Development and Implementation of Software Elements using State-of-the-Art Computational Methodology to Advance Modeling Heterogeneities and Mixing in Earth's Mantle

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CIG COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

1. GEOPHYSICAL MOTIVATION

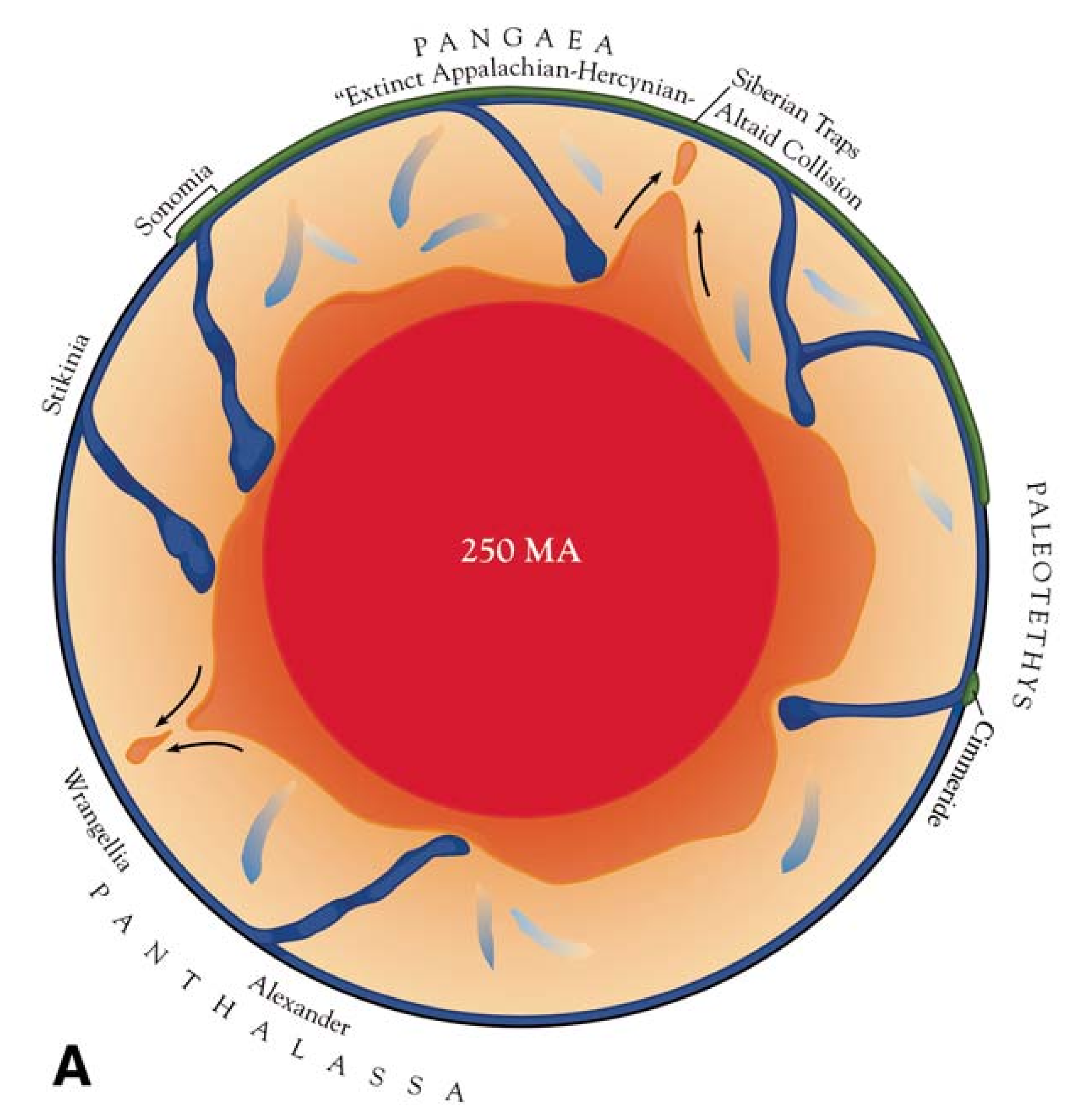


Figure 1: Schematic cross section of the Earth 250 MA (million years ago). Irregular zig-zag profile (or sector) through the Earth shows continental crust (green), oceanic crust (black), lithospheric plates (blue), lower mantle (yellow), hot abyssal layer (light orange), and core (red). Light-blue streaks are schematic representations of remnant slabs in lower mantle. Our Scientific Software Elements (SSEs) are enabling geodynamicists to make more accurate and efficient computations of the evolution of the structure of this and many other significant geodynamic processes that occur in the Earth's mantle.

