Three-dimensional numerical simulations of thermo-chemical multiphase convection in Earth's mantle

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Outline

1. Introduction: Previous studies on numerical models of thermo-chemical mantle convection.
2. Numerical models: Getting in sight to methods briefly.
3. Examples: Single-component phase changes system and multi-component phase change system.
4. Examples: Single-component phase changes with the post-perovskite phase change.
5. Summary.

Previous 3D studies

- Flow-scale and formation of thermo-chemical plumes in a rectangular box [Tackley, 1998; McNamara and Zhong, 2004 EPSL] and spherical shells [McNamara and Zhong, 2004 JGR].
- Heat flow scaling in a spherical shell [Oldham and Davies, 2004].
- All those studies have been done by a layered initial condition for the compositional field.
  - No melt-induced material differentiation with a uniform initial condition for the compositional field.

Previous studies on the melt-induced material differentiation in mantle convection models

- Formation of compositional stratification in the uppermost lower mantle due to the density crossover between olivine phase system and pyroxene phase system [Tackley and Xie, 2003; Ogawa, 2004].
- Those studies have been done in only two-dimensional cases.
- Investigating three-dimensional effects is essential for understanding thermo-chemical structure in Earth’s mantle.

Post-perovskite: Newly discovered phase change near the core-mantle boundary

- Discovered by high pressure mineral physics [Murakami et al., 2004; Oganov and Ono, 2004; Tsuchiya et al., 2004].
- Large positive Clapyeron slope (8 to 10MPa/K)
- Destabilize thermo-chemical boundary layer [Nakagawa and Tackley, 2005].
- Still worth to investigate a stability of thermo-chemical boundary layer above the CMB in a three-dimensional geometry.

In this study

- Checking the timing information on various types of CPU.
- Three-dimensional numerical simulations of thermo-chemical multiphase convection to investigate thermo-chemical structure in the uppermost lower mantle and mass transport across 660km depth.
- Adding newly discovered phase change near the core-mantle boundary and see what happens to chemically-dense layering above the CMB.

Numerical Method

- STAG3D: Finite Volume multigrid code for thermo-chemical multiphase convection in a compressible anelastic fluid as a modeled mantle.
- 128x128x64 resolution with 16 tracers in each cell to track the chemical composition and degree of melting.
- Melting tracers are instantaneously moved to the surface when it is erupted.
- Grid refinements are used in the surface, CMB and 660km to resolve thermal boundary layer.
- Simple core-cooling condition is applied to bottom thermal boundary condition.

CPUs that is using in this study

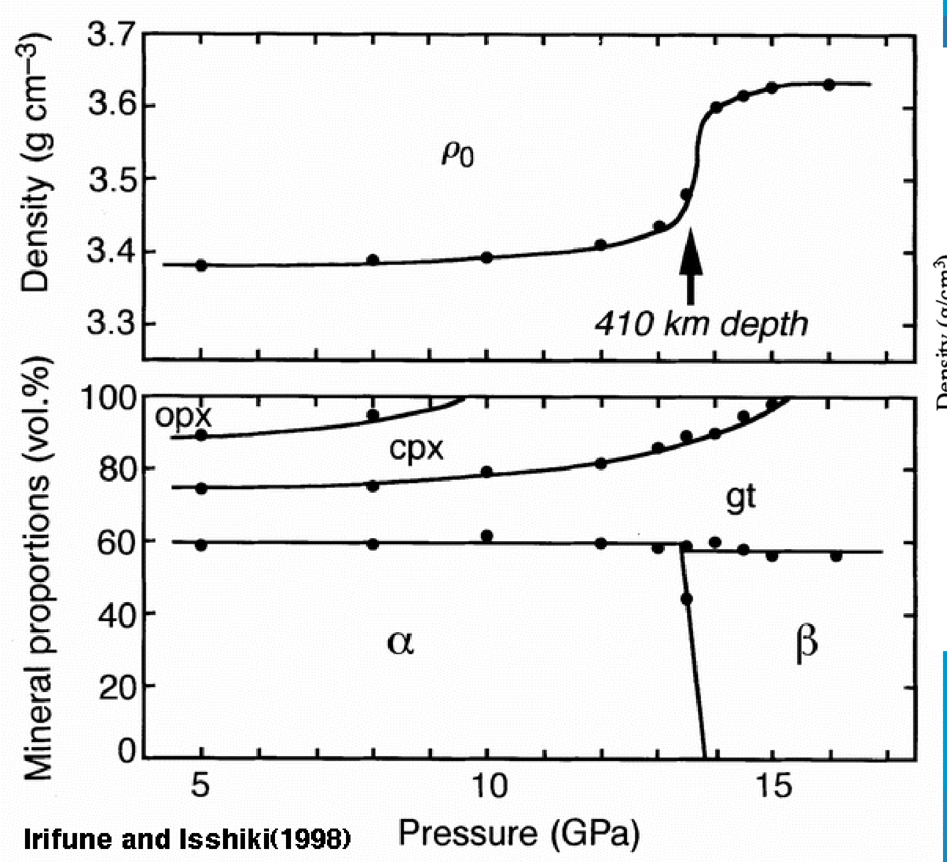
- Timing information: Using Intel P4 3.2GHz x 16 CPUs. (Integrating over 4.5Gyrs)
  - Approximately 5 days with using g77 compiler.
  - Approximately 4 days with using Intel Fortran Compiler.
  - Seems to be reasonable time to study three-dimensional cases systematically.
- Challenging the optimization to the Earth Simulator
  - Fails to vectorize STAG3D because special multigrid techniques that is required to simulate large viscosity variation due to temperature and yield stress has not been suitable for the vectorization.
  - Timing is the similar to Pentium 4.

