

Energy-conserving numerics and consistency

1. What is the role for the 2nd law in the formulation of energy-consistent subgrid physics and physics-dynamics coupling?
2. Do we separate physics from dynamics for good reasons? Is it an obstacle to some "better approaches"? Conversely are there good arguments in favor of not separating?
3. Should all physics be written as PDEs? Would that exclude certain approaches to parameterizing certain processes (e.g. deep convection)?
4. What needs to be specified in order to clarify which energetics we are talking about?
→ Total energy, thermodynamic potentials, dissipation rates ...
5. Suppose we find a way to do everything right, and it is not affordable.
How do we minimize the errors induced by inevitable compromises? Monitor errors?
6. What to expect / demand in terms of accuracy / convergence?
7. What approaches could we learn from other fields?

5. Correctness vs. Cost

Correctness

- Have we split the problem correctly?
- Correctly solving the mathematical problem?

Accuracy:

- Is higher-order worth it?
- Is implicit worth it?

Feasibility:

- Efficient calculation (time, resources)?
- “Grey zone” confidence?

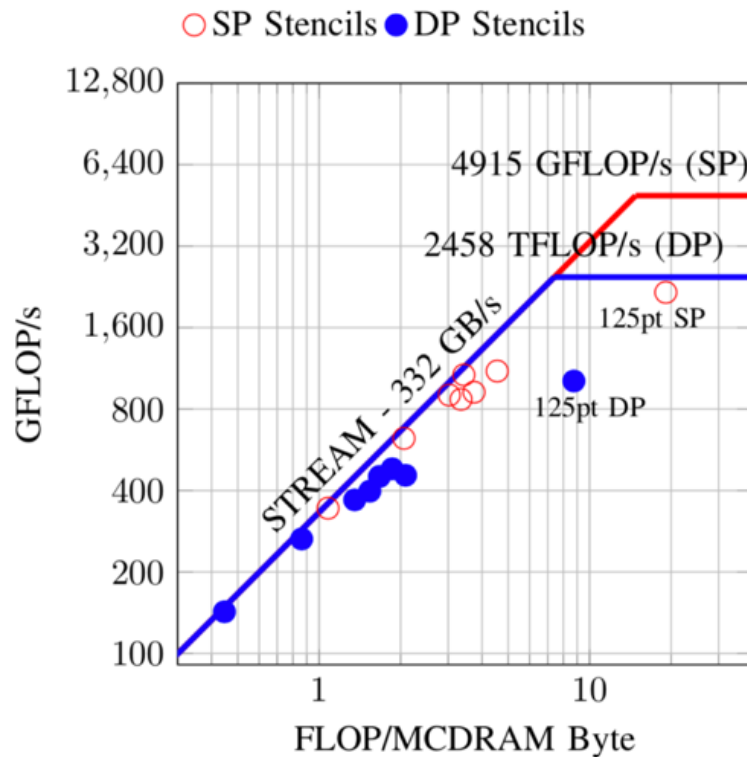
Current state-of-the-art:

- Non-hydrostatic with good asymptotics?
- Conservation, energy, entropy?

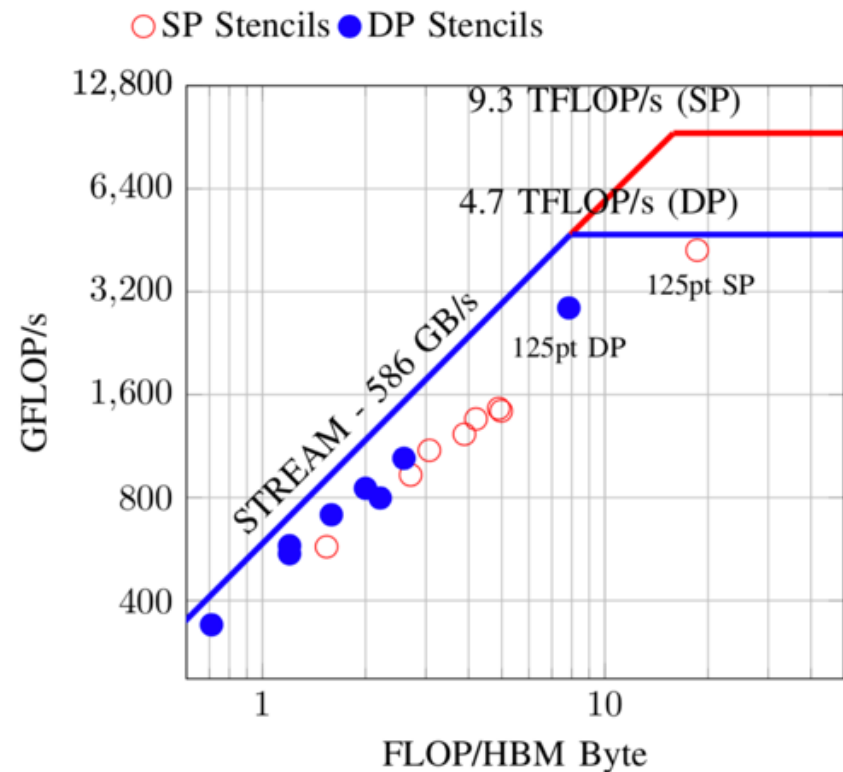
- Higher-order HEVI schemes?
- Numerical convergence in space/time?

- AMR + block-structured efficiency?
- More rigorous tests?

Block-structured stencils, “brick” code-generation



Intel KNL 7250



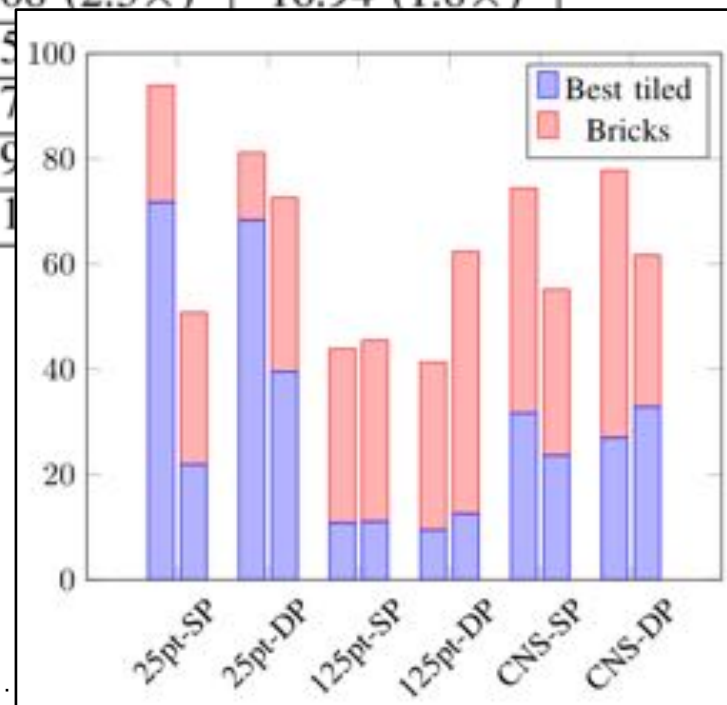
NVIDIA P100

Bricks can be faster for higher-order, coupled stencils

| Name | Brick GStencil/s & Speedup | | | |
|-------|----------------------------|--------------|--------------|--------------|
| | KNL SP | KNL DP | P100 SP | P100 DP |
| 7pt | 26.46 (0.9×) | 10.96 (0.7×) | 41.04 (1.4×) | 24.25 (1.1×) |
| 13pt | 24.93 (1.0×) | 10.59 (0.8×) | 35.79 (1.8×) | 21.06 (1.4×) |
| 19pt | 24.35 (1.2×) | 9.98 (0.9×) | 32.18 (2.1×) | 18.84 (1.7×) |
| 25pt | 21.83 (1.3×) | 9.20 (1.2×) | 29.08 (2.3×) | 16.94 (1.8×) |
| 27pt | 20.84 (1.0×) | 8.59 (0.9×) | 26.5 | |
| 125pt | 8.67 (4.1×) | 4.08 (4.4×) | 16.7 | |
| iso | 14.24 (1.1×) | 6.52 (1.0×) | 19.9 | |
| CNS | 1.98 (2.3×) | 1.03 (2.9×) | 3.1 | |

