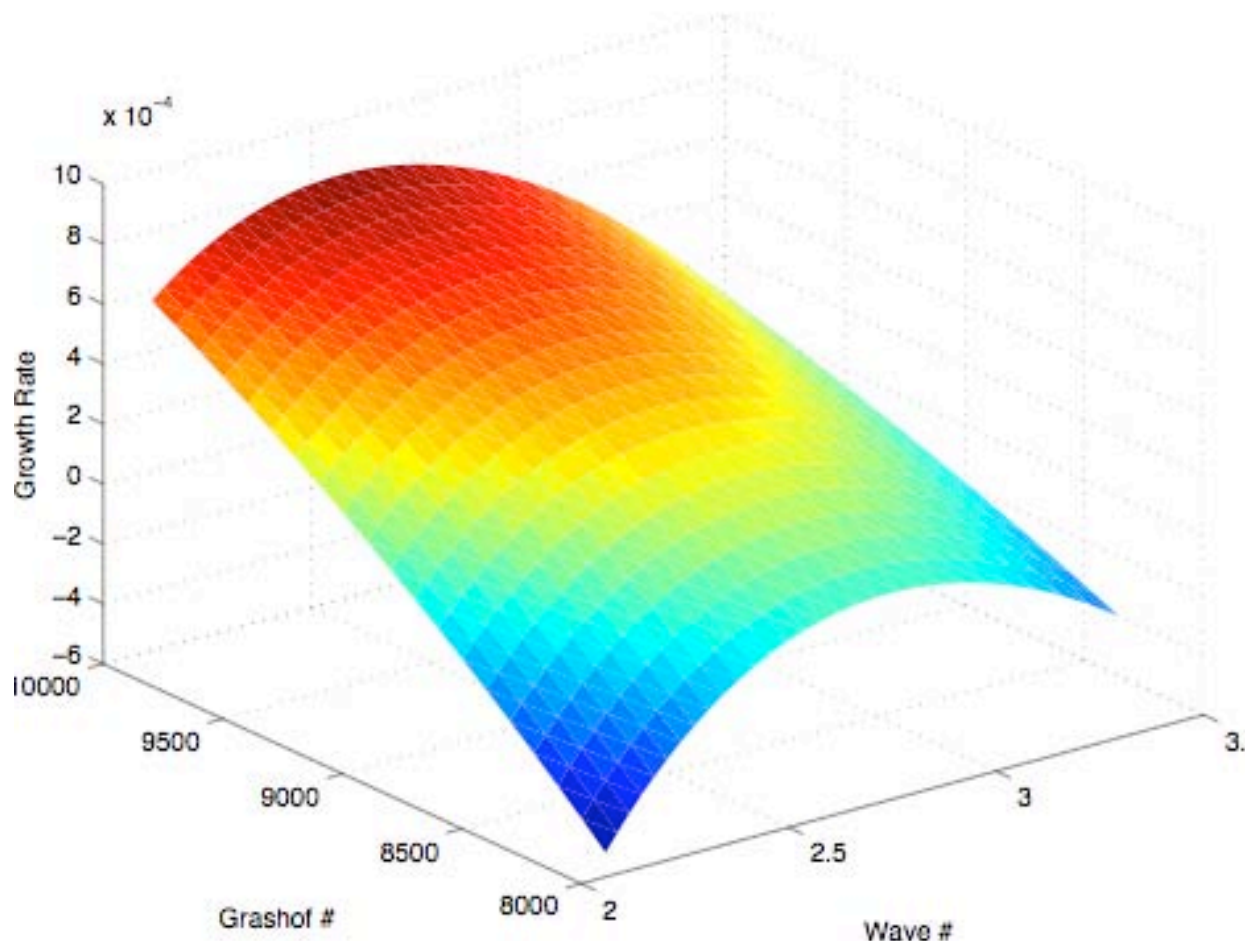


Linear Stability Analysis Extension

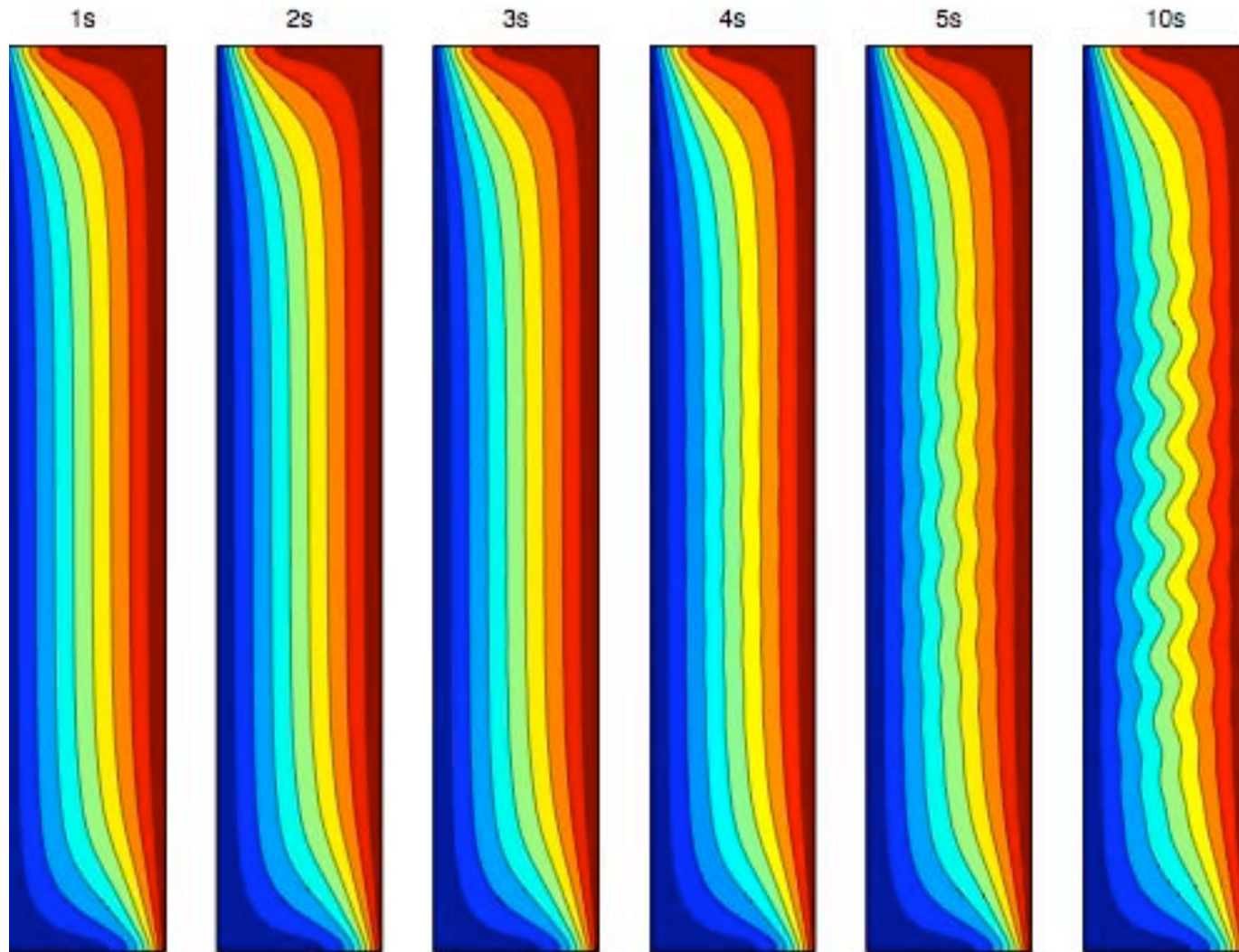
- **Keep time derivative - no longer looking for stable states but unstable transition**