2. THE NEED FOR IMPROVED NUMERICS

- **ONE EXAMPLE:** In many numerical methods for transporting or *advecting* a quantity in a fluid flow, the quantity may exceed its natural bounds. For example, it is unphysical for the density ρ or the viscosity ν to be less than zero. Yet, without some ad hoc workaround, this was known to occur in all of the codes designed to model processes in the Earth's mantle.

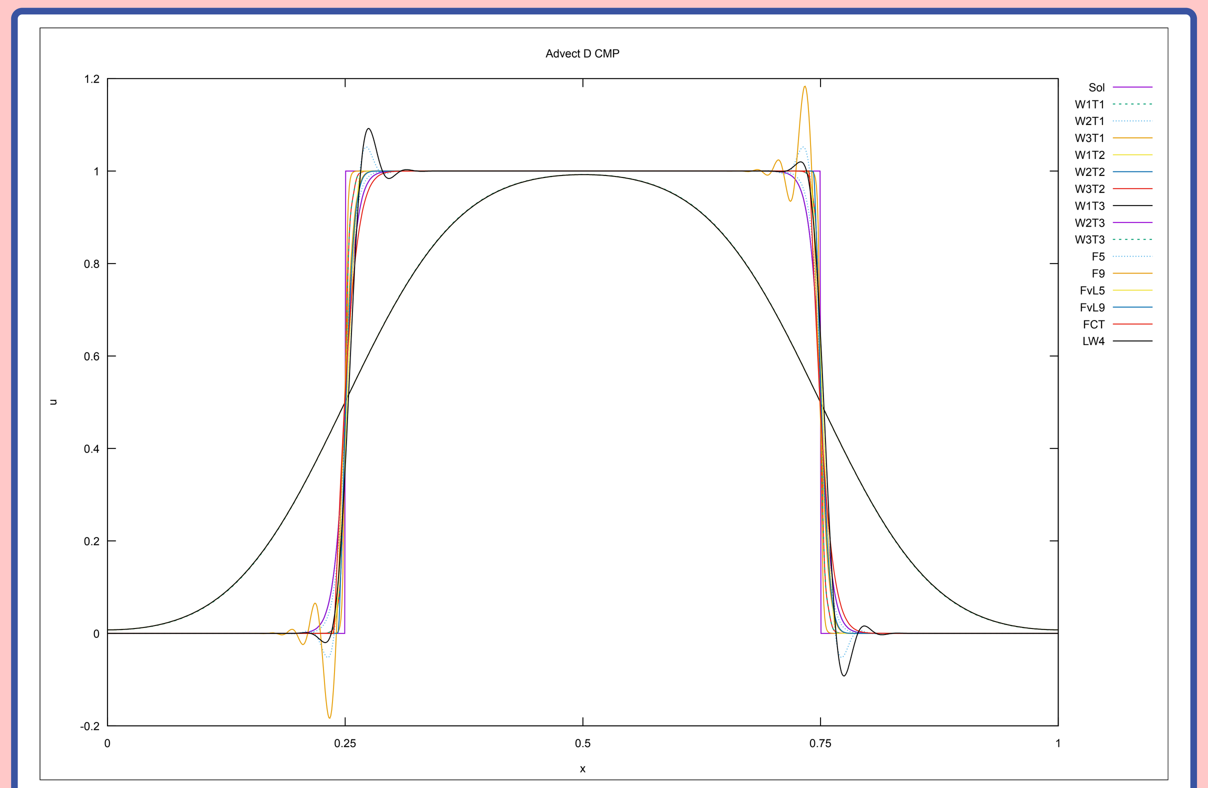


Figure 2: Square wave $S(x)$ advecting right at constant velocity. Godunov's Theorem states overshoot / undershoot will occur for *all* high-order (i.e., ≥ 2) *linear* methods. *Nonlinear* high-order methods with limiters preserve the correct bounds $0 \leq S(x) \leq 1$.