Speed-up depends on a lot of factors:

- Aggressive 6D tiling w/ auto-tuning baseline
- Very low HBM (& L1) data movement compared to tiling larger array sizes
- Greatly reduces # of streams, cache misses



↑ Higher is better

Nonlinear column solves use batched

Column solvers are an issue

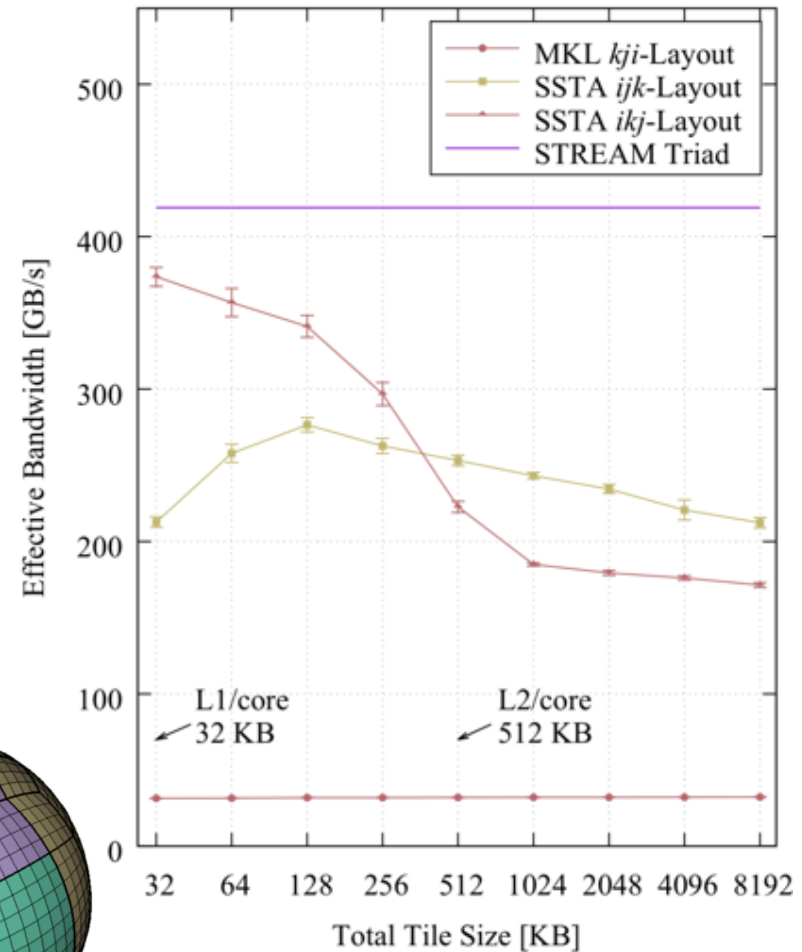
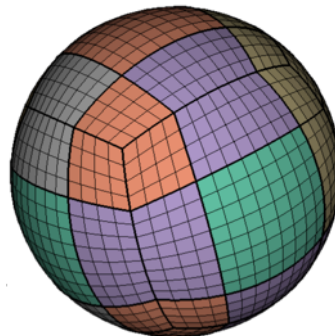
- Non-linear for numerical accuracy, asymptotics
- Typically 1-3 iterations
- k-major or i-major?