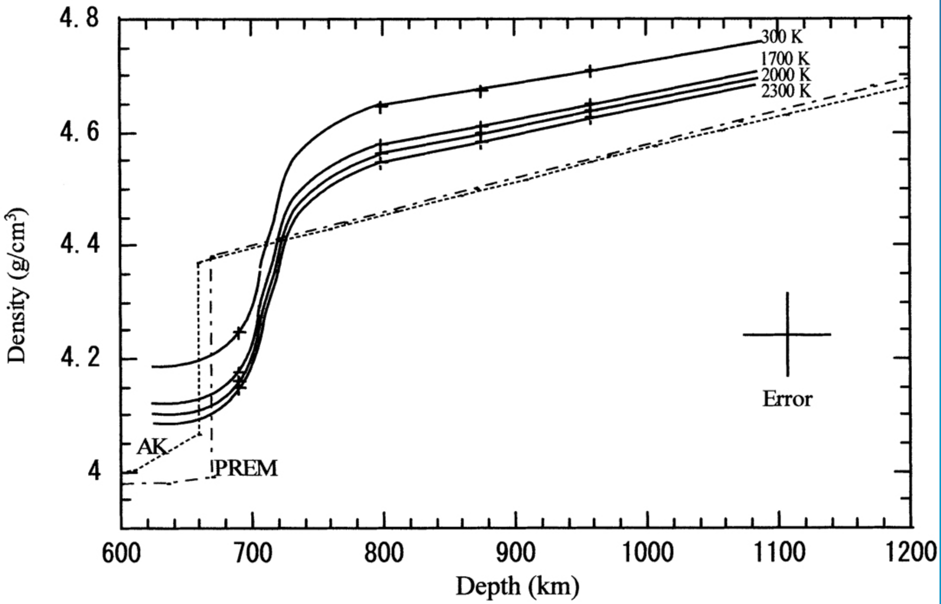
Important material properties

- Viscosity: Temperature- (an order of six), depth (an order of two) and yield stress-dependent viscosity under Bingham fluid approximation [Trampert and Hansen, 1998; Stein et al., 2004].

- Phase changes: olivine-spinel-perovskite-post perovskite and pyroxene-garnet-perovskite-post perovskite systems are assumed.

Phase diagram and density profiles from experimental studies



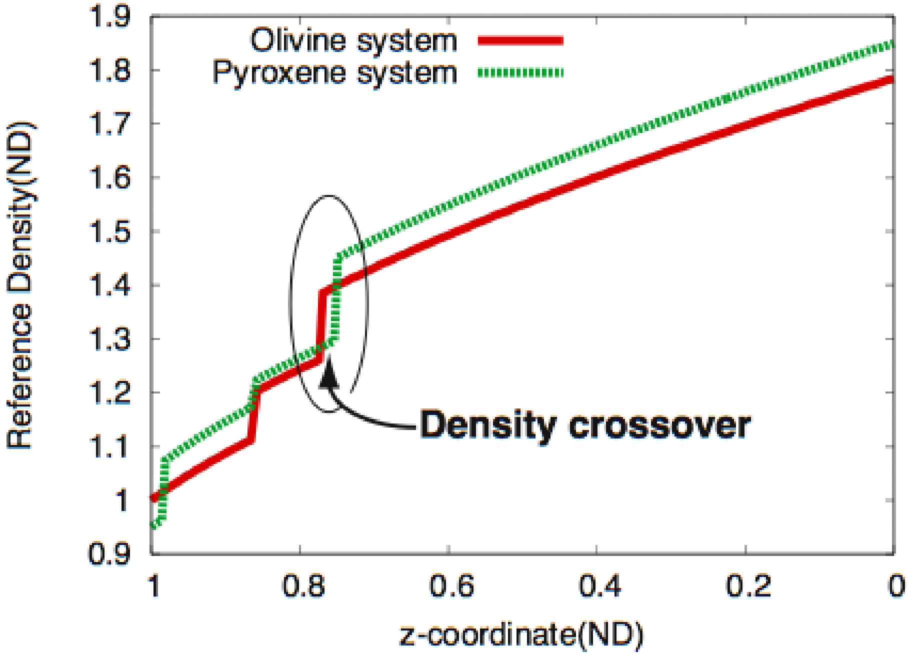


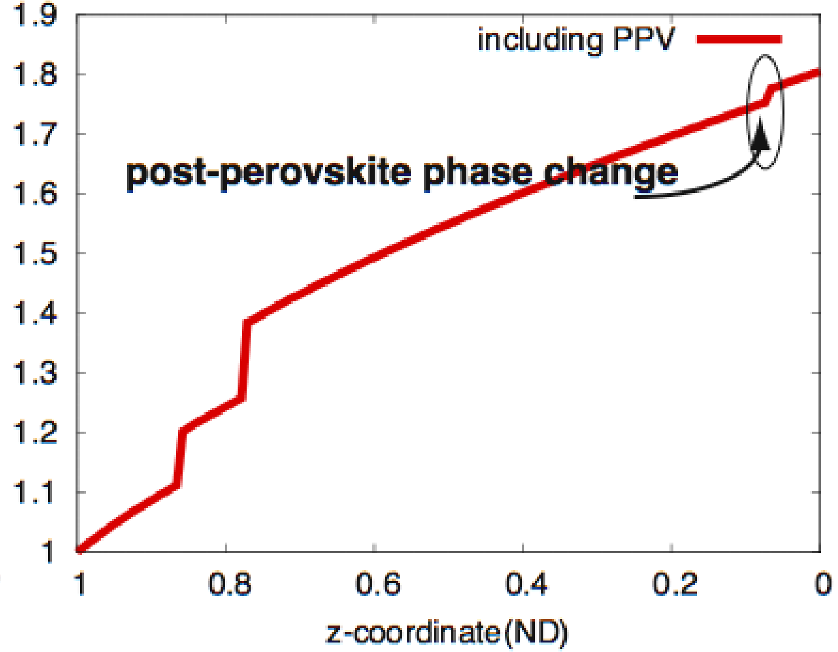
Lower mantle density for MORB (Ono et al., 2001)