3. NEW METHODOLOGY - SSEs

- (1) Volume-of-Fluid (VOF) Interface Tracking, (2) Bound Preserving Discontinuous Galerkin methods (DG-BP) & (3) Active tracer particles
- SSEs (1) and (2) have never been used in this field
- All use Adaptive Mesh Refinement (AMR) & have excellent parallel scaling

4. VAN KEKEN PROBLEM

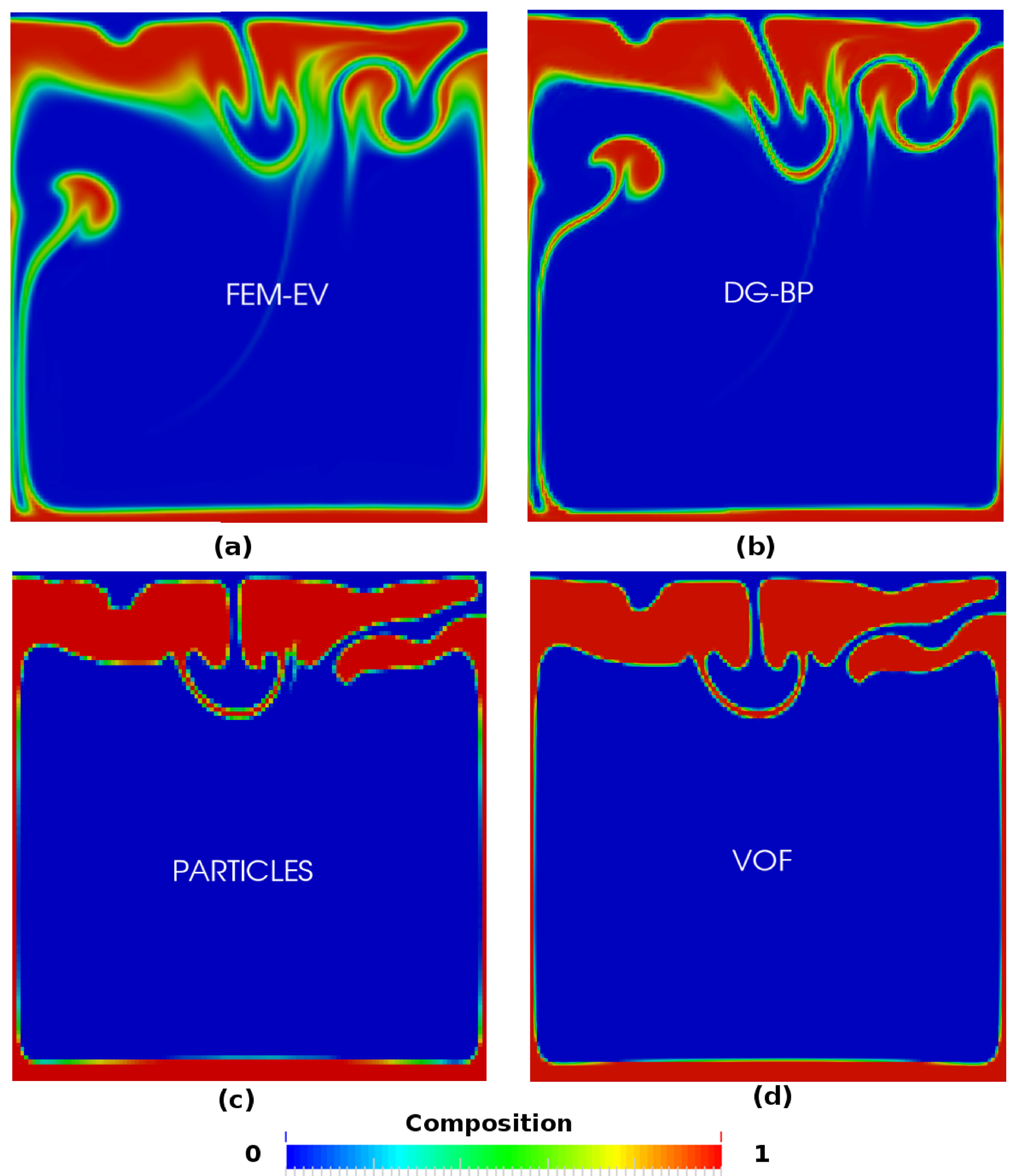
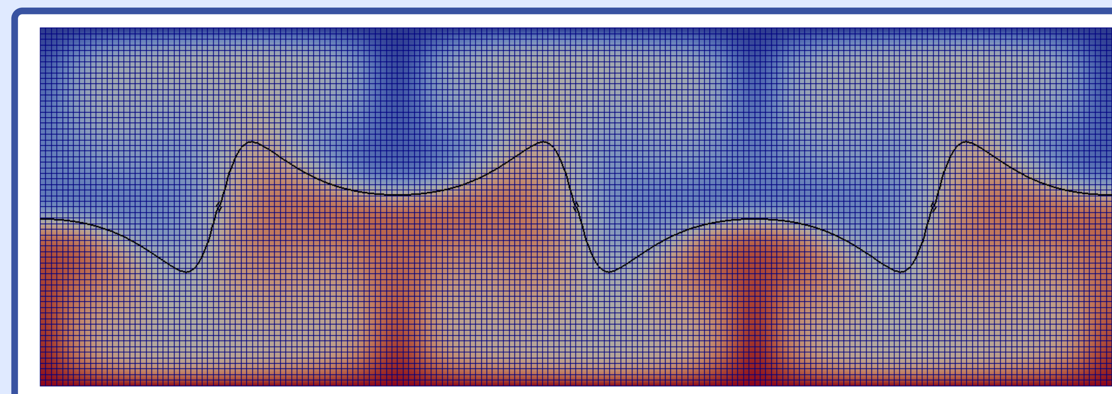