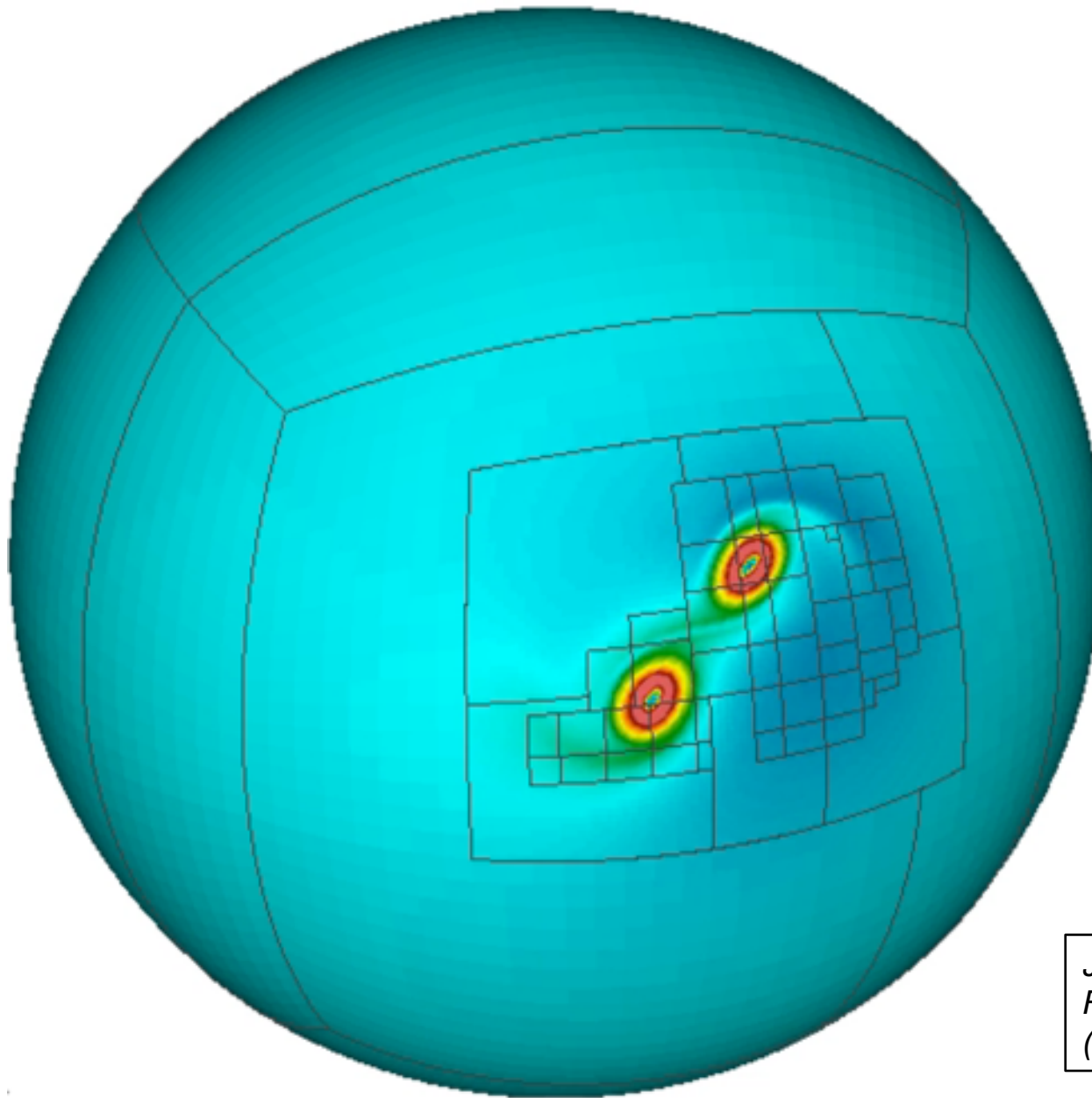
Banded solvers are bw-bound

- Despite lots of flops, also requires same order of data
- Fast divides/reciprocal on KNL mean memory bw-bound
- Even batched MKL library calls have overhead, generalities

Porting to GPU and MPI optimizations in progress

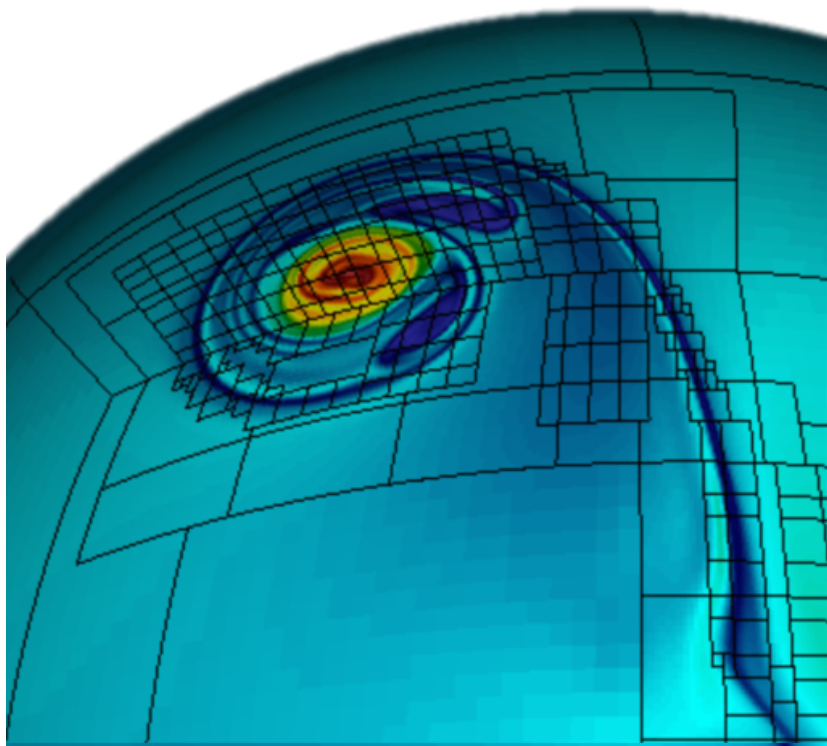
...



