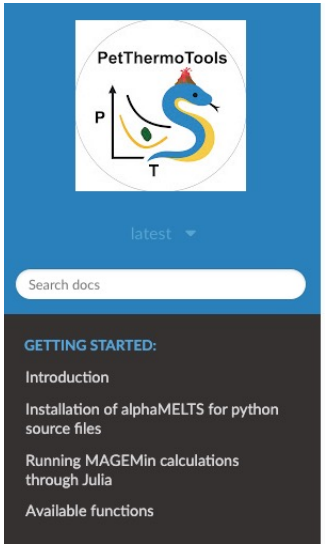
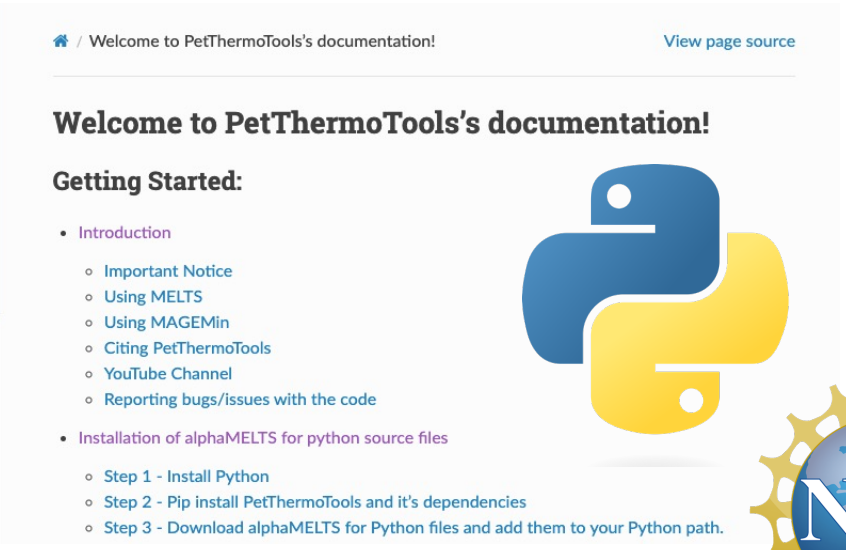
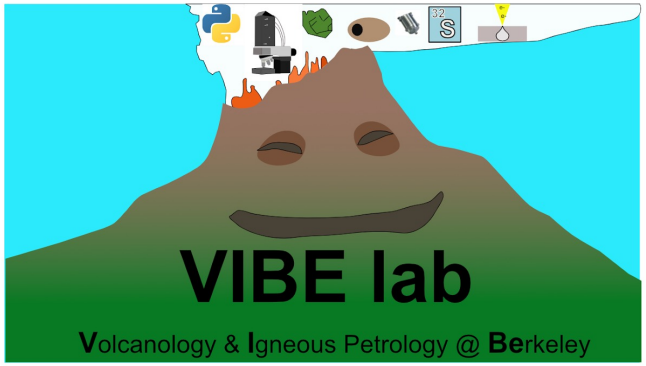
PetThermoTools – a Python3 package for fast, easy, and flexible thermodynamic calculations

Please have at a look at our documentation:
https://petthermotools.readthedocs.io/en/latest/index.html