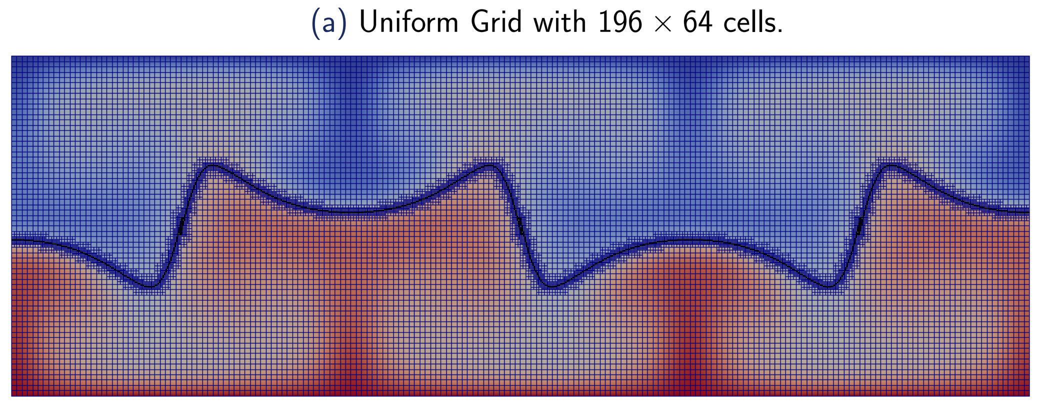


Figure 3: The van Keken problem is a standard test problem in computational mantle convection The problem is unstable, as are many problems in the Earth's deep interior. Hence, different numerical methods can cause large changes in the final solution

5. VOF INTERFACE TRACKING & AMR



(a) Uniform Grid with 196 × 64 cells.