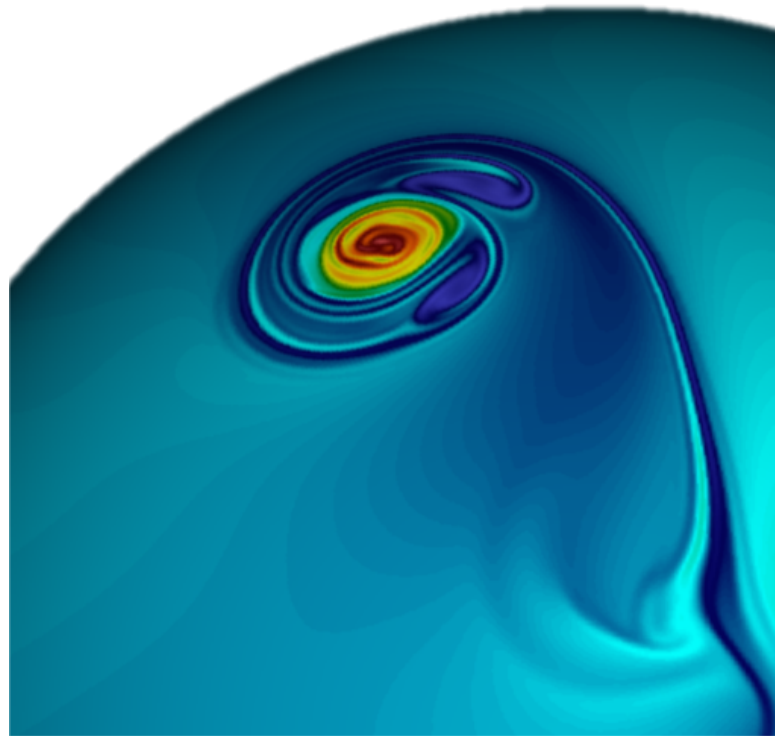


*Joint work with
Ferguson, Jablonowski
(U. Michigan)*

Example: Vorticity dynamics, AMR vs. uniform



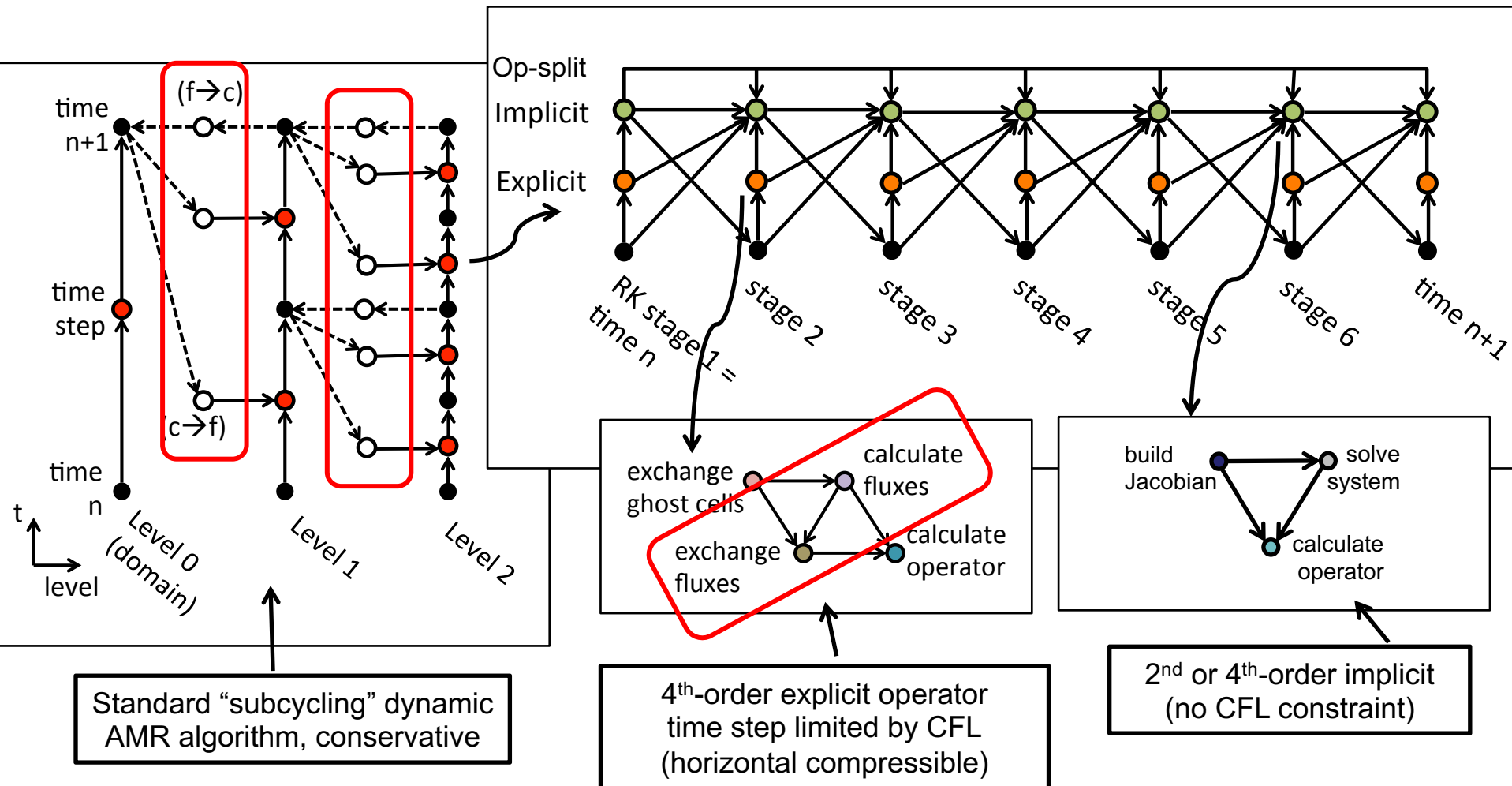
3x AMR C1024



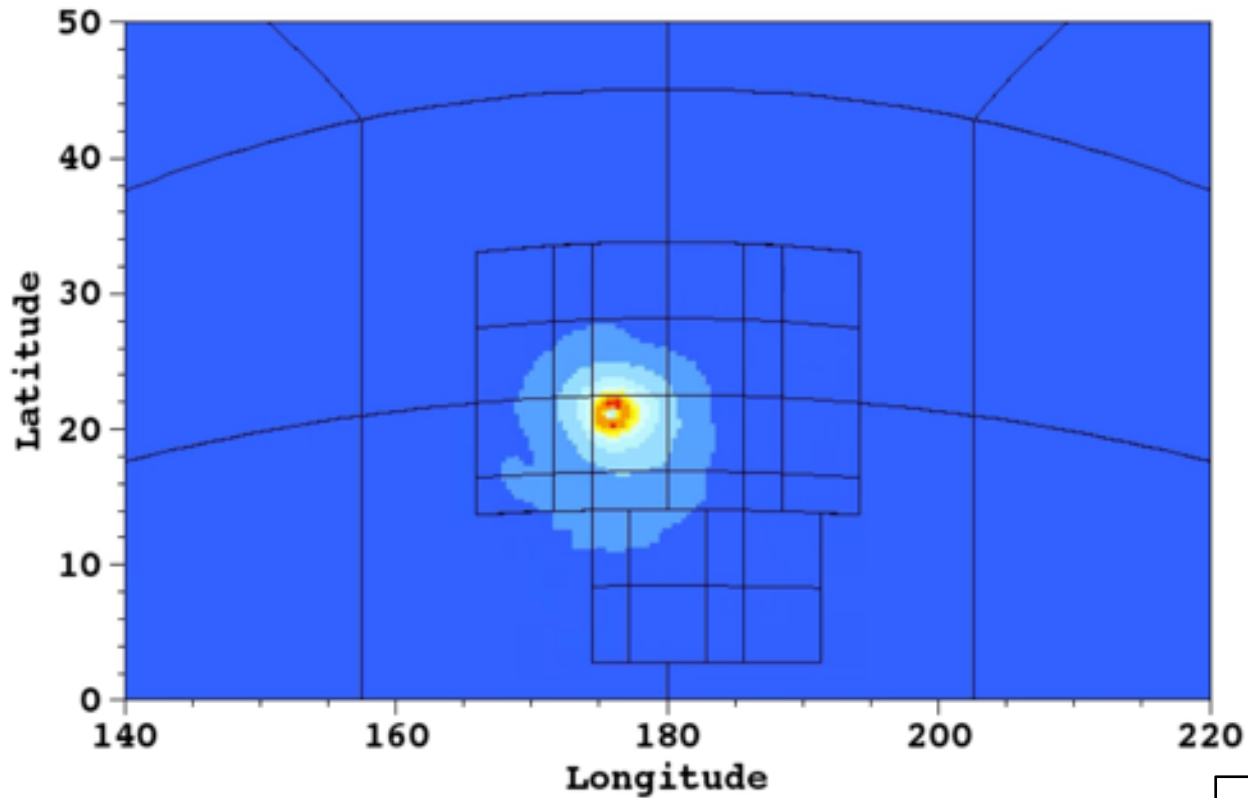
Uniform C1024

*Joint work with
Ferguson, Jablonowski
(U. Michigan)*

AMR time stepping: RK ImEx, but also SDC, R-W, QSS, ...



3D AMR: Idealized Tropical Cyclone



c64/c256 (~160/40 km)

Joint work with
Ferguson, Jablonowski
(U. Michigan)

AMR Time accuracy across refinement boundaries?

- AMR in “grey zone:” hydrostatic ($> 20\text{km}$, large aspect ratios) vs. non-hydrostatic ($< 10\text{ km}$)?
- Aspect ratios depend on horizontal resolution, orography, kinked/stretched vertical mappings
- Implicit solver should asymptote to Richardson’s eqn / hydrostatic vertical velocity

$$\frac{\partial p^H}{\partial t} = w\rho g - g \int_r^\infty \nabla^\perp \cdot (\rho \mathbf{u}^\perp) dr'$$

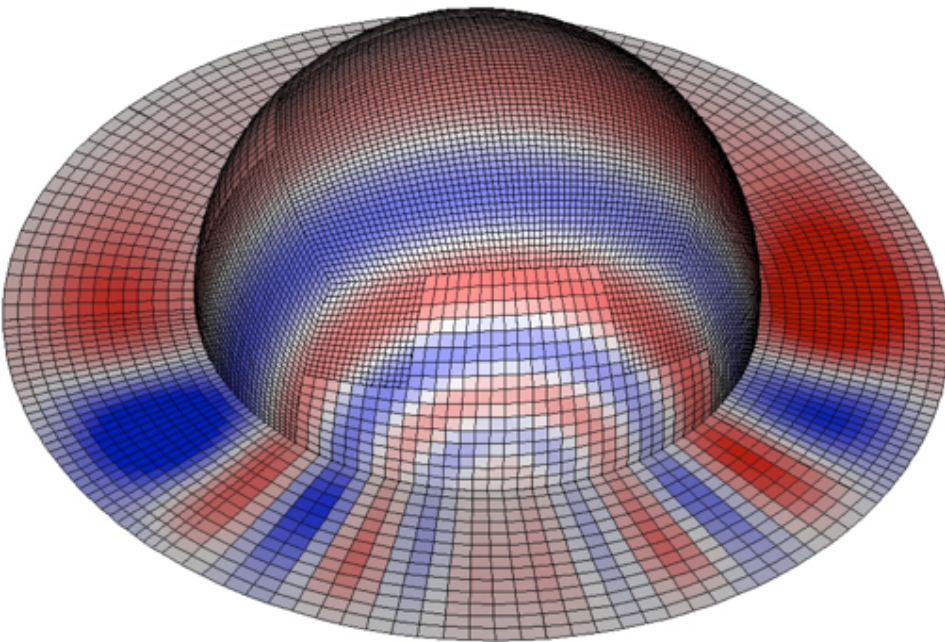
$$\frac{\partial w}{\partial t} + \frac{1}{\rho} \frac{\partial \pi}{\partial r} = -\mathbf{u}^\perp \cdot \nabla^\perp w - w \frac{\partial w}{\partial r},$$