$$\begin{aligned} & \left(\frac{\partial}{\partial t} + \bar{v} \frac{\partial}{\partial y} \right) u' - \frac{1}{Gr} \Delta u' + \frac{\partial p'}{\partial x} = 0 \\ \left(\frac{\partial}{\partial t} + \bar{v} \frac{\partial}{\partial y} \right) v' + u' \frac{\partial \bar{v}}{\partial x} - \frac{1}{Gr} \Delta v' - \frac{1}{Gr} \frac{\partial^2 \bar{v}}{\partial x^2} + \frac{\partial p'}{\partial y} - \frac{1}{Gr} T = 0 \\ & \frac{\partial u'}{\partial x} + \frac{\partial v'}{\partial y} = 0 \\ & \left(\frac{\partial}{\partial t} + \bar{v} \frac{\partial}{\partial y} \right) T' + u' \frac{\partial \bar{T}}{\partial x} - \frac{1}{Gr Pr} \Delta T' = 0 \end{aligned}$$

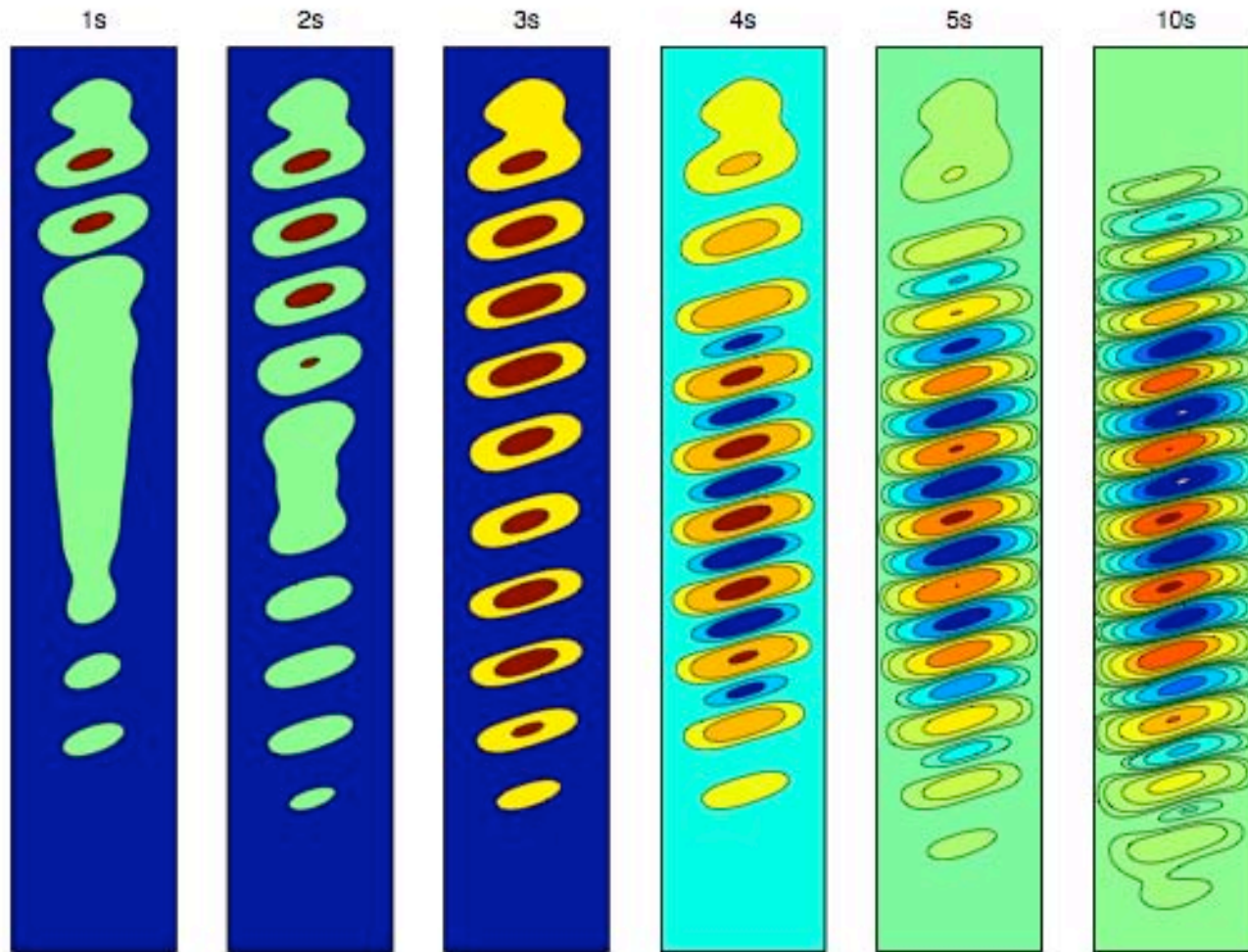
Linear Stability Analysis: Surface of Solutions for Pr=0.71