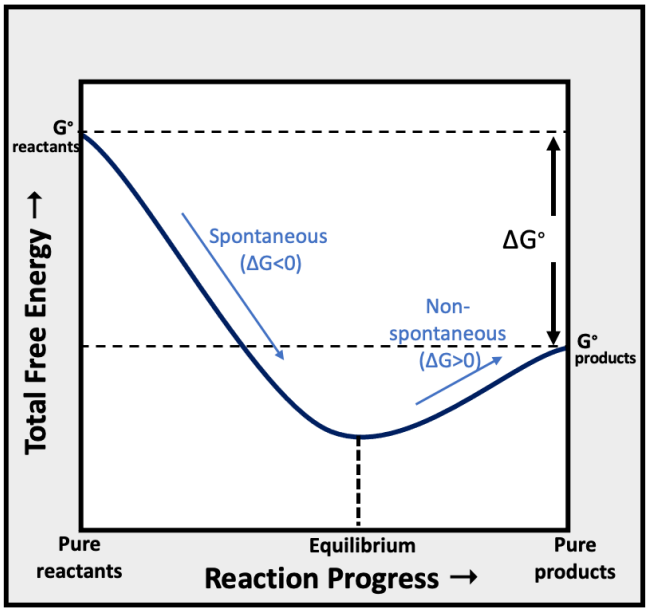
Berkeley
UNIVERSITY OF CALIFORNIA

Caltech

NSF

MAGMA

Thermodynamic modelling – the basics

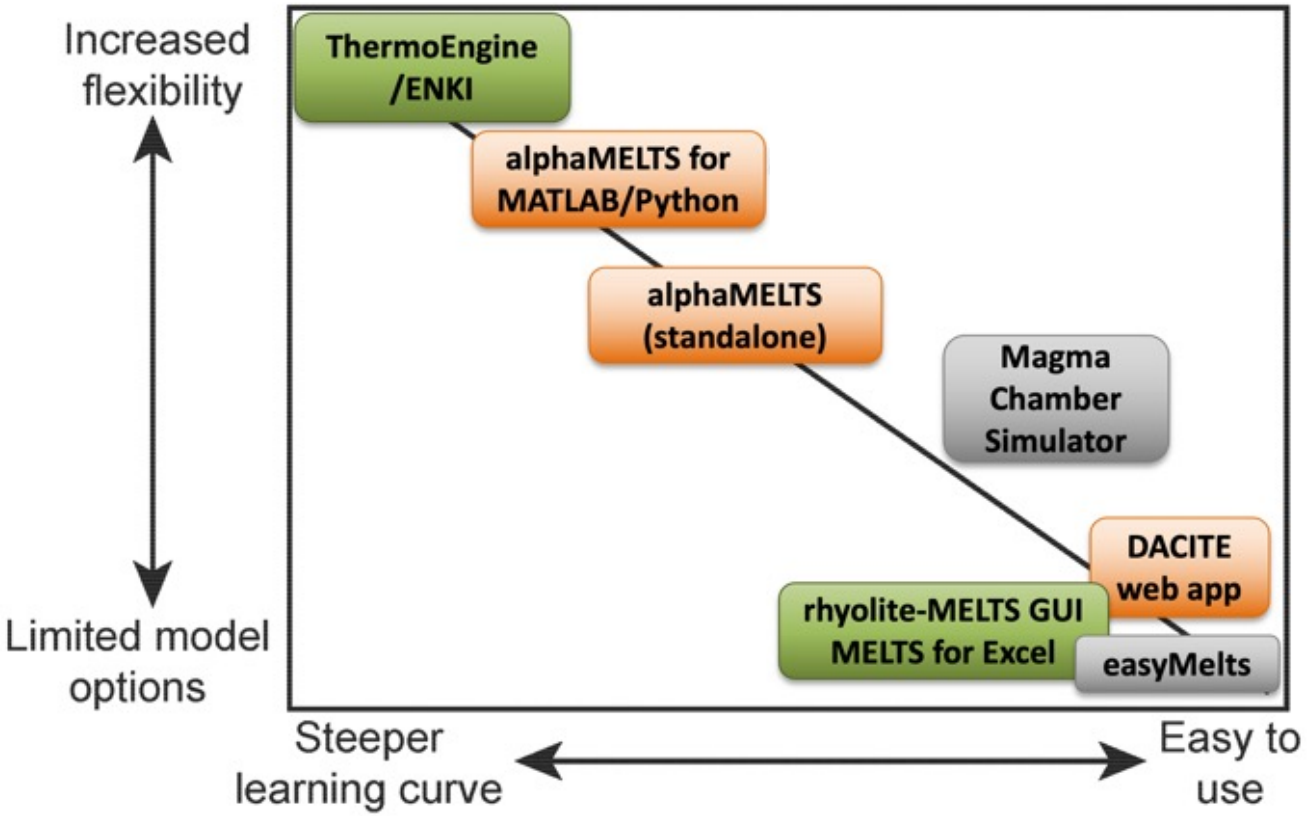


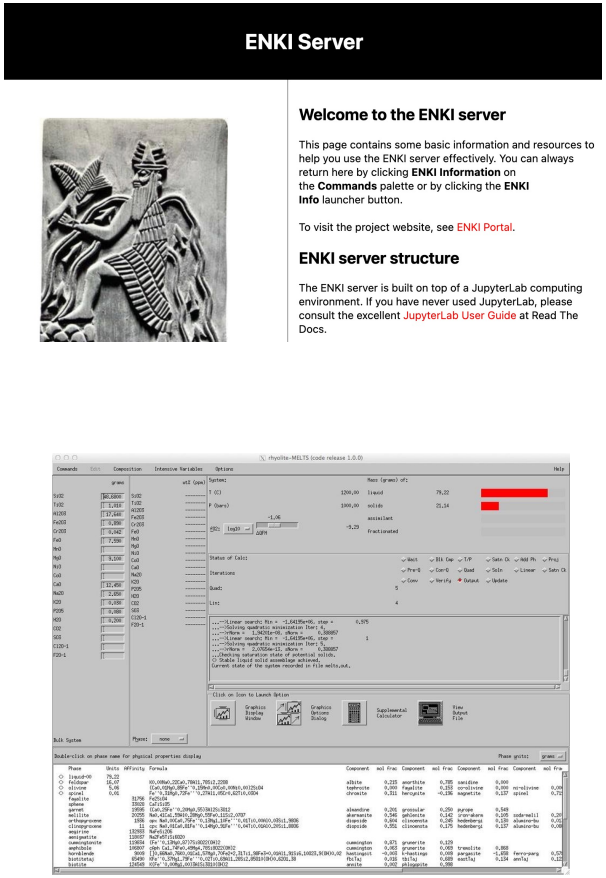
Given

- Bulk composition (masses of each component)
- Two independent intensive parameters [*P* or *V*; *T*, *S*, or *H*]
- and (optionally) fO_2 and/or a_{H2O} …

Calculate equilibrium by finding the distribution of the mass of each component among all known phases that minimizes the appropriate thermodynamic potential

Providing something new?





Main aims of PetThermoTools

alphaMELTS@CIT

DOI 10.5281/zenodo.17861695

alphaMELTS started as a text menu-driven interface to subroutine versions of the MELTS (Ghiorso & Sack, 1995), pMELTS (Ghiorso et al., 2002), and pHMELTS (Asimow et al., 2004) models of thermodynamic equilibrium in silicate