$$\frac{\partial \pi}{\partial t} + \rho c^2 \frac{\partial w}{\partial r} = g \int_r^\infty \nabla^\perp \cdot (\rho \mathbf{u}^\perp) dr' - \rho c^2 \nabla^\perp \cdot \mathbf{u}^\perp - \mathbf{u}^\perp \cdot \nabla^\perp p^H - \mathbf{u} \cdot \nabla \pi$$

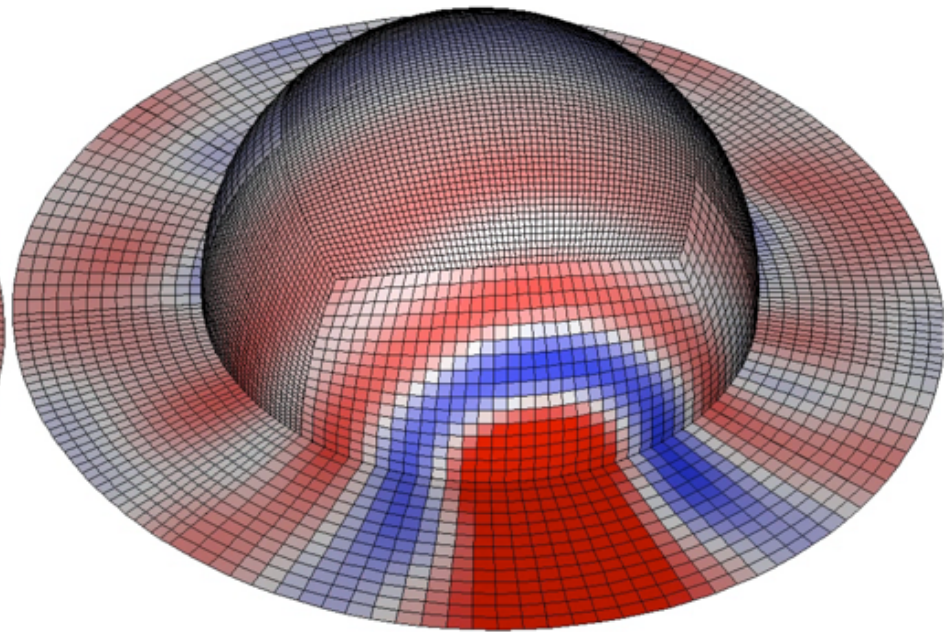
$$\Rightarrow \rho c^2 \frac{\partial w}{\partial r} = g \int_r^\infty \nabla^\perp \cdot (\rho \mathbf{u}^\perp) dr' - \rho c^2 \nabla^\perp \cdot \mathbf{u}^\perp - \mathbf{u}^\perp \cdot \nabla^\perp p^H$$