Temperature contours for $Gr=8700$



Time Integration: Secondary flow cells develop within the background flow



T Contours:

+/- .001

+/- .002

+/- .005

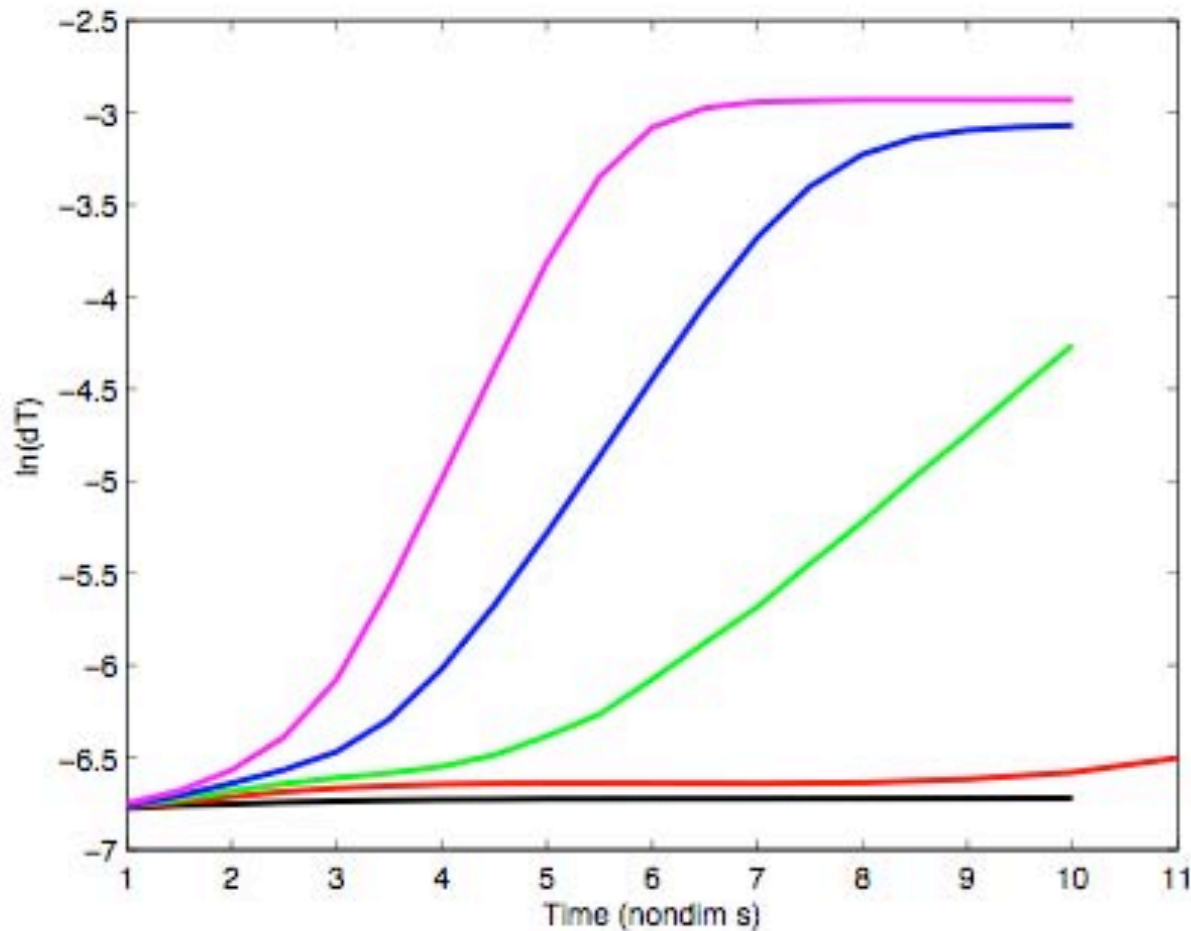
+/- .01

+/- .02

+/- .03

+/- .05

Time Integration: Growth of dT



Gr=8700 Magenta
Gr=8600 Blue
Gr=8500 Green
Gr=8400 Red
Gr=8200 Black

HOMME: High-Order Method Modeling Environment

- **Spectral element, cubed sphere dynamic core option of the Community Atmospheric Model**
- **Explicit and semi-implicit solver options**
- **Global atmosphere model developed in part through the DOE CCPP program at NCAR**
- **Principal HOMME Developers:**
 - **John Dennis (NCAR/CU)**
 - **James Edwards (NCAR)**
 - **Rory Kelly (NCAR)**
 - **Ramachandran D. Nair (NCAR)**
 - **Amik St-Cyr (NCAR)**
 - **Mark Taylor (Sandia)**



Atmospheric Climate Model Test Cases: Shallow Water Equations

$$\frac{\partial \mathbf{v}}{\partial t} = -(\zeta + f)\hat{k} \times \mathbf{v} - \nabla \left(\frac{1}{2} \mathbf{v} \cdot \mathbf{v} + gH \right),$$
$$\frac{\partial h}{\partial t} = -\nabla \cdot (h\mathbf{v})$$

