Density variations driving mantle convection depend on phase transformations that are typically described by *hydrostatic* thermodynamics (i.e, assuming isotropic stress). However, the mantle is under *non-hydrostatic* stress, which laboratory experiments show significantly impacts phase transformations (Wheeler, 2014, 2018, 2020). Our group at the University of Liverpool is exploring the impact of stress on phase transformations by applying Material Science models to quantify olivine $\rightarrow$ wadsleyite reaction rates under stress (Lu & Wheeler, 2024). My hackathon goal is to add a new `PhaseFieldModel` class to ASPECT that bridges the gap from our nanoscale model to the macroscale—thereby enabling an optional feedback between macroscopic reaction rates and compressible mantle flow. To date I am not aware of any numerical geodynamic software that has this capability.

The new `PhaseFieldModel` class will link two distinct length scales, each with its own "phase" parameter that have different interpretations. On the macroscopic scale, we define X as the proportion of phase a in a representative volume of mantle that is large with respect to grain size. X ranges between 0 and 1 and evolves in accordance with a stress-dependent rate law:

$$\frac{DX}{Dt} = \frac{\partial X}{\partial t} + \vec{u} \cdot \nabla X = f(X, T, \sigma) \tag{1}$$

To derive $f(X, T, \sigma)$, a detailed description of microscopic reactions under stress (at scales much smaller than grain size) is required. In Materials Science the powerful "phase field modeling" technique facilitates this. It is based on a "phase field variable" $\phi(\vec{r}, t)$ which is 0 for phase a and 1 for phase b. Intermediate values occur within narrow regions that represent diffuse interfaces, but are not physical mixtures of the two phases. Time evolution of ϕ represents interface velocity and, consequently, reaction rates at a larger scale (after Steinbach, 2009):

$$\frac{\partial \phi}{\partial t} = -M \frac{\partial F}{\partial \phi} \tag{2}$$

where M is a "mobility constant" related to interface velocity, and $F(\phi, T, \sigma)$ is a free energy function that drives macroscopic reaction rates. F is a linear combination of the Helmholtz free energy F_0 at zero stress and the and elastic energy E:

$$F = F_0(\phi, T) + E(\phi, T, \sigma) \tag{3}$$

where E depends on the stress via material coefficients like the elastic modulus. Conventional thermodynamic and mechanical data for mineral phases are readily available, and ongoing work by another PDRA at the Liverpool group has demonstrated how Equation 2 can be solved and upscaled to determine the local reaction rate DX/Dt through volume averaging:

$$X(t) = \frac{1}{V_0} \int_{V_0} \phi(\vec{r}, t)\, dV \tag{4}$$

In contrast to the `PhaseFunctionDiscrete` and `PhaseFunction` classes in ASPECT (source/material_model/utilities.cc), the new `PhaseFieldModel` class requires thermodynamic/mechanical mineral data. Thus, it will depend on the PT lookup table EOS (thermodynamic_table_lookup.cc), or be an option limited to certain material models that already use PT lookup tables (entropy_model.cc, grain_size.cc, steinberger.cc). Moreover, because X evolves with time, it will need to be tracked as either a compositional field or via particles. Otherwise, the new `PhaseFieldModel` class will follow the same general structure and usage as the `PhaseFunctionDiscrete` and `PhaseFunction` classes.

References

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