Nonhydrostatic Gravity vs. Acoustic Waves

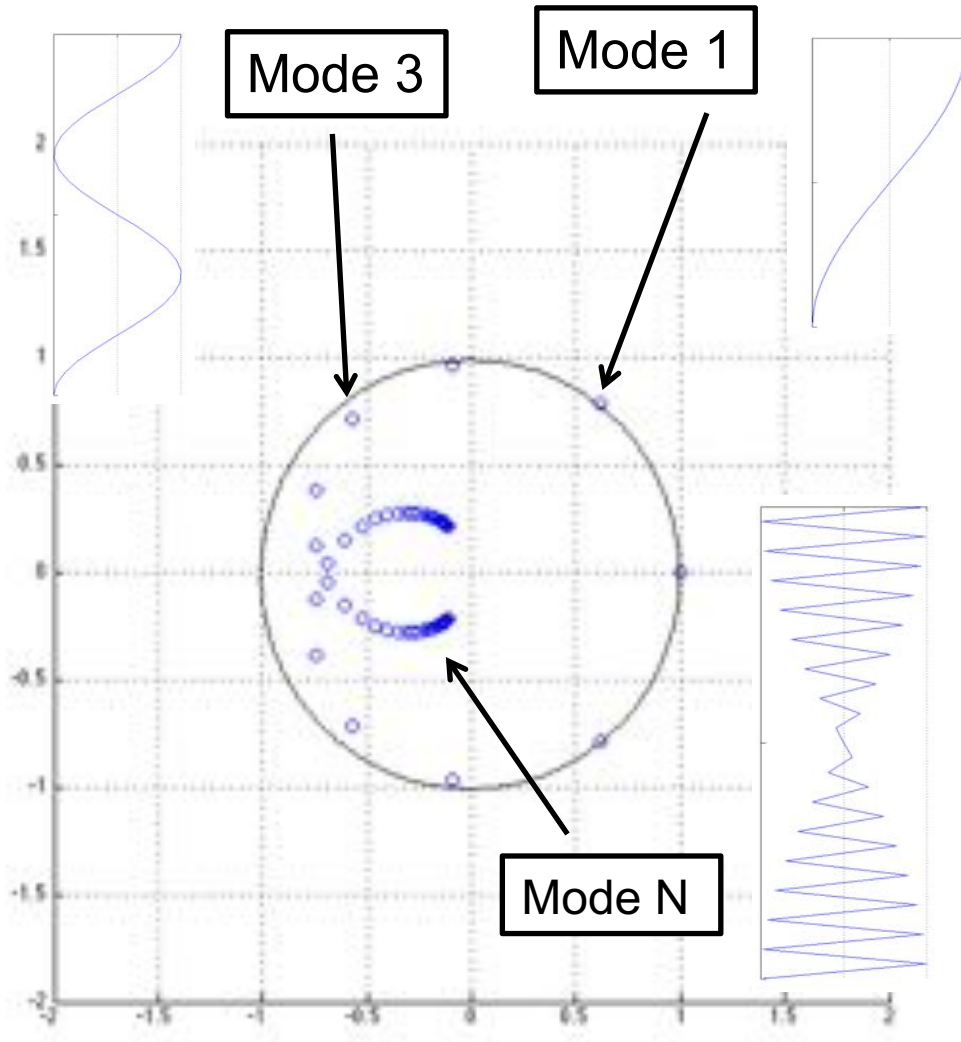
Potential temperature



Pressure perturbation

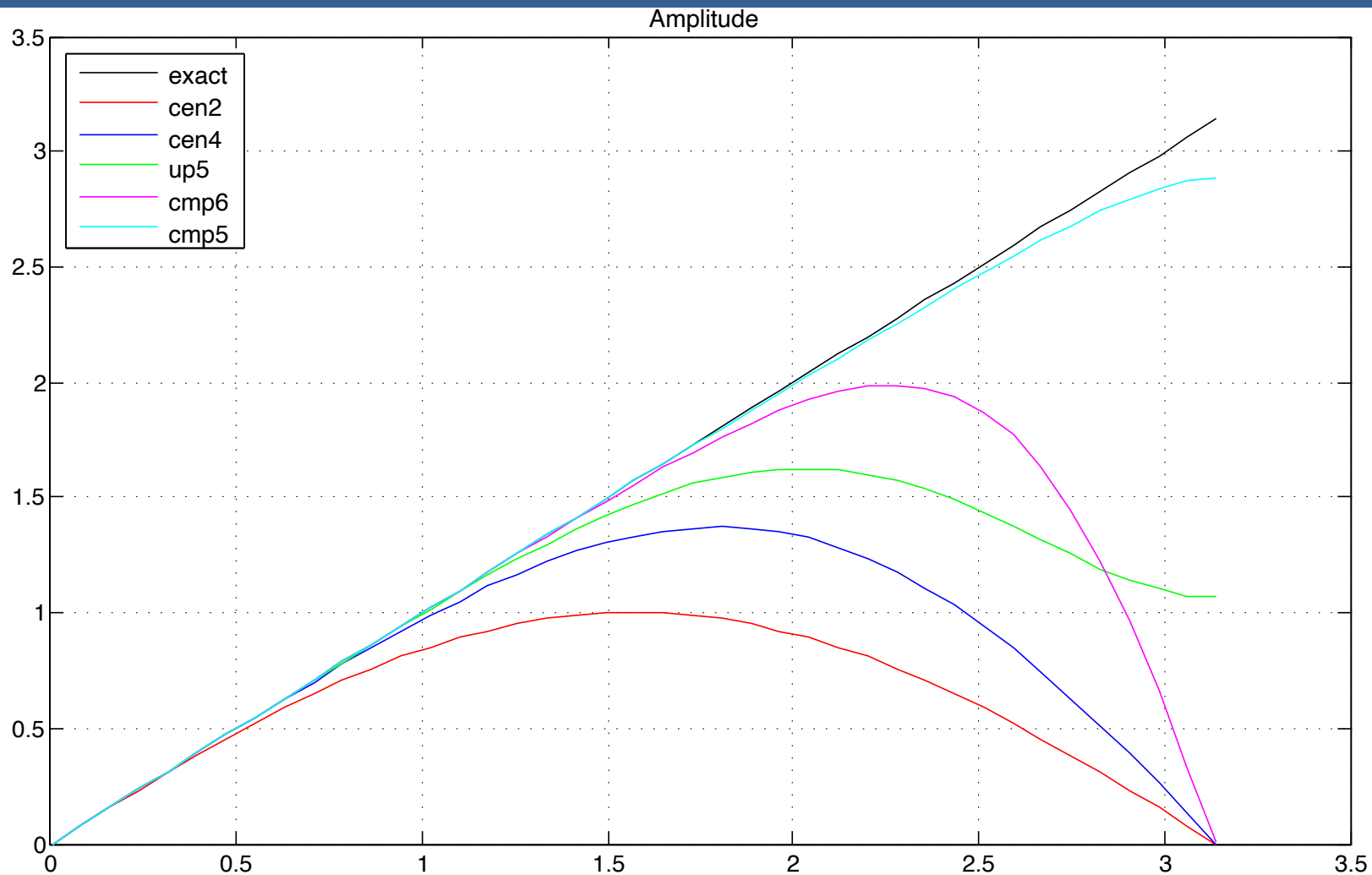


Vertical AMR Challenges

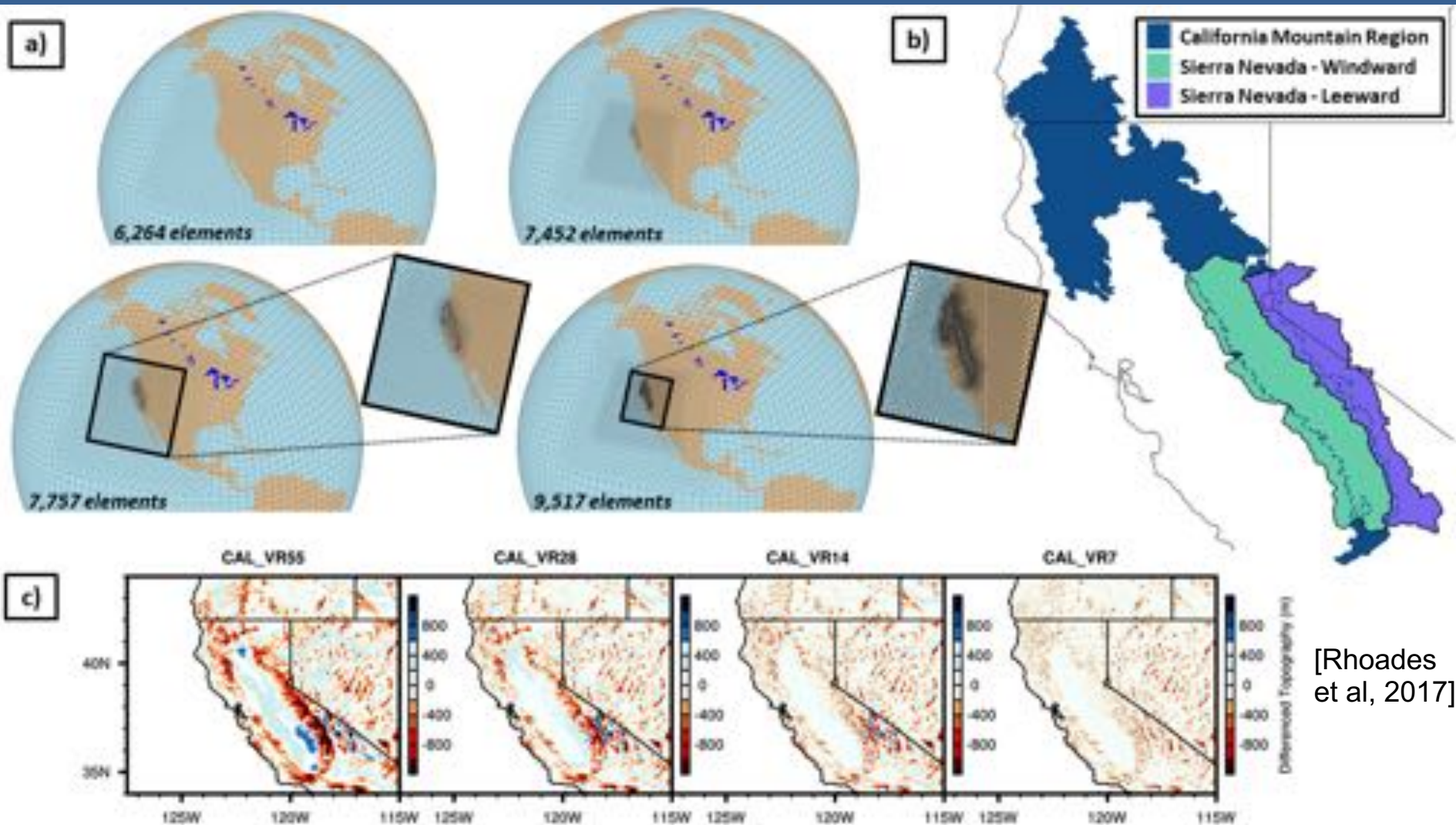


- Coupling implicit wave equation, “volume discrepancy,” and physics
→ *as in complex combustion codes*
- At coarse resolutions, system only good for 1-2 modes at 10x CFL
- Fast modes damp rapidly, but oscillate
→ Very under-resolved, phase error flips signs every solve
- Kinked vertical mappings exacerbate with eigenmode shapes
- AMR complications – space-time convergence vs. vertical refinement?