where

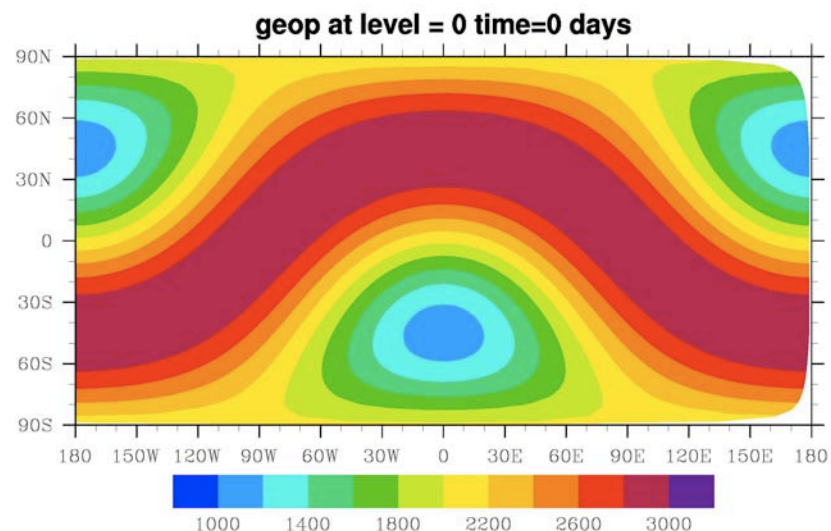
$$H = h + h_s,$$

$$\zeta = \hat{k} \cdot \nabla \times \mathbf{v},$$

$$f = 2\Omega \sin \theta$$

SW Test Case 2. Steady-State nonlinear geostrophic flow for 12 days, $\alpha = \pi/4$

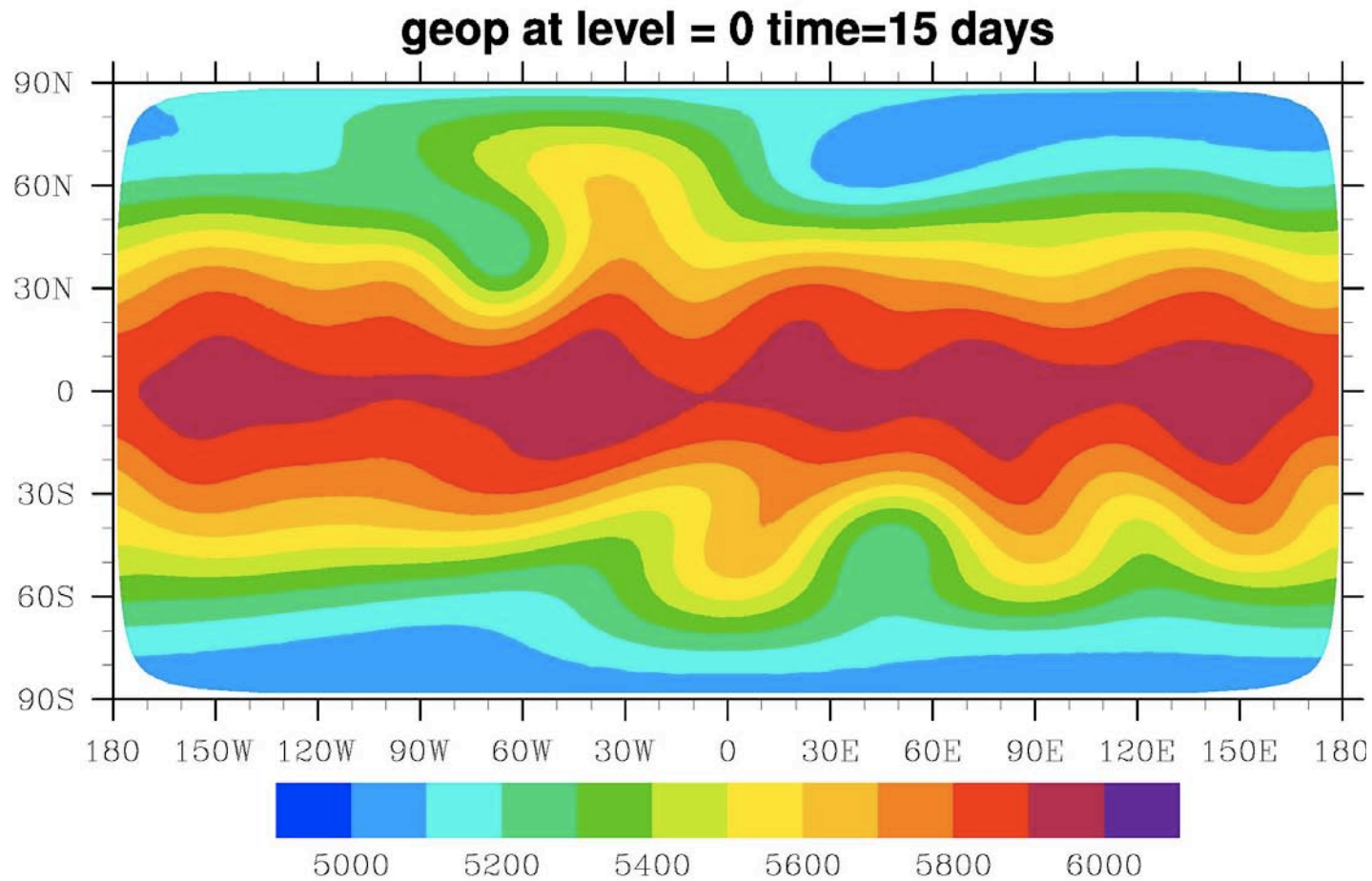
- Steady state, nonlinear zonal flow.
- Wind corresponds to solid body rotation
- Tests performance and treatment of nonlinearities
- #elements=216, NP=12 (~150km resolution)