systems. Formerly known as 'Adiabat_1ph', and described in a software brief in G-cubed (Smith & Asimow, 2005), it evolved to 'alphaMELTS' via Adiabat_1ph → A1ph → Alph → alpha → alphaMELTS.

- alphamelts-py-2.3.1-linux.zip
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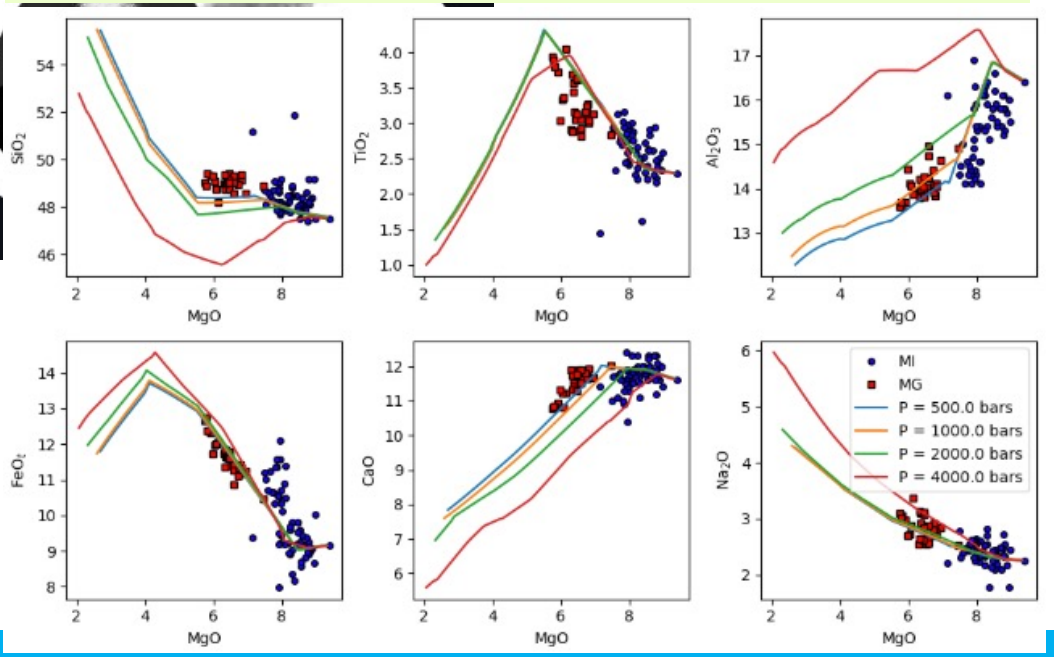
- alphamelts-py-2.3.1-macos-x86_64.zip
- alphamelts-py-2.3.1-win64.zip

```
Isobaric_Xtal_CO2 = ptt.isobaric_crystallisation(Model = "MELTSv1.2.0",
    bulk=starting_comp,find_liquidus=True,P_bar=np.array([500,1000,2000,4000]),
    T_end_C=1050,dt_C=2,fO2_buffer="FMQ",fO2_offset=-1.0,
    Frac_solid=True,Frac_fluid=True,H2O_init=0.4,CO2_init=0.5,label="P_bar")
```

```
ptt.harker(Results = Isobaric_Xtal_CO2, data = {'MI': MI, 'MG': MG},
    d_color = ['b','red'], legend_loc = [1,2],
    y_axis = ['SiO2', 'TiO2', 'Al2O3', 'FeOt', 'CaO', 'Na2O'])
```