Phase diagram and upper mantle density (Irifune and Isshiki, 1998)

Realistic mantle: 60% olivine system and 40% pyroxene system with the density crossover between 660km and 720km depths.

Reference density profiles





Implementations for phase changes

Γ: Sheet mass anomalies for
 olivine-spinel-perovskite phase changes
 pyroxene-garnet-perovskite phase changes

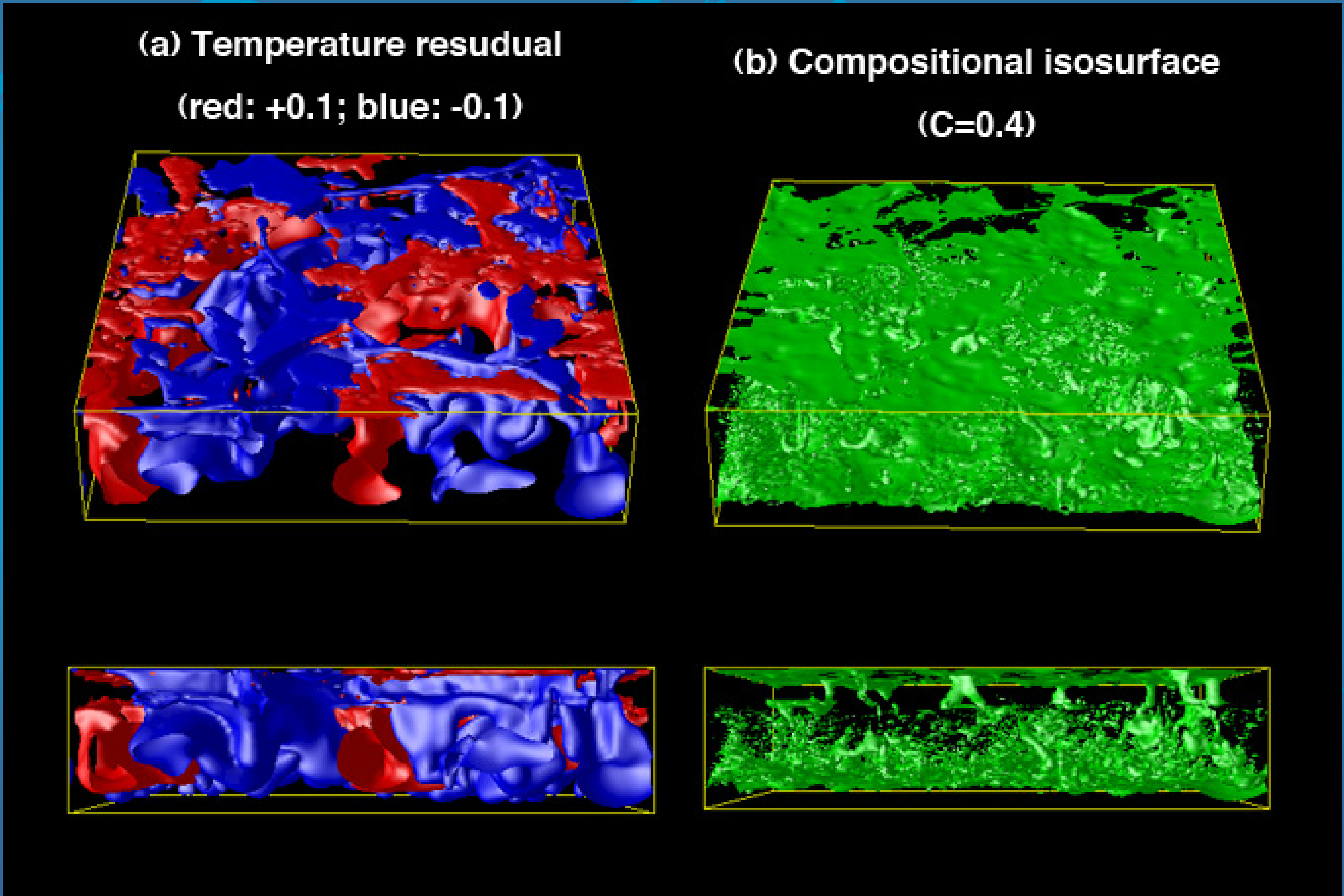
For the post-perovskite phase change:

Two series of numerical simulations

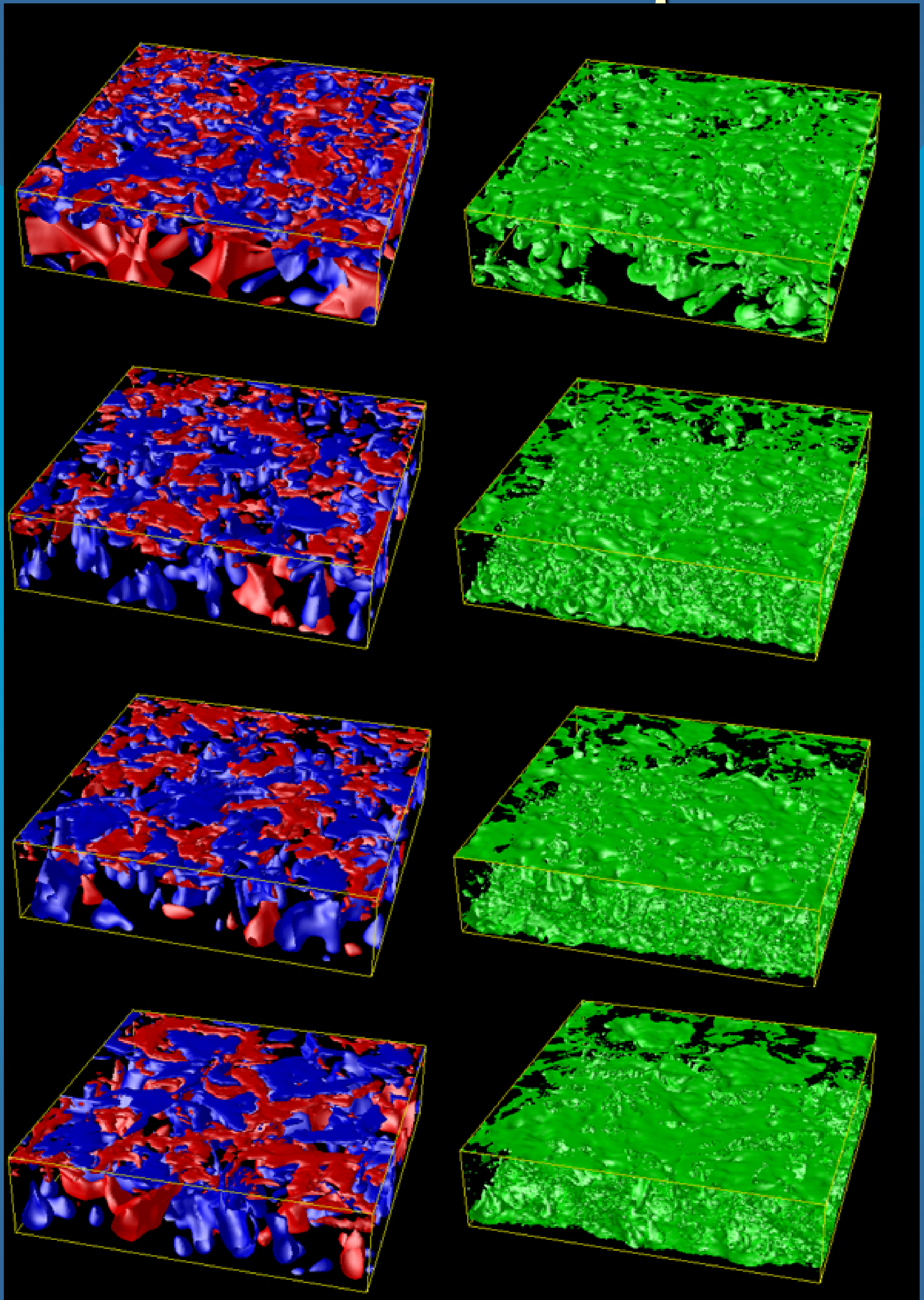
- Multiphase thermo-chemical convection:
  - No post-perovskite effects
  - 60% olivine and 40% pyroxene .
  - 100% olivine cases are done for comparing with realistic composition cases.
- Effects of post-perovskite phase change:
  - No pyroxene phase change system.
  - Two cases (+16MPa/K with 2% density difference between basaltic material and harzburgite, +0MPa/K with 2% density anomalies).