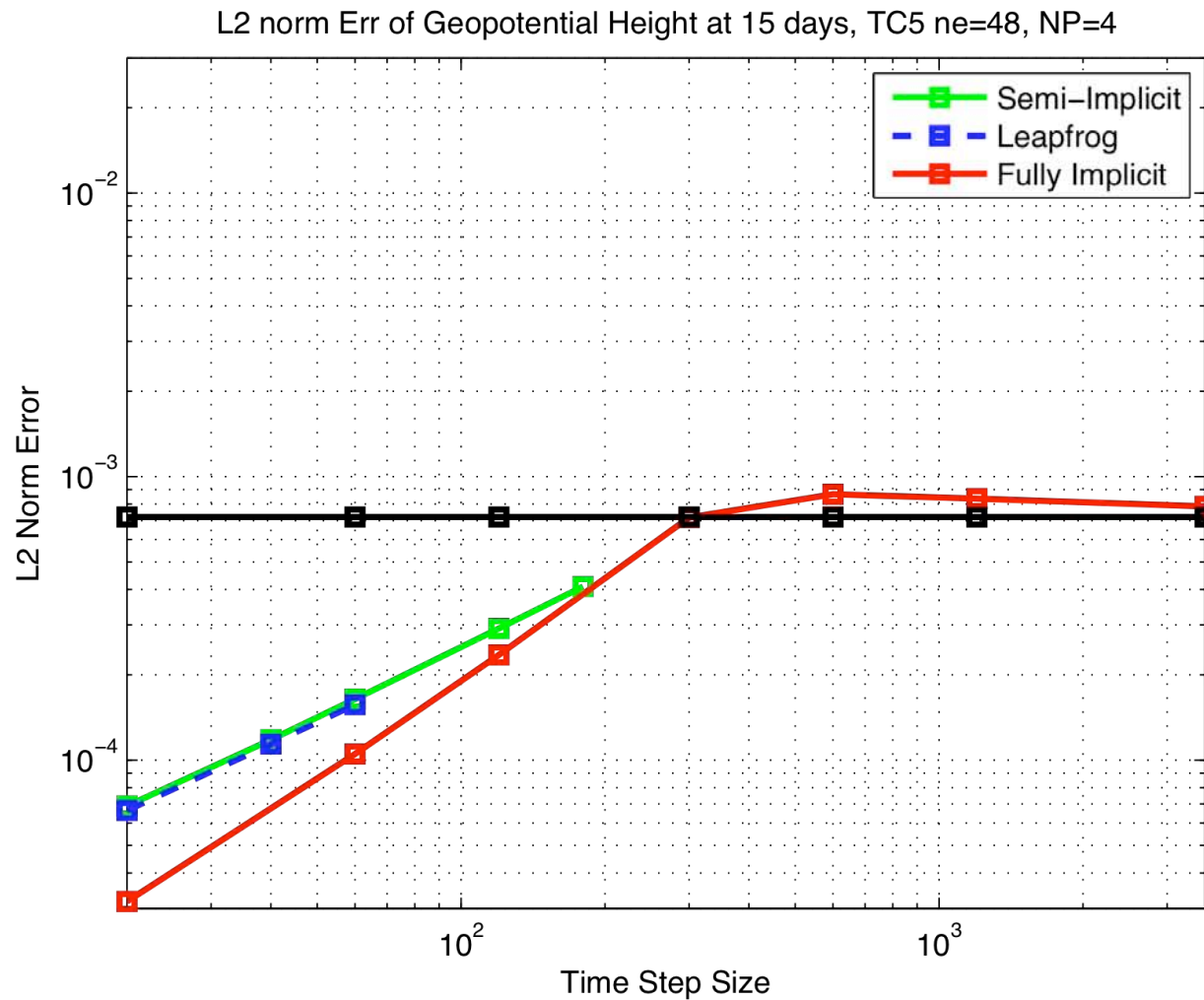
Time Integration Method	Time Step	Wall Clock (s)	L2 error
Leapfrog	100s	1m2s	6.0e-16
BDF2	86400s	8.3s	1.9e-15

The implicit configuration took 1 Newton iterations, 56 Krylov iterations for the one time step.

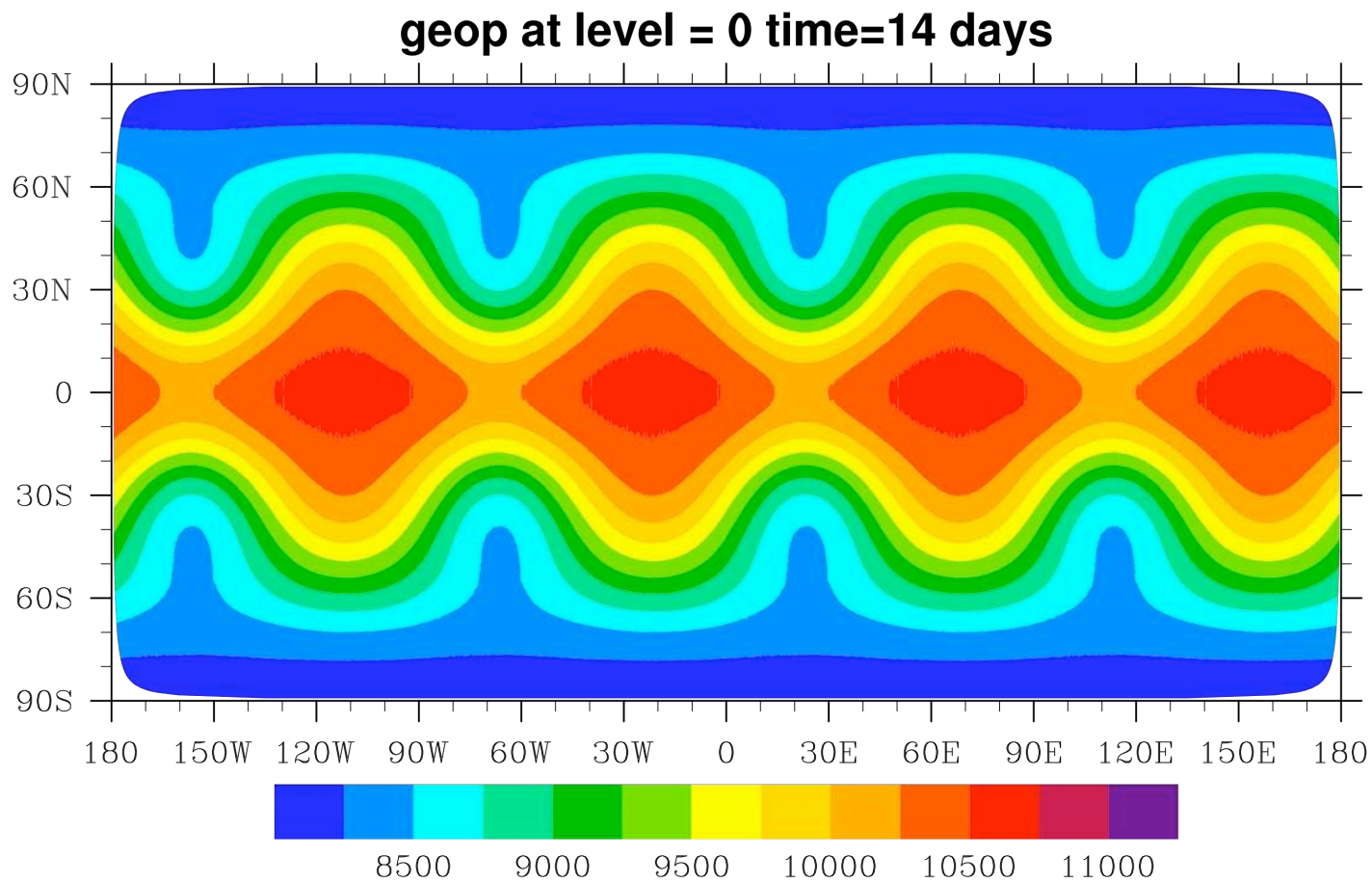
Test case 5: flow over a mountain feature