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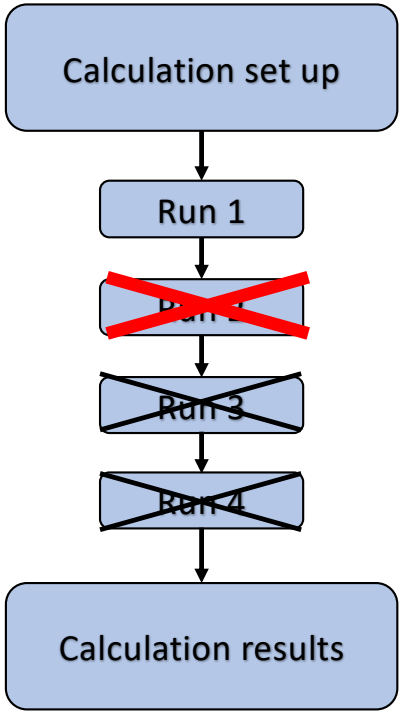
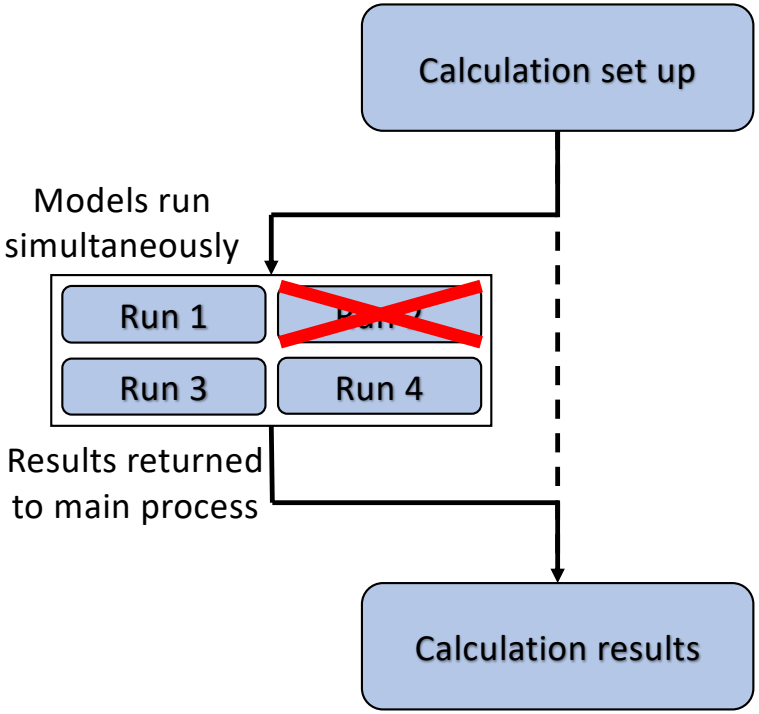
- alphamelts-py-2.3.1-macos-x64.zip
- alphamelts-py-2.3.1-win64.zip

```
MELTS:libraryAlreadyInitialized.
Could not re-initialize MELTS library! Please check stderr (console or terminal).
```

