Moving the Earth with thermodynamics and python

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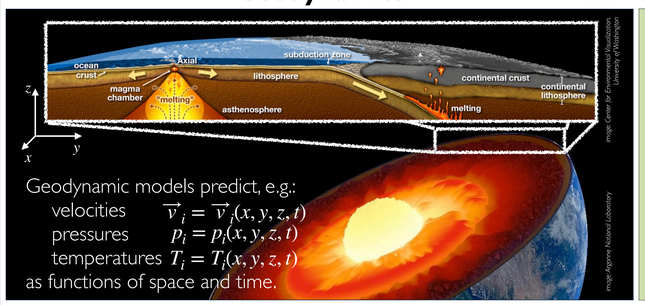
The Problem

Geodynamics is driven by **Thermodynamics**



Geodynamic models predict, e.g.:
velocities $\vec{v}_i = \vec{v}_i(x, y, z, t)$
pressures $p_i = p_i(x, y, z, t)$
temperatures $T_i = T_i(x, y, z, t)$
as functions of space and time.

Thermodynamic models predict, e.g.:
densities
$\rho_i = \rho_i(p_i, T_i, n_i^0, \ldots, n_i^{K_i})$
thermal expansivities
$\alpha_i = \alpha_i(p_i, T_i, n_i^0, \ldots, n_i^{K_i})$
heat capacities
$C_{pi} = C_{pi}(p_i, T_i, n_i^0, \ldots, n_i^{K_i})$
chemical potentials
$\mu_i^k = \mu_i^k(p_i, T_i, n_i^0, \ldots, n_i^{K_i})$
entropies
$S_i = S_i(p_i, T_i, n_i^0, \ldots, n_i^{K_i})$
at a single point but as functions of a high-dimensional parameter space.

Olivine

We model the thermo-mechanical evolution of the Earth using ordinary and partial differential equations (O/PDEs) that describe conservation laws in space and time.

The high-dimensionality of thermodynamic models typically means that geodynamic models rely on inconsistent thermodynamic approximations and other simplifying assumptions. This limits our ability to apply experimental petrology data to large-scale simulations or consistently model open reactive systems.

Our Solution

Given a model for the free energy of a thermodynamic phase:

$$G_i(p_i, T_i, n_i^k)$$

differentiation gives consistent thermodynamic parameters

$$S_i = -\frac{\partial G_i}{\partial T_i} \qquad \frac{M_i}{\rho_i} = \frac{\partial G_i}{\partial p_i} \qquad \mu_i^k = \frac{\partial G_i}{\partial n_i^k}$$

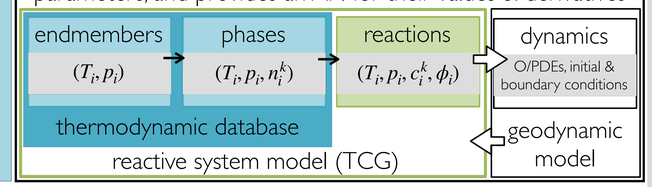
$$\frac{C_{pi}}{T_i} = \frac{\partial S_i}{\partial T_i} = -\frac{\partial^2 G_i}{\partial T_i^2} \qquad \alpha_i \frac{M_i}{\rho_i} = \frac{\partial \frac{M_i}{\rho_i}}{\partial T_i} = \frac{\partial^2 G_i}{\partial p_i^2} \qquad \frac{\partial^2 G_i}{\partial T_i c_i^k}, \frac{\partial^2 G_i}{\partial p_i c_i^k}$$

$$\ldots \frac{\partial^3 G_i}{\partial T_i^3}, \frac{\partial^3 G_i}{\partial T_i^2 p_i}, \frac{\partial^3 G_i}{\partial T_i p_i}, \frac{\partial^3 G_i}{\partial p_i^3}, \ldots$$

The relationships between the thermodynamic parameters and the (e.g. Gibbs) free energy make them ideal candidates for symbolic representation, differentiation and code generation, allowing thermodynamic models to be rapidly implemented for use in geodynamic simulations. We have developed ThermoCodegen for this purpose.

ThermoCodegen (TCG)

describes free energy models of thermodynamic endmembers & phases, & reactions between them using SymPy, automatically generates code for the thermodynamic parameters, and provides an API for their values & derivatives



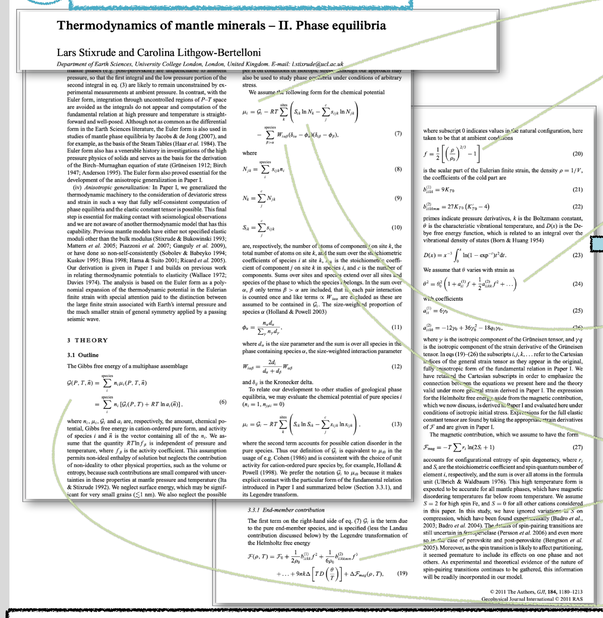
Find us on gitlab: gitlab.com/ENKI-portal/ThermoCodegen