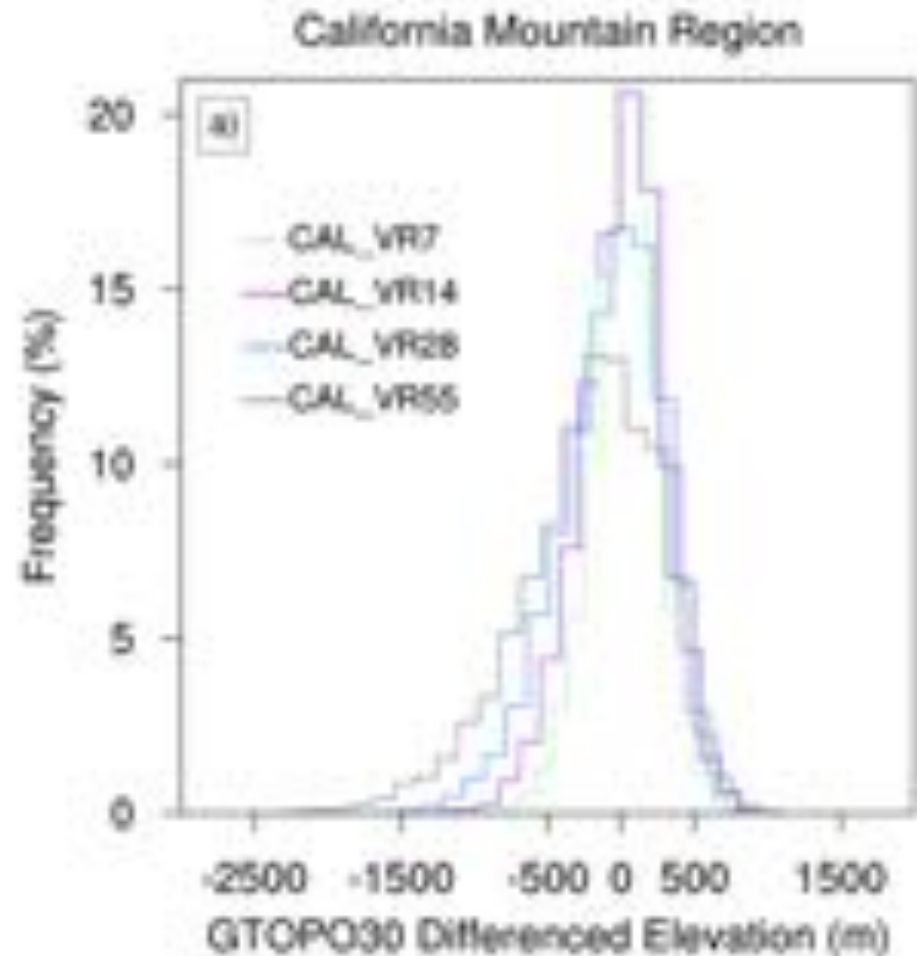
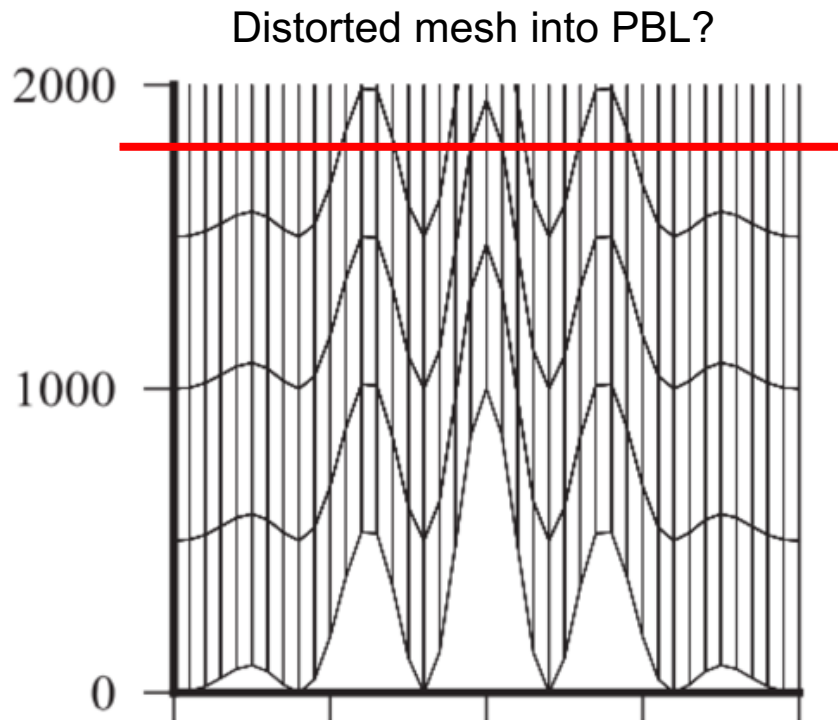
Space-time accuracy, spectral resolution matters



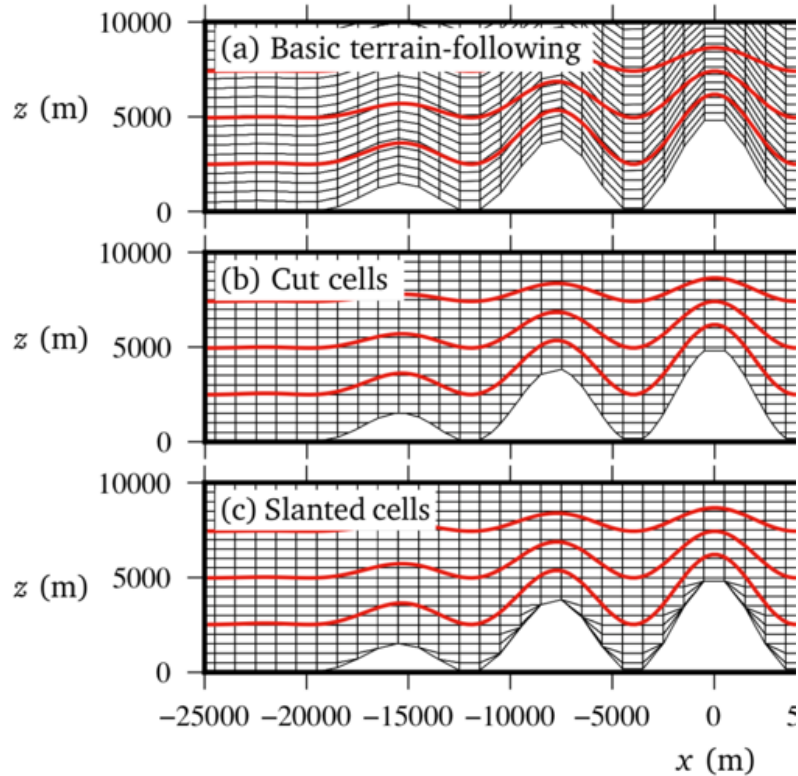
Global simulations at coarse resolutions?