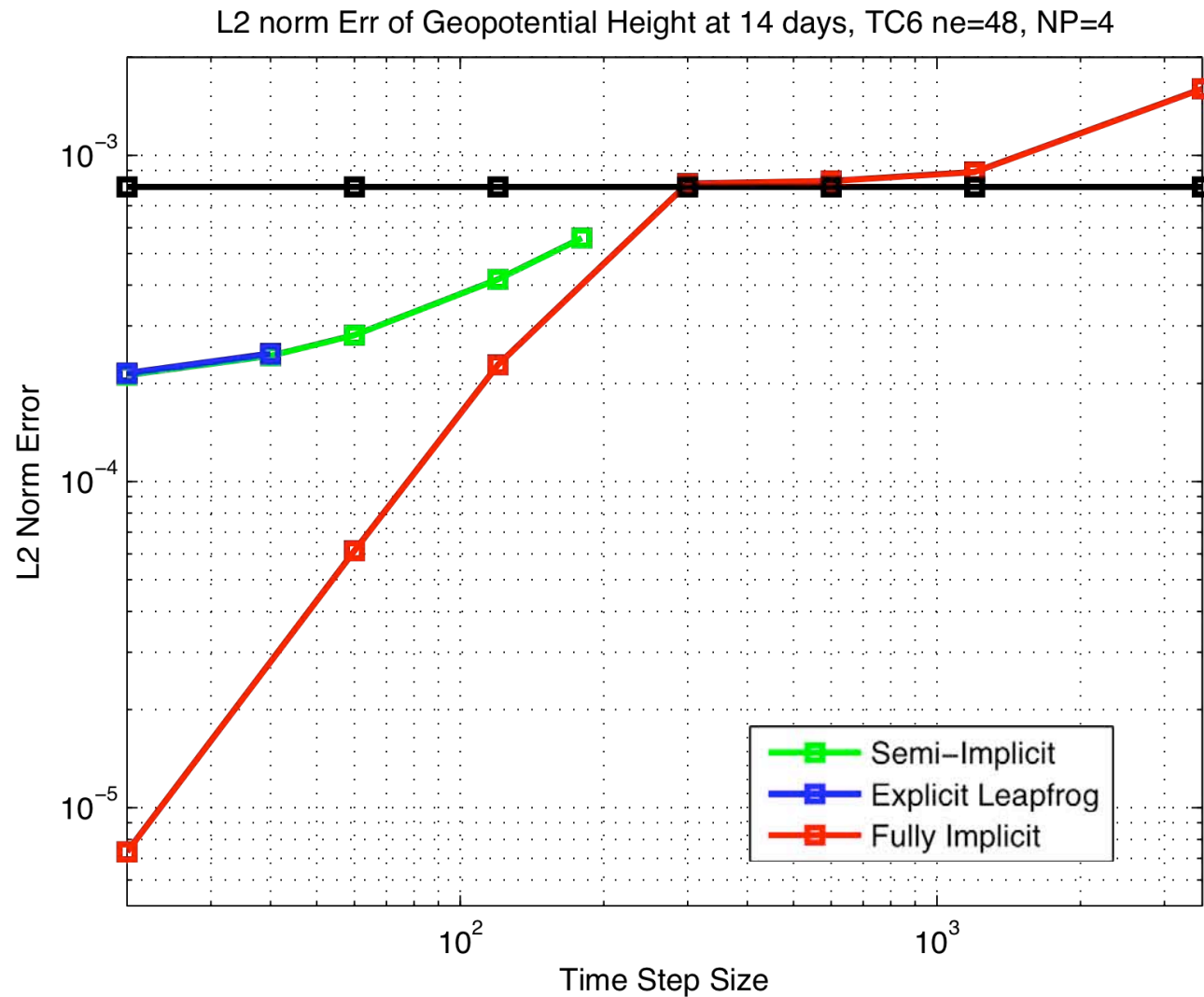
Test Case 5: Time integration method versus a small time step size benchmark