PetThermoTools – parallel processing for speed and stability



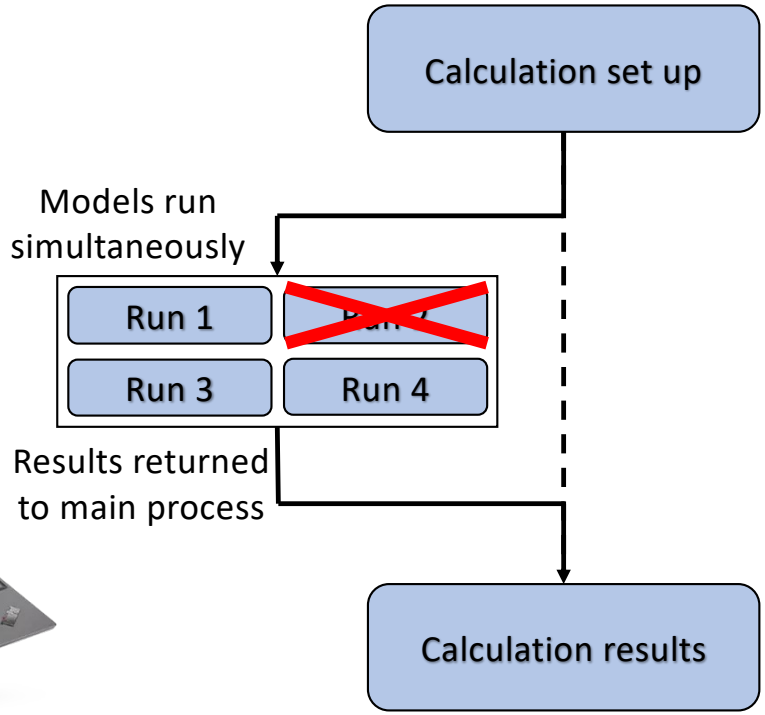


PetThermoTools – parallel processing for speed and stability

PetThermoTools automatically runs calculations in parallel to optimize your computer.

8 calculations at a time
2-4X speed improvement

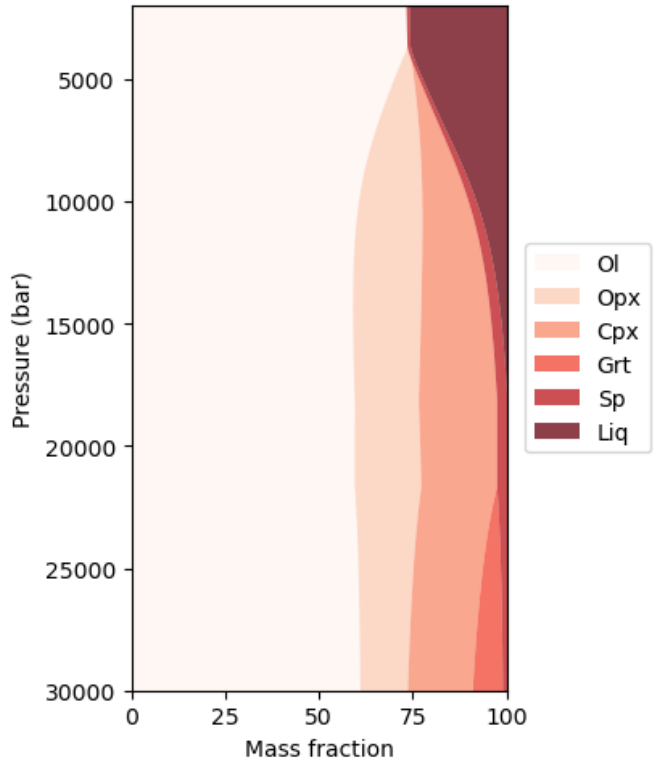
1000 Fraction Crystallization models:
Normally ~1 hours!
Now… ~15 minutes – 30 minutes.



PetThermoTools – easy-to-use functions for common calculations

Adiabatic Mantle Melting as an example

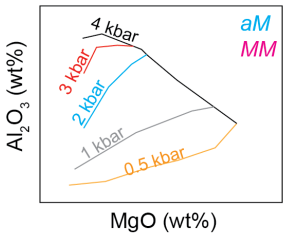
Full example available on ReadTheDocs!



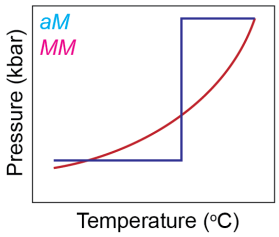
*aM - **compatible with alphaMELTS for Python***
*MM - **compatible with MAGEMin_C***

a) Crystallisation calcs

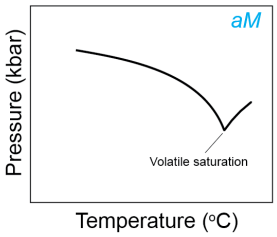
isobaric_crystallisation()



polybaric_crystallisation_onestep()
polybaric_crystallisation_path()