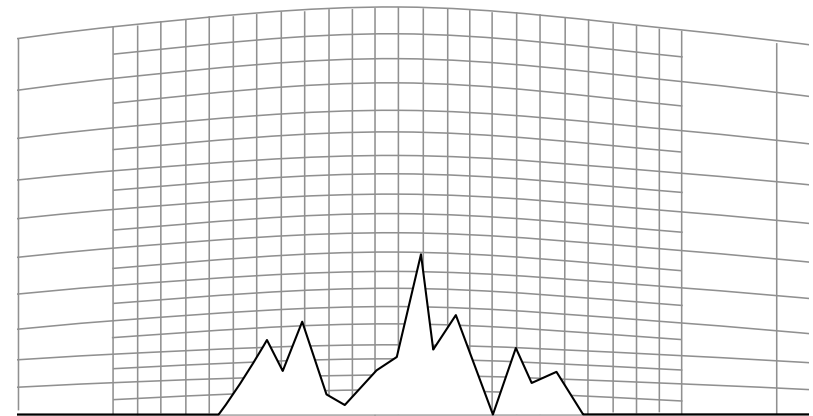
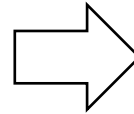
Complex orography \leftrightarrow non-smooth mappings?



Complex orography with cut cells, smooth mappings?

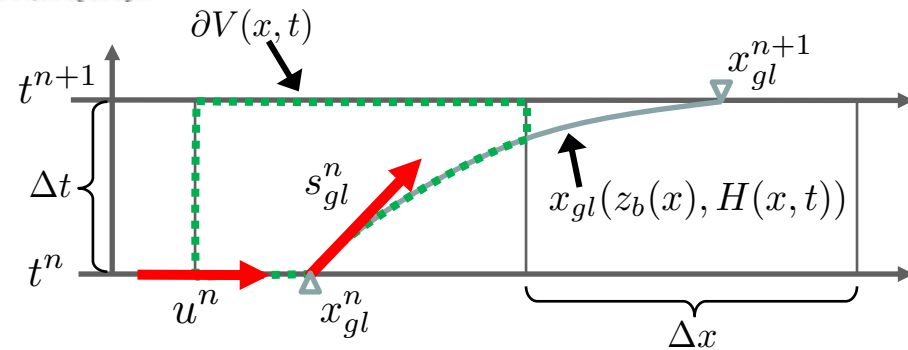
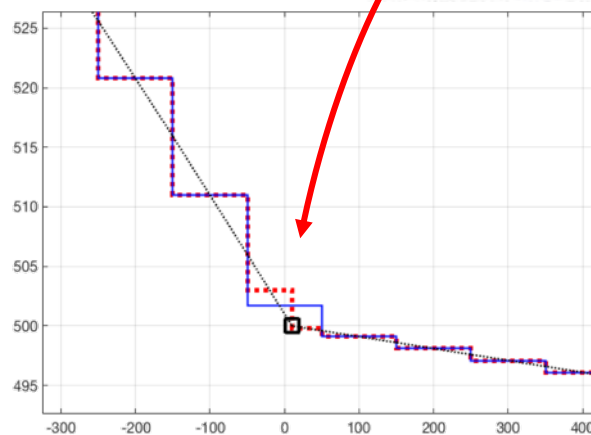
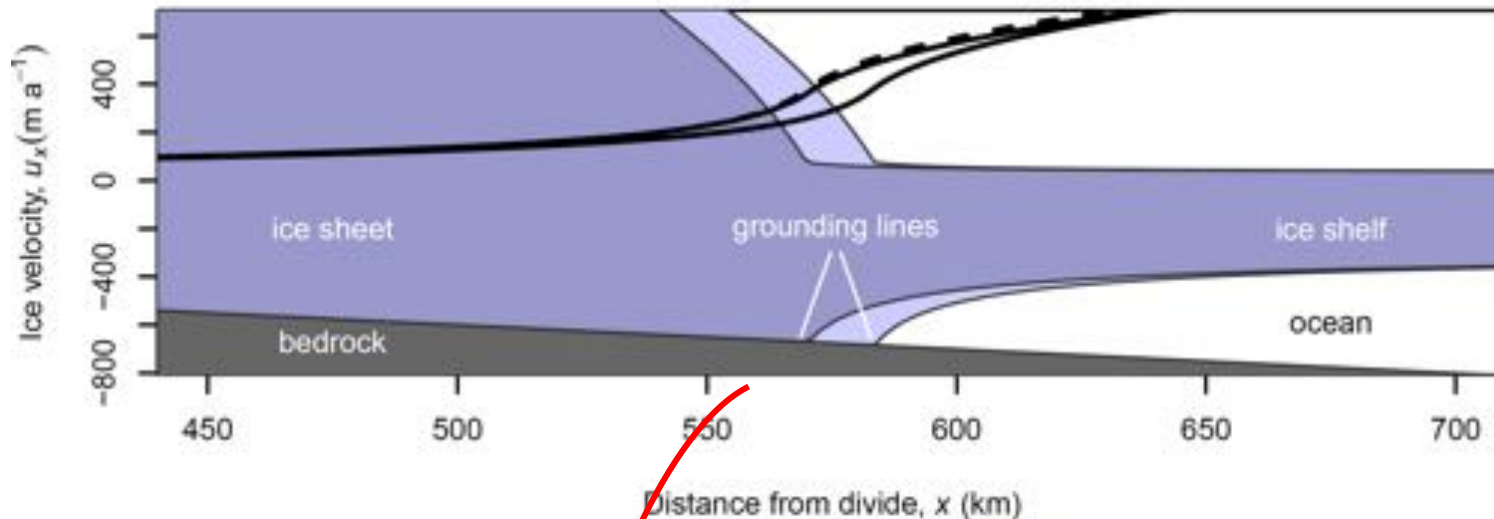


[Shaw, Weller 2016]



AMR + cut cells have the potential to correctly represent topography at all resolutions, *without* smoothing terrain or distorting mapping.

Example: Grounding line as a Multifluid Interface



Energy-conserving numerics and consistency

1. What is the role for the 2nd law in the formulation of energy-consistent subgrid physics and physics-dynamics coupling?
2. Do we separate physics from dynamics for good reasons? Is it an obstacle to some "better approaches"? Conversely are there good arguments in favor of not separating?
3. Should all physics be written as PDEs? Would that exclude certain approaches to parameterizing certain processes (e.g. deep convection)?
4. What needs to be specified in order to clarify which energetics we are talking about?
→ Total energy, thermodynamic potentials, dissipation rates ...
5. Suppose we find a way to do everything right, and it is not affordable.
How do we minimize the errors induced by inevitable compromises? Monitor errors?
6. What to expect / demand in terms of accuracy / convergence?
7. What approaches could we learn from other fields?