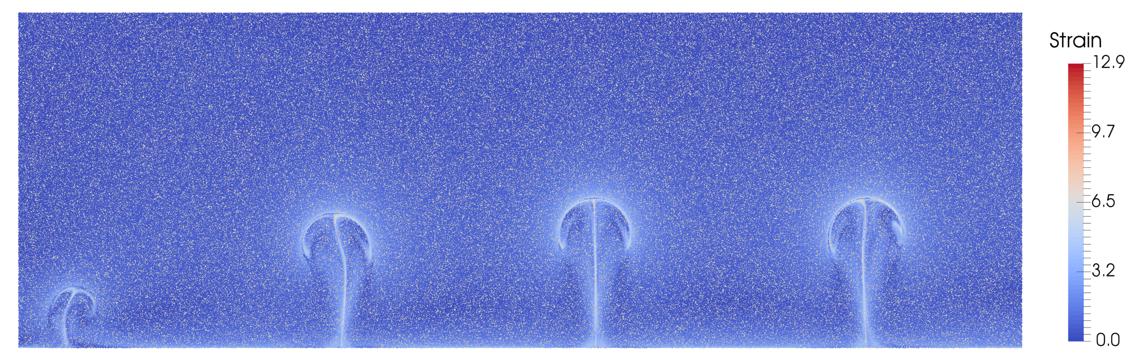


(b) Two additional levels of AMR on the interface *only*

Figure 4: Computations of an idealized model of the interface between the lower mantle and the hot abyssal (primordial) layer shown in Figure 1

6. UTILITY OF PARTICLE METHODS

- Particles facilitate history dependent material properties; e.g., strain
- More accurate than compositional fields



7. 3D PARTICLE MODEL OF SUBDUCTION

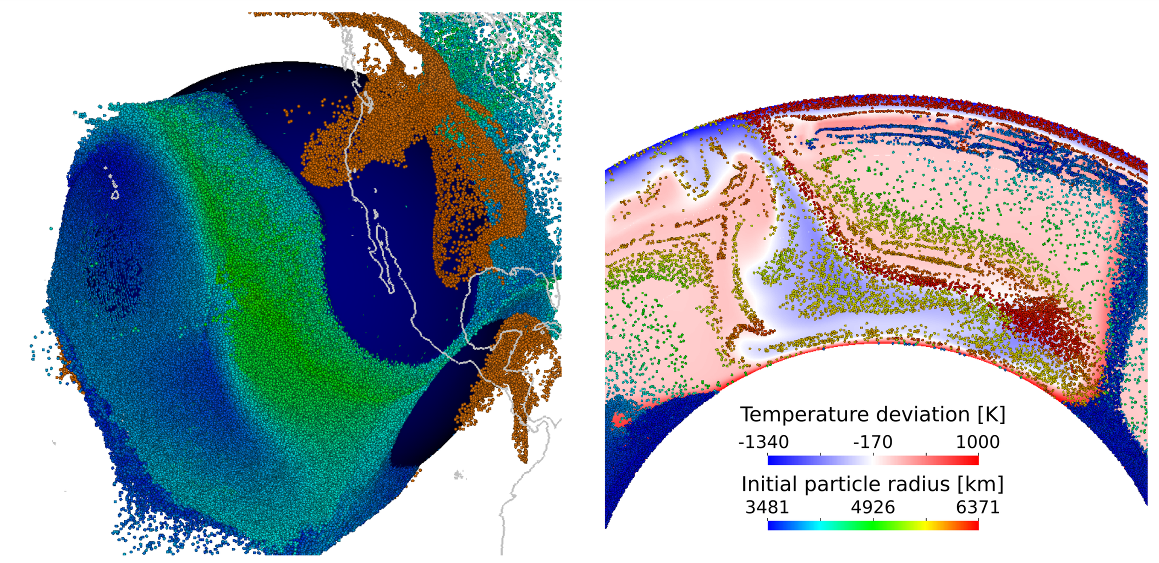


Figure 5: 3D mantle convection computation with particles. Left: Subducting plates below the Western U.S.; Brown particles push material at the core-mantle boundary (CMB) (dark blue sphere) towards the west. Only some of these particles are shown, each colored by the distance from its initial position (blue: small; green: large). Right: Vertical slice through the subduction zone. Particles close to the slice are shown, colored by the radius of their initial position (red: surface; blue: CMB).