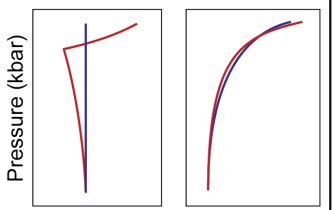
isochoric_crystallisation()



b) Decompression calcs

aM

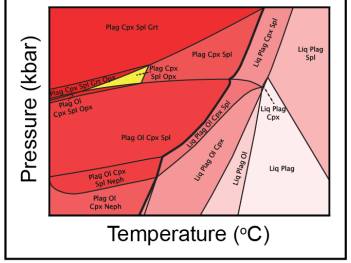
isothermal_decompression()
isentropic_decompression()



c) Phase Diagram calcs

aM
MM

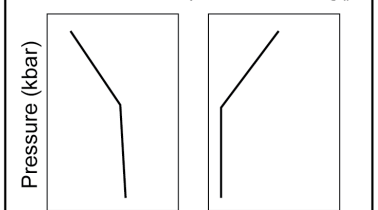
phaseDiagram_calc()



d) Melting calcs

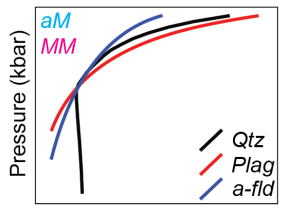
aM
MM

AdiabaticDecompressionMelting()

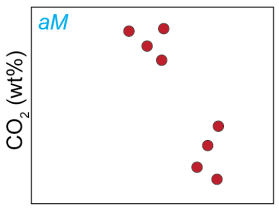


e) Barometry calcs

mineral_cosaturation()



saturation_pressure()



f) Additional core funcitons

findLiq_multi() - load in an Excel spreadsheets of liquids as a DataFrame and calculate their liquidus temperatures

findCO2_multi() - given a melt composition, pressure and H2O content, find the maximum CO2 content of the melt phase (aM only)

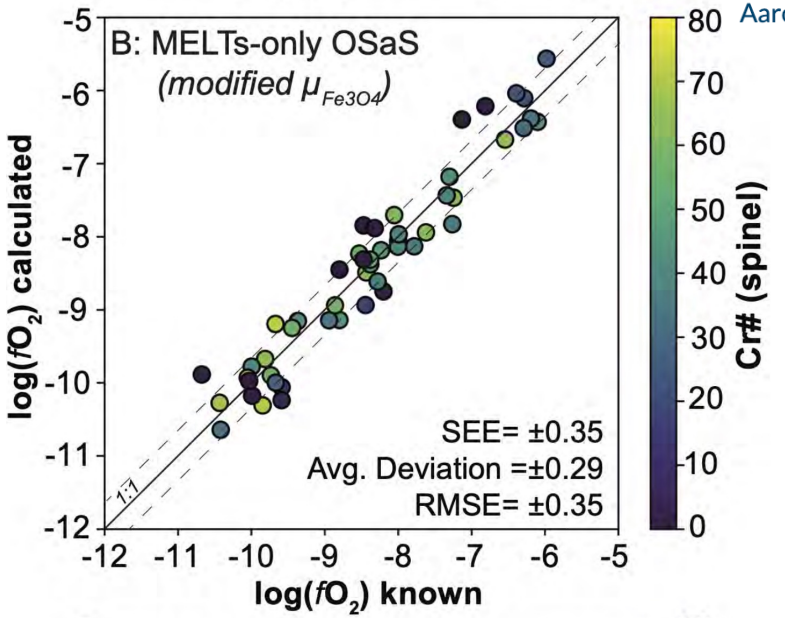
equilibrate_multi() - takes multiple input variables and returns data for phase composition, abundance, and thermodynamic properties at set P&T

PetThermoTools – continuing to expand…

RESEARCH ARTICLE | JANUARY 01, 2025

The olivine-spinel-$a_{SiO_2}^{melt}$ (OSaS) oxybarometer: A new method for evaluating magmatic oxygen fugacity in olivine-phyric basalts

Aaron S. Bell; Laura E. Waters; Mark Ghiorso



PetThermoTools – comparison of different models

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- alphamelts-py-2.3.1-win64.zip