Read our docs: enki-portal.gitlab.io/ThermoCodegen

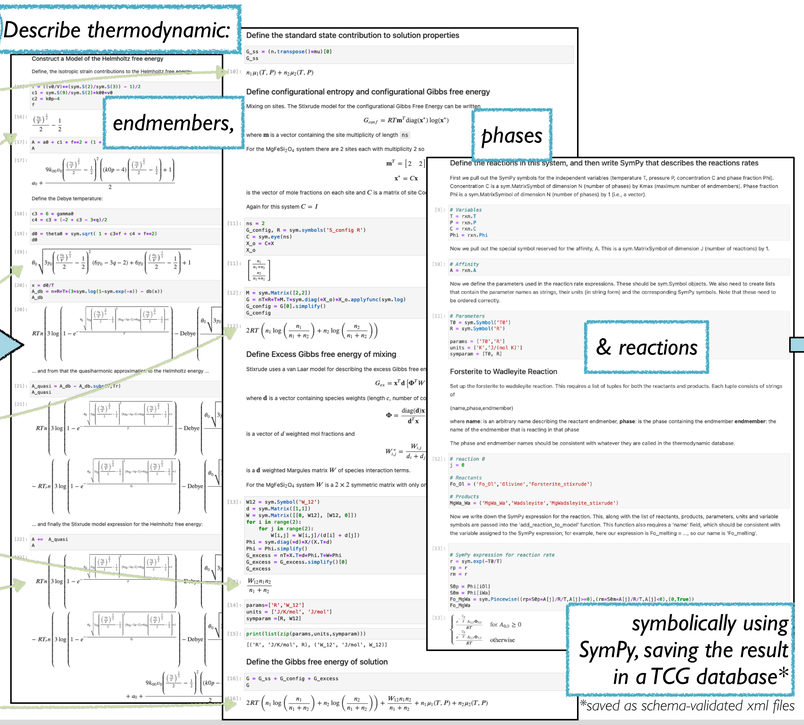
JOSS paper: NEW doi.org/10.21105/joss.04874

Our Workflow

1 *Choose (or design) a database of thermodynamic models, e.g.:*



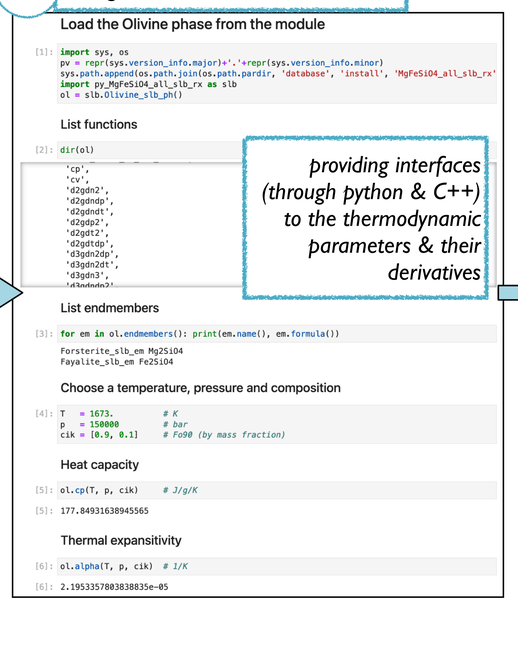
2 *Describe thermodynamic:* *endmembers,* *phases* *& reactions*



*symbolically using SymPy, saving the result in a TCG database**

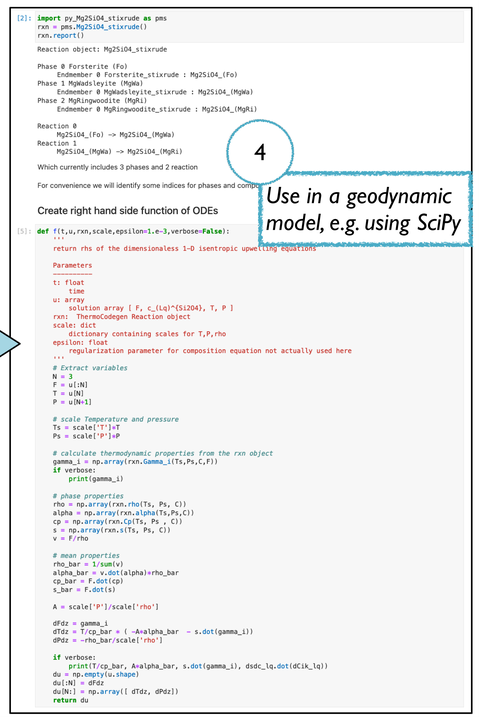
**saved as schema-validated xml files*

3 *TCG generates & builds C/C++ code:*



providing interfaces (through python & C++) to the thermodynamic parameters & their derivatives