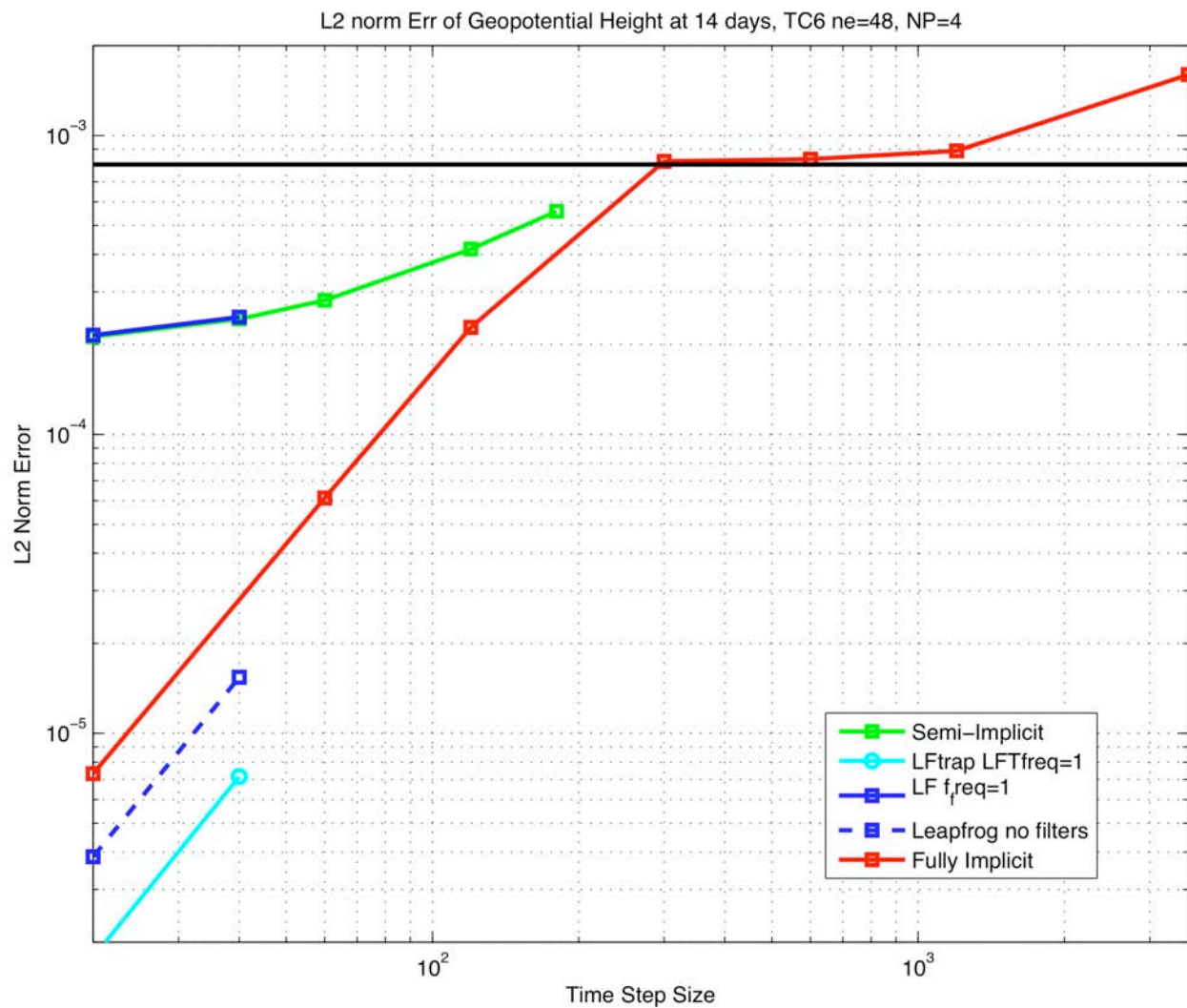
Test case 6:



Test Case 6: Time integration method versus a small time step size benchmark



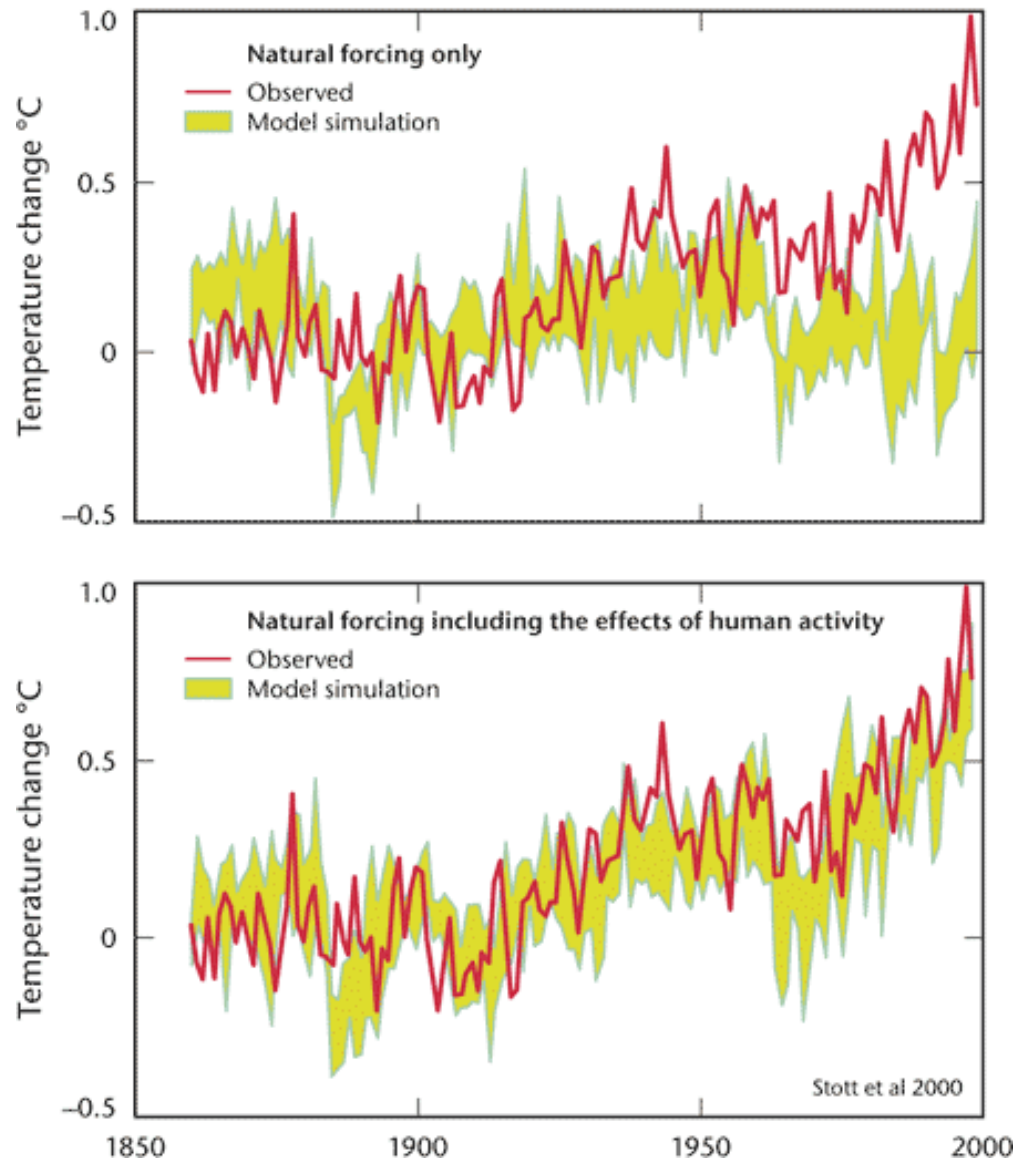
Test Case 6: Time integration method versus a small time step size benchmark