Geochemistry, Geophysics, Geosystems

Research Article | Open Access

MAGEMin, an Efficient Gibbs Energy Minimizer: Application to Igneous Systems

N. Riel, B. J. P. Kaus, E. C. R. Green, N. Berlie

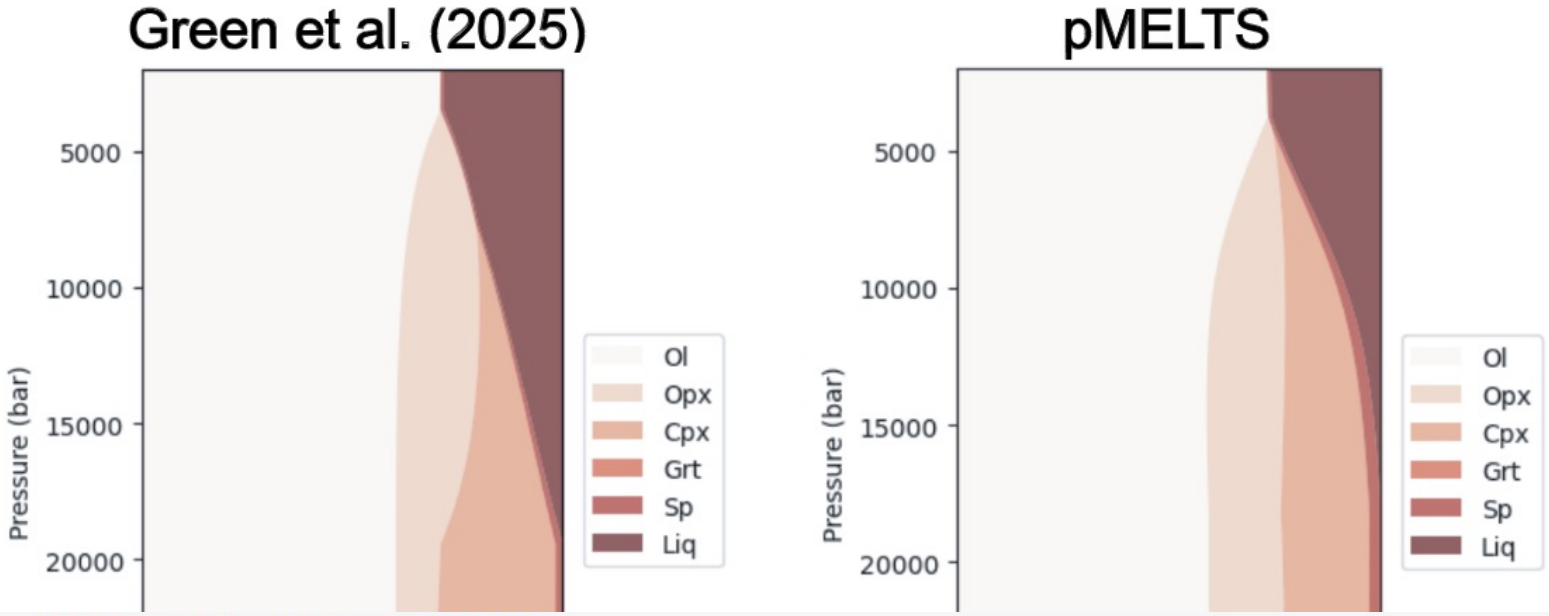
First published: 04 July 2022 | https://doi.org/10.1029/2022GC010427 | VIEW METRICS

MAGEMin_C.jl

docs dev | CI passing | DOI

Julia interface to the MAGEMin C package, which performs thermodynamic equilibrium calculations.

PetThermoTools – comparison of different models



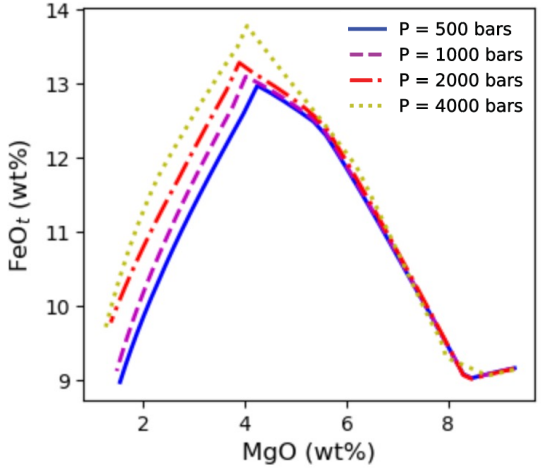

```
Model = ['pMELTS', 'Green2025']
Results = {}
for m in Model:
    Results[m] = ptt.AdiabaticDecompressionMelting(Model = m, bulk = "KLB-1",
        Tp_C = 1350.0, P_start_bar = 30000.0, P_end_bar = 2000.0, dp_bar = 200.0)
```

PetThermoTools – integration with other Python toolkits

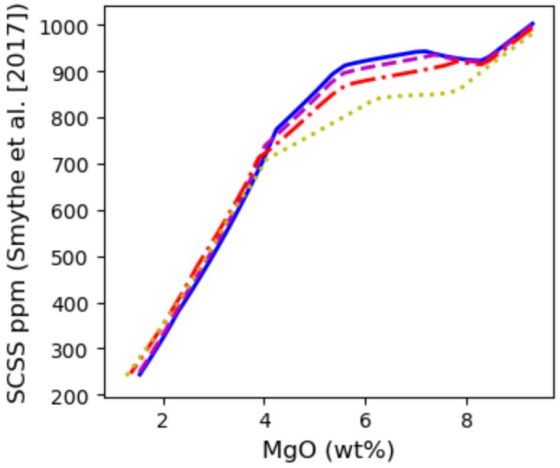
Perform fractional crystallization model with PetThermoTools

```
Isobaric_Xtal = ptt.isobaric_crystallisation(
    Model = "MELTSv1.2.0", bulk = starting_comp, find_liquidus = True,
    P_bar = np.array([500,1000,2000,4000]), T_end_C = 1000, dt_C = 5,
    fO2_buffer = "FMQ", fO2_offset = -1.0,
    Frac_solid = True, Frac_fluid = True, label = "pressure")
```