4 *Use in a geodynamic model, e.g. using SciPy*

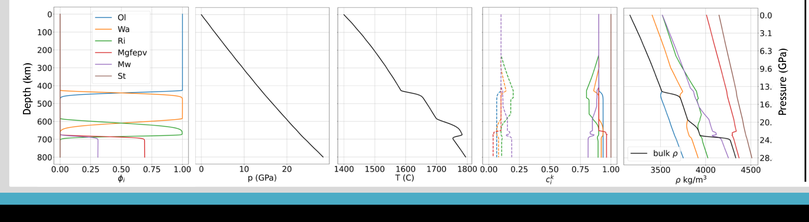


Some Applications

Global scale solid-state mantle convection with reactive-disequilibrium phase changes, e.g. isentropes calculated using SciPy+TCG

Phases
Olivine (Ol)
Wadsleyite (Wa)
Ringwoodite (Ri)
Perovskite (Pv)
Magnesiowüstite (Mw)
Stishovite (St)

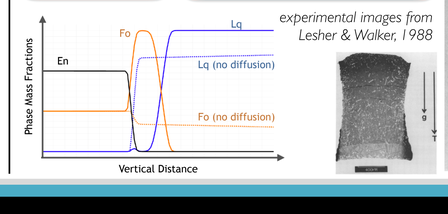
Reactions
$[Mg,Fe]_2SiO_{4\_(Ol,Ol,Wa)} \rightleftarrows [Mg,Fe]_2SiO_{4\_(Wa,Ri,Ri)}$
$[Mg,Fe]_2SiO_{4\_(Ol,Wa,Ri)} \rightleftarrows [Mg,Fe]SiO_{3\_(Pv)} + [Mg,Fe]O_{\_(Mw)}$
$[Mg,Fe]_2SiO_{4\_(Ol,Wa,Ri)} \rightleftarrows 2\ [Mg,Fe]O_{\_(Mw)} + SiO_{2\_(St)}$
$[Mg,Fe]SiO_{3\_(Pv)} \rightleftarrows [Mg,Fe]O_{\_(Mw)} + SiO_{2\_(St)}$
$MgSiO_{3\_(Pv)} + FeO_{\_(Mw)} \rightleftarrows FeSiO_{3\_(Pv)} + MgO_{\_(Mw)}$



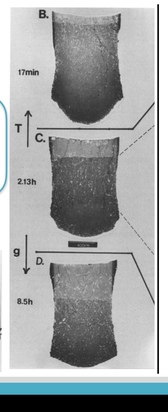
Laboratory scale disequilibrium reaction-diffusion melting experiments, modeling performed using FEniCSX+PETSc+TCG

Phases
Forsterite Solid (Fo)
Orthopyroxene Solid (En)
Quartz Solid (Qz)
Melt Liquid (Lq)

Reactions
$Mg_2SiO_{4\_(Fo)} \rightleftarrows Mg_2SiO_{4\_(Lq)}$
$MgSiO_{3\_(En)} \rightleftarrows 1/2\ Mg_2SiO_{4\_(Lq)} + 1/4\ Si_2O_{4\_(Lq)}$
$SiO_{2\_(St)} \rightleftarrows 1/2\ Si_2O_{4\_(Lq)}$



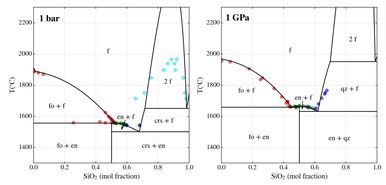
experimental images from Lesher & Walker, 1988

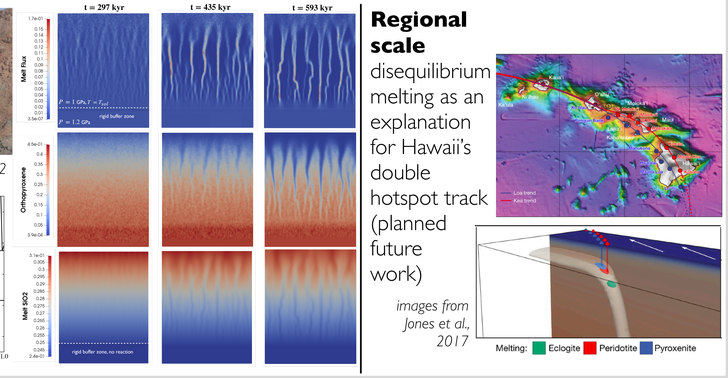


Outcrop scale disequilibrium reactive-channeling simulations, modeling performed by Lucy Tweed using TerraFERMA+TCG

field image from Kelemen et al., 2022

same reactive system as in the laboratory scale results





Regional scale disequilibrium melting as an explanation for Hawaii's double hotspot track (planned future work)

images from Jones et al., 2017

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