Example 1: Non-olivine effects

100% Olivine



Time variation of temperature and composition



t = 0.00236

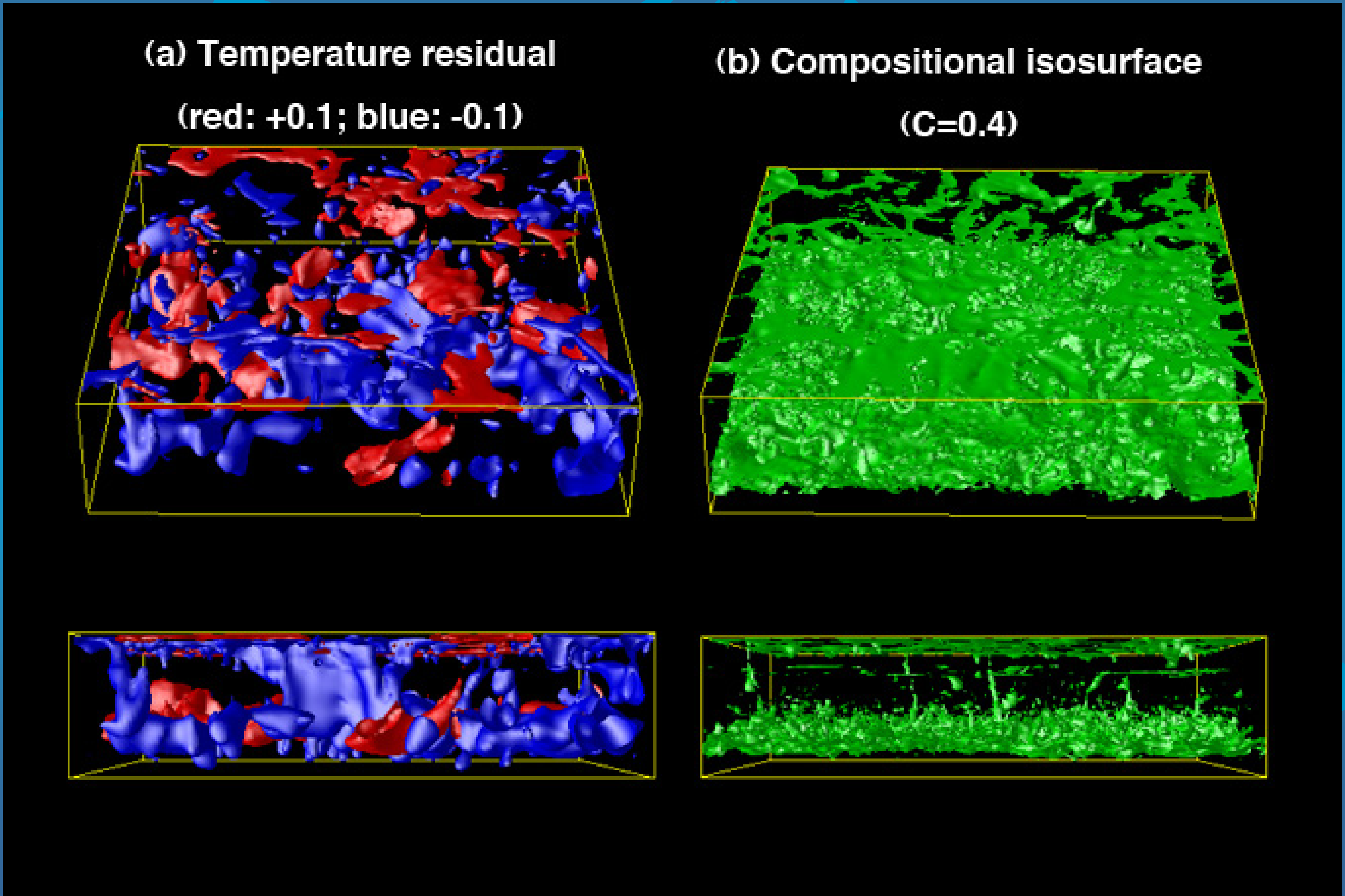
t = 0.00472

t = 0.00708

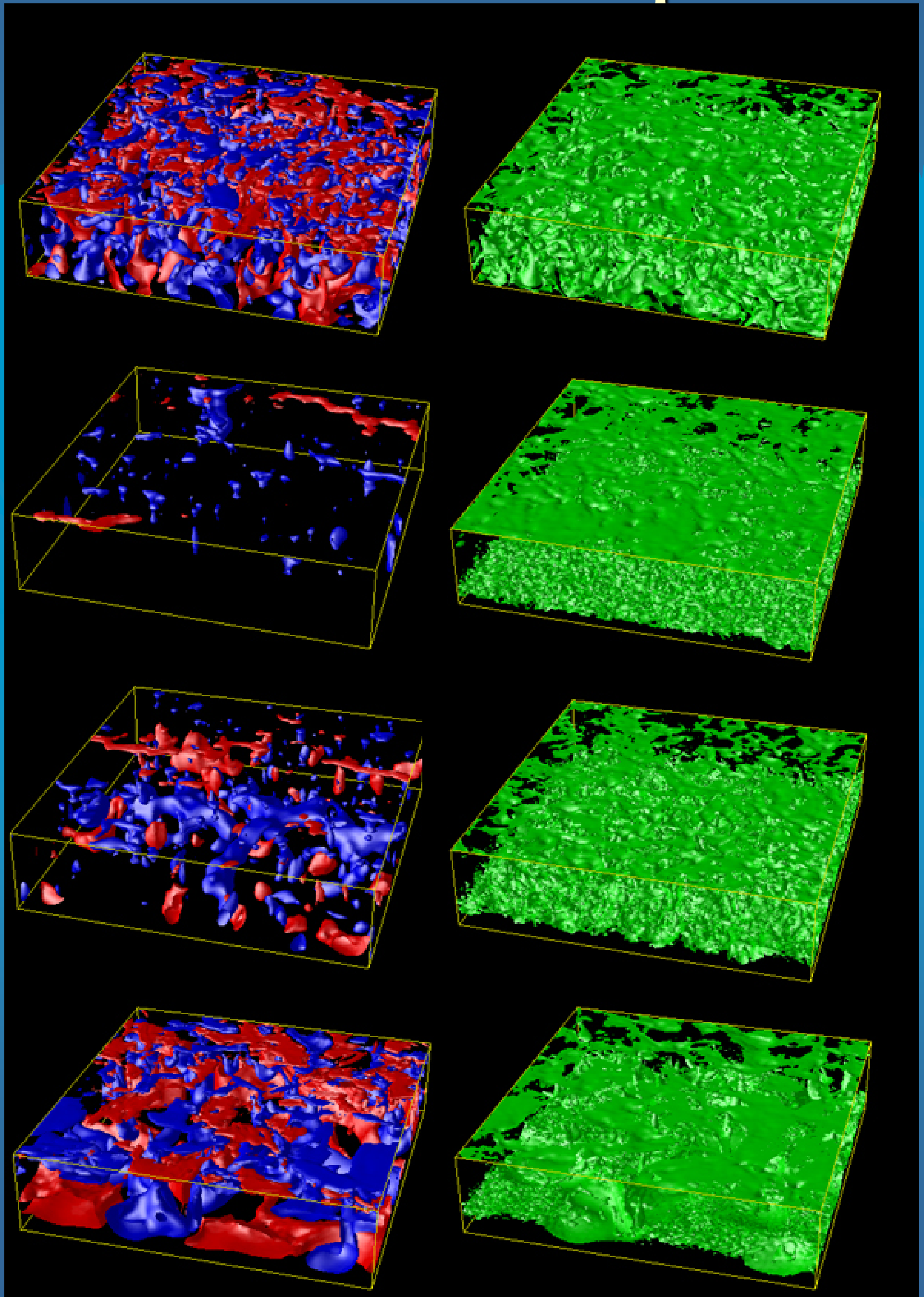
t = 0.00944

Example 1: Non-olivine effects

60% Olivine + 40% Pyroxene (referred as 60/40)