8. LOAD BALANCING AMR vs PARTICLES

- On a uniform mesh particles exhibit excellent weak and strong scaling
- MPI transfer is handled as non-blocking point-to-point communication
- Sorting and advecting the particles is the main computational cost

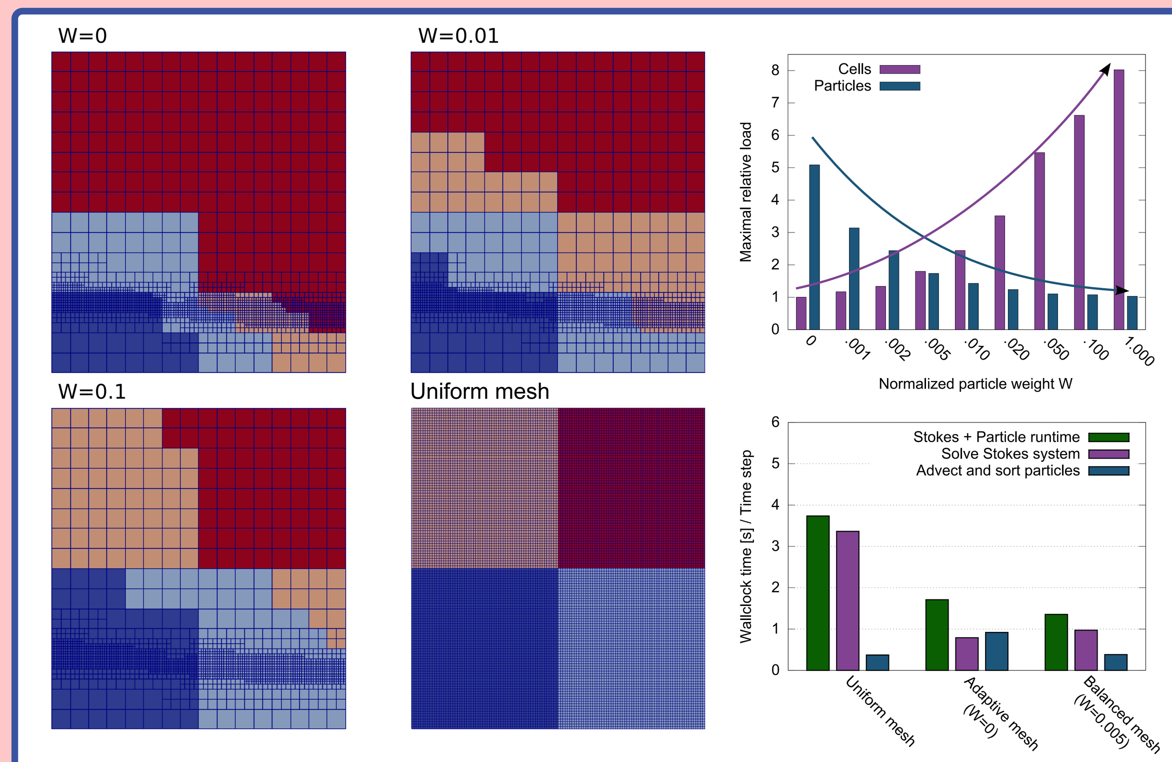
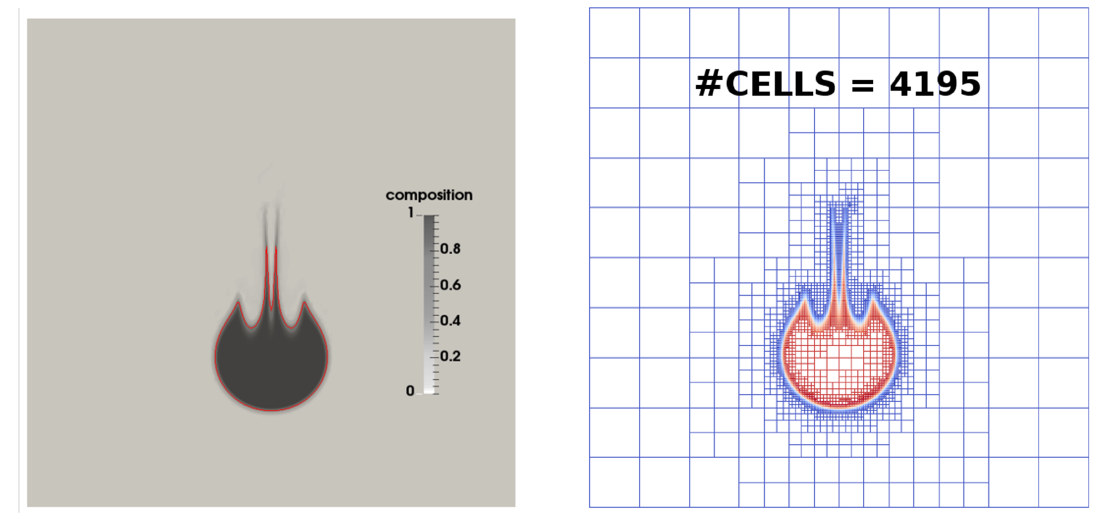


