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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The Geophysical Motivation

At the elevated pressures and temperatures of Earth's deep interior, mantle rock responds to stress by slow, creeping solid-state flow. The resulting convection in the Earth's mantle is the driving mechanism of plate tectonics, volcanism, earthquakes, mountain building, and other geologic activity.



plunges into the hot interior of the mantle.

Since the Earth's mantle is not accessible to direct observation, we rely on a combination of inferences from direct and indirect observations of geophysical and geochemical datasets, combined with laboratory analogs and computational / numerical models of mantle convection.

A Subduction Dynamics Computation

The Need for Computational Models

Left: Temperature (blue 273K to red 2400 K). Black contours are temperature (300 K). Blue lines follow mineral phase transitions. Red lines mark compositional layer boundaries in the slab. **Right:** Viscosity (red 1018 Pa-s to blue 1024 Pa-s). White lines mark compositional layers in the slab. Red lines are mineral phase transitions. The subducting plate sinks beneath the (left) overriding plate (right). There is a jump in viscosity at the mineral phase transition at the upper-lower mantle boundary (660 km). The slab is in the process of folding as it meets resistance sinking at the upper-to-lower mantle boundary. Accurate tracking of the compositional layers and computation of the temperature field is required. *Temperature over-shoots commonly* occur at the tip of the slab in these types of computations causing incorrect computational results.

The Computational Infrastructure for Geodynamics (CIG)

is an NSF funded, community-driven CIG organization, headquartered at the University of California, Davis, for advancing Earth science by developing and disseminating software for geophysics and related fields. All computational models of mantle convection currently in the CIG code repository produce significant overshoot and undershoot in the neighborhood of sharp gradients in temperature.

A Simple Overshoot / Undershoot Example

The temperature field from a simple, two dimensional model problem computed with **CitcomS**, a mantle convection code maintained and disseminated by CIG. The initial state is shown on the left and the state after ten time steps is shown on the right. Note that in a neighborhood of the interface between the two regions of different temperatures (blue and yellow) the temperature field on the right is both higher and lower than the maximum and minimum values of the initial temperature distribution. For these boundary conditions this is *physically incorrect.* The cause of these overshoots and undershoots is a numerical artifact, which is well-known and wellunderstood in other fields, such as the computational shock physics community.



Our Scientific Software Elements

The goal of this project is to design, develop, and implement state-of--the-art Scientific Software Elements (SSEs) for computing problems in mantle convection in which an essential feature of the problem is the presence of one or more moving boundaries, interfaces, or steep gradients in temperature, composition, or viscosity. In particular, we are developing high-order accurate, monotone numerical methods for the advection and diffusion of the temperature field, which will preserve the physically correct maximum and minimum values of the computed quantities. These SSEs will address critical issues that currently limit modern mantle convection computations. They will be implemented in **ASPECT**, which is opensource software specifically designed for modeling mantle convection. It is the most advanced of the computational models of mantle convection in the CIG code repository.



This map shows the location of all users who downloaded **ASPECT** from the **CIG** repository within the past year.





COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

ASPECT Users Map

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