Time variation of temperature and composition



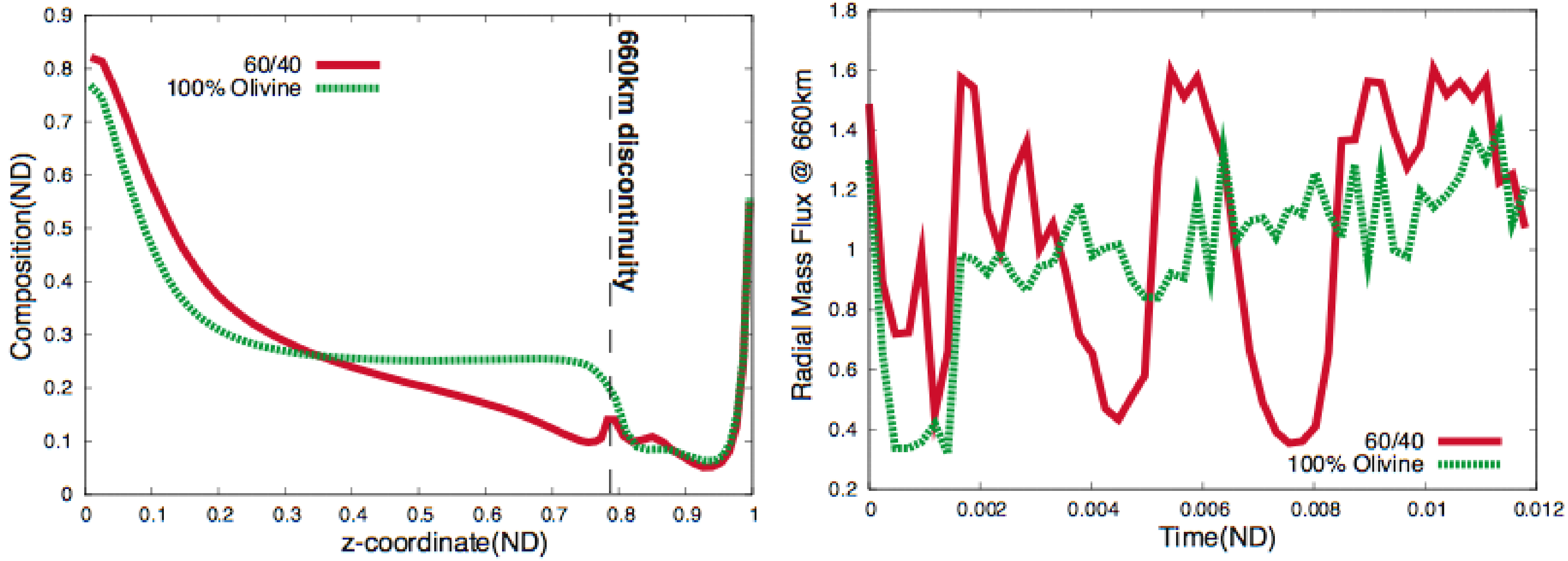
t = 0.00236

t = 0.00472

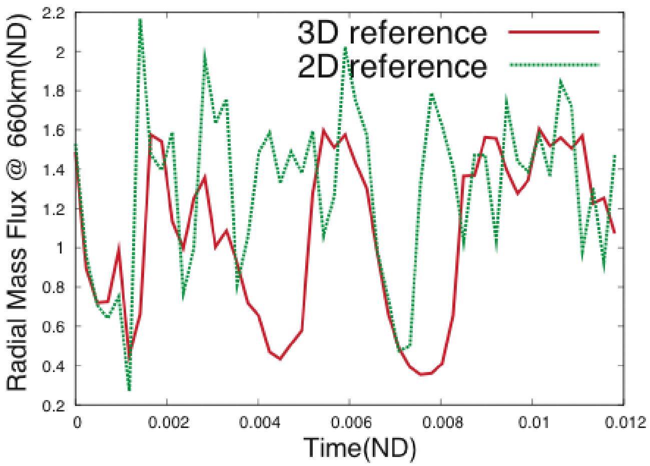
t = 0.00708

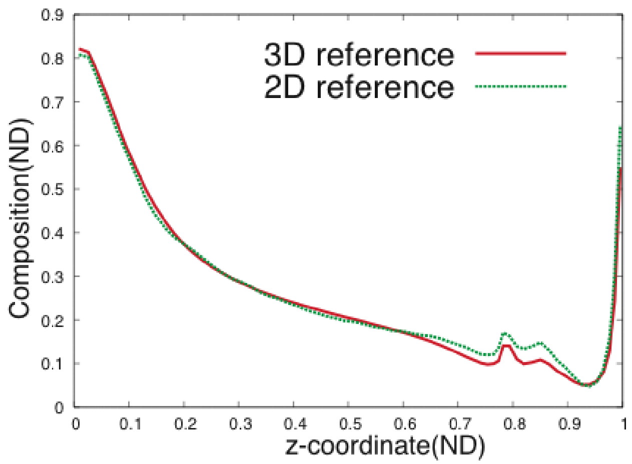
t = 0.00924

Comparison of diagnostics



Diagnostics (Compositional structures and mass flux) compared to two-dimensional cases