Figure 6: AMR reduces the time spent for the FEM solve and sorting particles, but it increases the overall particle cost due to a load imbalance (lower RH corner).

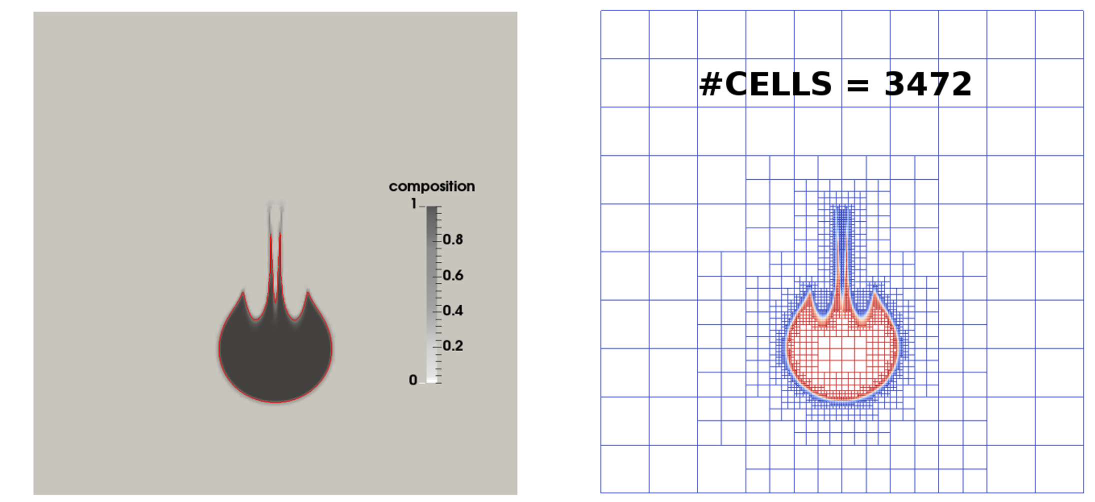
- Idea: Introduce weight W so weighted sum of cells and particles is balanced
- Increased balancing of particles decreases balancing of cells
- The optimal weight W is problem-dependent
- Can reduce runtime by 30% for this example problem