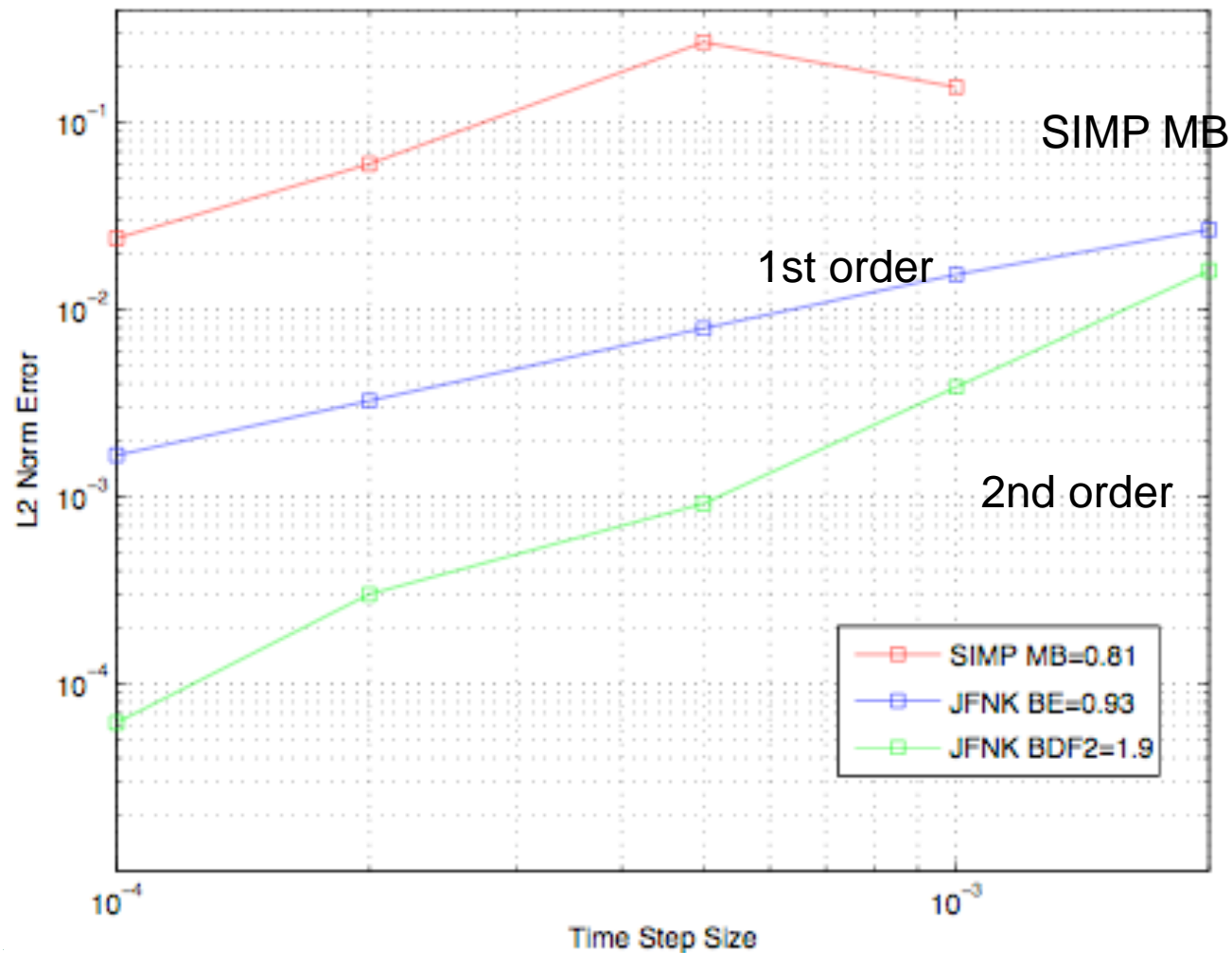
Analysis:

- **All the methods implemented in HOMME can improve upon the previously established limit of accuracy when the benchmark solution is temporally (and spatially) converged.**
- **The second order discretized methods with no time splitting or filters are second order accurate**
- **The implicit method is able to run 20x greater time step size than the gravity wave CFL and maintain accuracy at the diffusion limit. Test case 5 can be run at about 30x tss larger at the diffusion accuracy limit.**

Questions?



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



Inner linear Krylov loop (GMRES) produces an update for the Newton loop:

$$J_{\mathbf{v}} \simeq \frac{F(\mathbf{x} + \epsilon \mathbf{v}) - F(\mathbf{x})}{\epsilon}$$

JF designation: only $J_{\mathbf{v}}$ is used, and generated with a finite differencing approximation

With GMRES, storage grows with each iteration, so a quality preconditioner is crucial. Ideally we want the number GMRES iterations to be flat with increasing problem size.

Spectral Element Spatial Discretization

Spectral Transform Methods

Finite Element Methods

High order Accuracy

High convergence rate

Geometric flexibility

Minimal Communication

Best of both

- **Cubed sphere grid; each face is subdivided into square elements**
- **Variables within each element are approximated by polynomial expansions**
- **Communication only needed at element edges (Galerkin)**
- **Mesh refinement can occur via adding elements or increasing order of spectral degree**