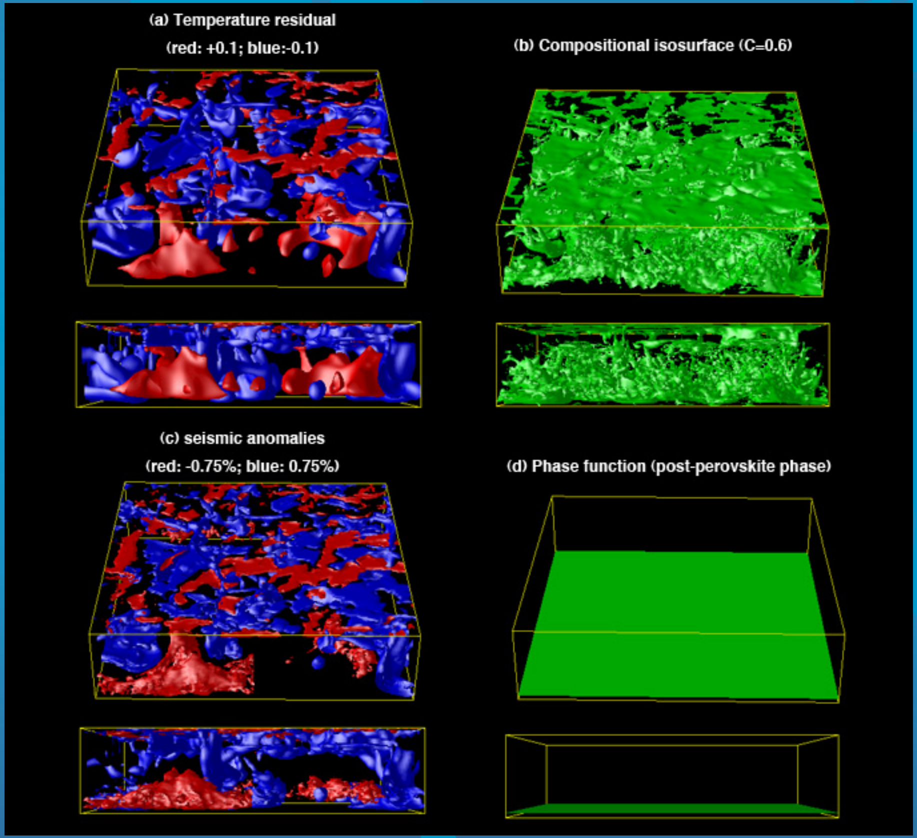
Top: Radial Mass Flux @ 660km
Bottom: Horizontally-averaged C
Both plots are 60/40 cases.

Time variation for mass flux:
3D case has longer term variation

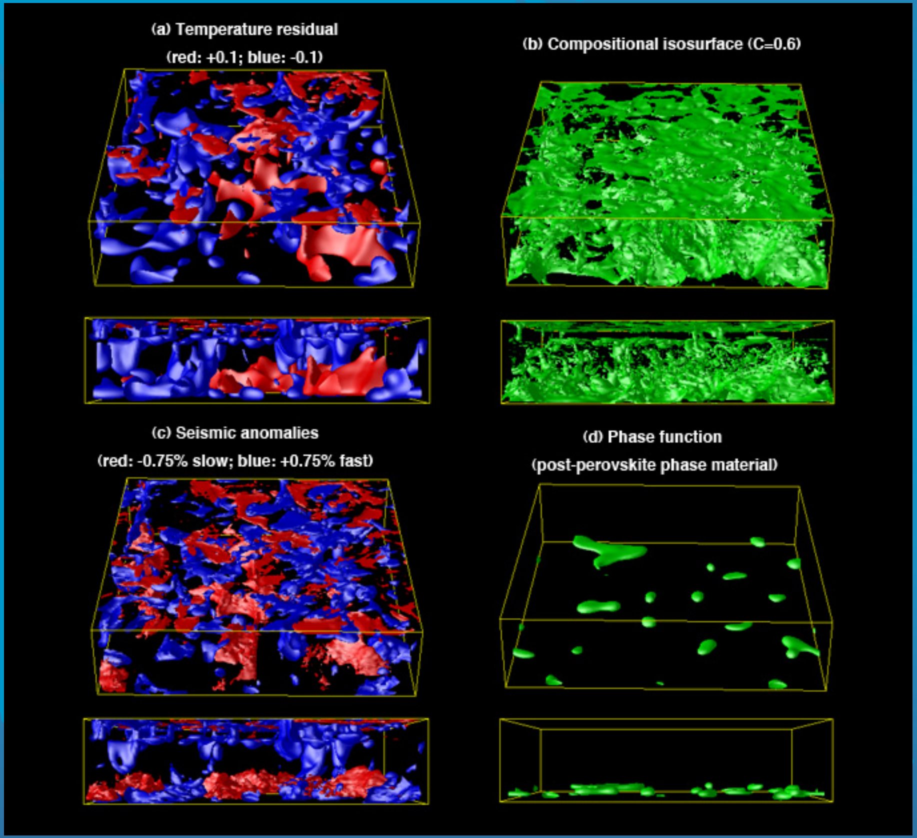
Vertical structure of C:
Not quite different between both cases