5. THE SINKING BLOCK BENCHMARK

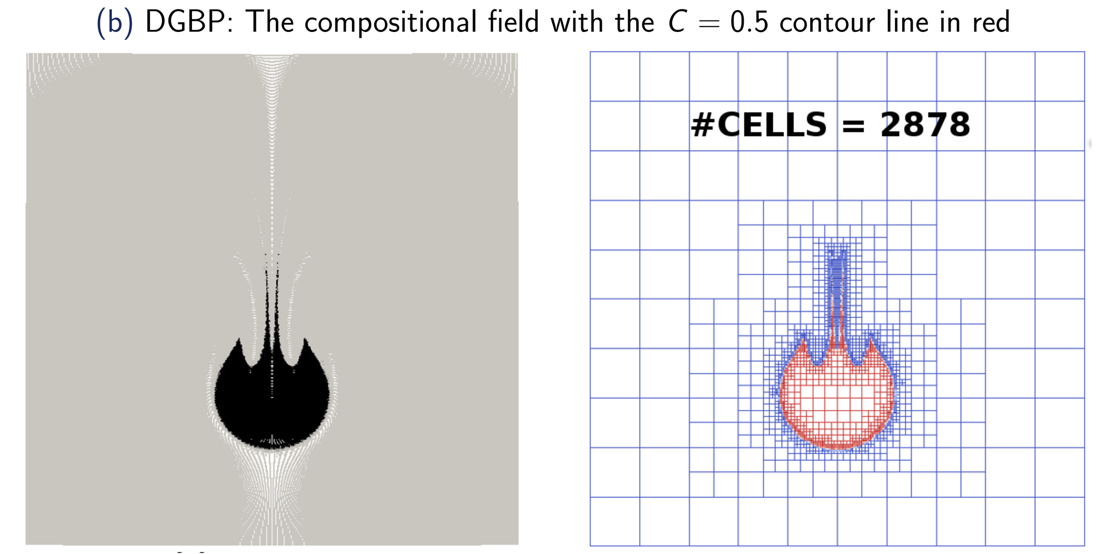
- Idealized model of subduction and similar processes
- Initially square block falls in less dense medium
- VOF interface tracking best reproduces edge of block with fewer grid cells



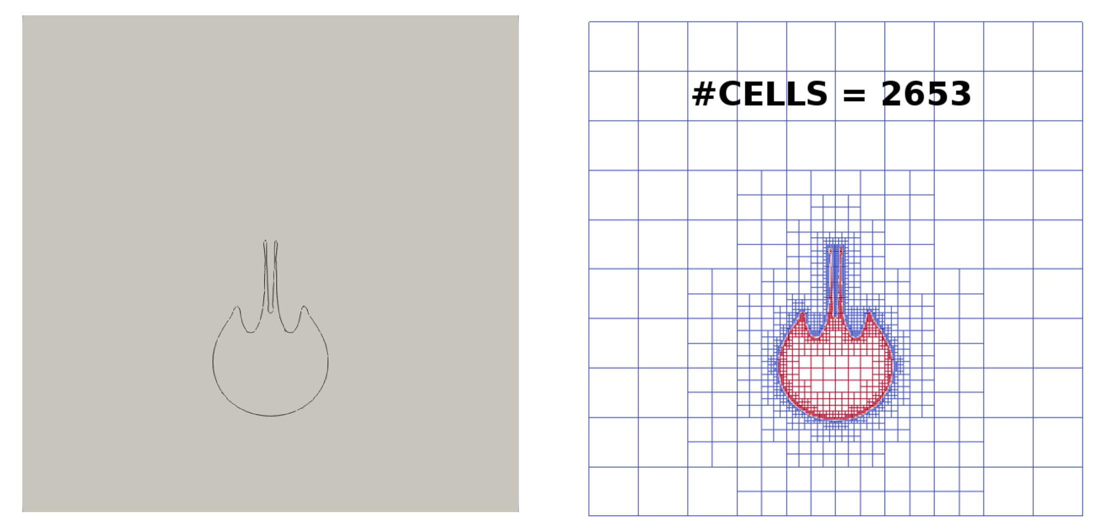
(a) Standard FEM method with 'entropy viscosity' to diffuse over/under shoots



(b) DGBP: The compositional field with the $C = 0.5$ contour line in red



(c) PARTICLES: white spaces are regions where there are no particles



(d) The reconstructed VOF interface is drawn in black on the left

Figure 7: Computations in ASPECT of the Gerya-Yuen 'Sinking Block' problem with AMR. All four computations have the same refinement criterion and input parameters. The initial coarse mesh is a uniform grid with 10 × 10 cells.

ACKNOWLEDGEMENTS AND AVAILABILITY

All SSEs shown here were developed under the auspices of NSF Award No. ACI–1440811 and are included in ASPECT, an open source code for modeling convection and other processes in the Earth's mantle. ASPECT is licensed under the GNU GPL v3.0 (or newer) license and is available at
`https://geodynamics.org/cig/software/aspect/`

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