Example 2: Effects of post-perovskite phase change near the core-mantle boundary

Zero Clapeyron slope

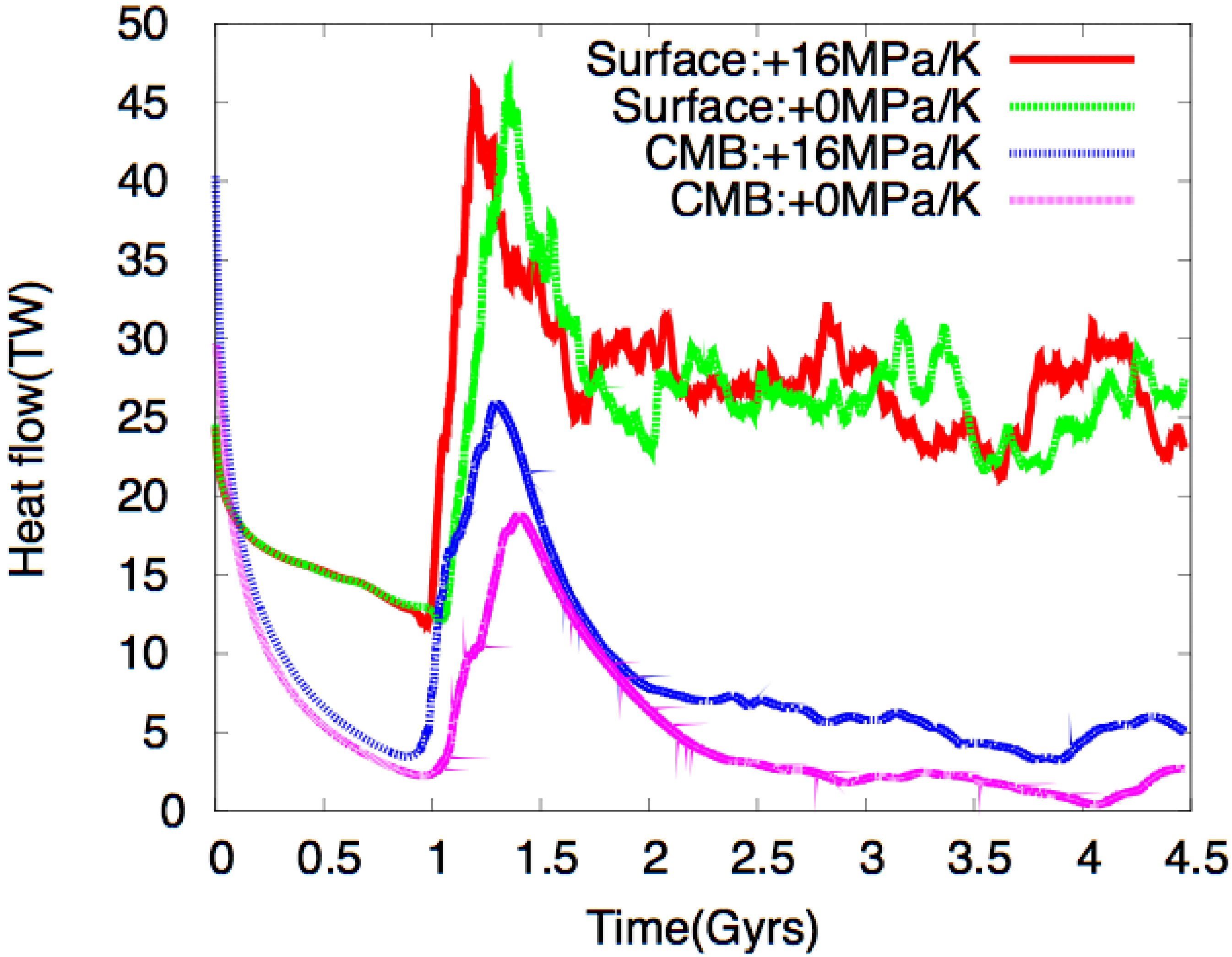


Exaggerated Clapeyron slope (+16MPa/K)



Both cases are 2% density difference between basaltic and harzburgite

Heat flow as a function of time



Summary

- Three-dimensional numerical simulations of thermo-chemical multiphase convection in Earth's mantle including the melt-induced differentiation can be done for a realistic computational time.
- Two examples of complicated phase changes and newly discovered phase change are shown using three-dimensional cases.
- Comparing between two- and three-dimensional results, flux across a certain boundary is longer time scale for 3D cases than for 2D cases.
- Higher heat flow across the CMB is expected when the post-perovskite phase change is taken into account, which is consistent with preliminary two-dimensional results [Nakagawa and Tackley, 2004].
- Necessary to expand a spherical geometry for STAG3D and investigate more realistic thermo-chemical evolution in Earth's mantle in the future.

Next direction (due date: AGU Fall meeting ?)

- Non-olivine effects cases: Change the compressibility in the lower mantle and comparing to 2D cases for the formation of the dense piles.
- Post-perovskite phase change cases: See what happens the cases of realistic Clapeyron slope and doing various cases (0% density difference and more denser cases).
  - Comparing with 2D cases as well.

おしまい!

The End !