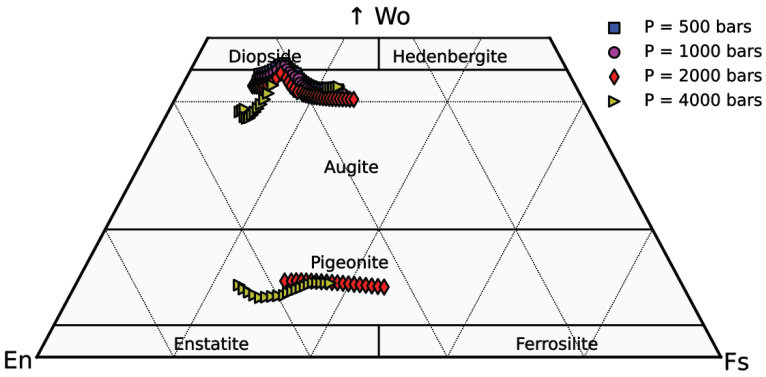
In-built plotting tools



SCSS calculations with PySulfSat



Mineral classification diagrams with Thermobar

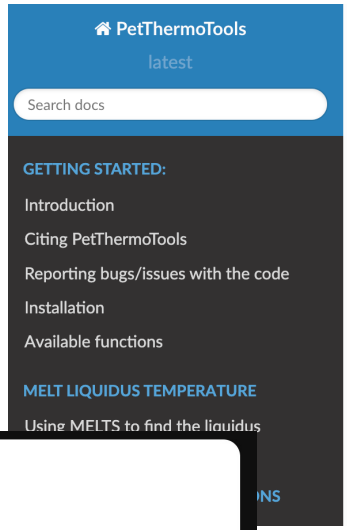


Please visit our documentation to find out more!

If you're interested in getting involved or have any ideas please get in touch!
gleesonm@berkeley.edu

https://www.youtube.com/@PetThermoTools

https://petthermotools.readthedocs.io/en/latest/index.html



Melt liquidus temperature

- Using MELTS to find the liquidus temperature

Crystallisation calculations

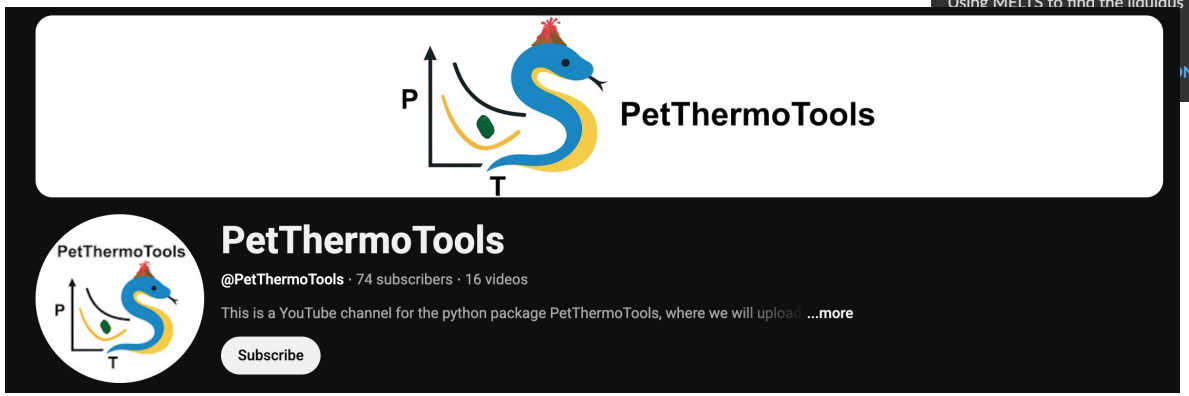
- Modelling liquid-line-of-descents

Melting calculations

- Adiabatic Decompression melting of peridotite and pyroxenite mantle sources
  - Examining the influence of source lithology on melting behaviours
  - Utilizing outputs to calculate the SCSS of mantle melts

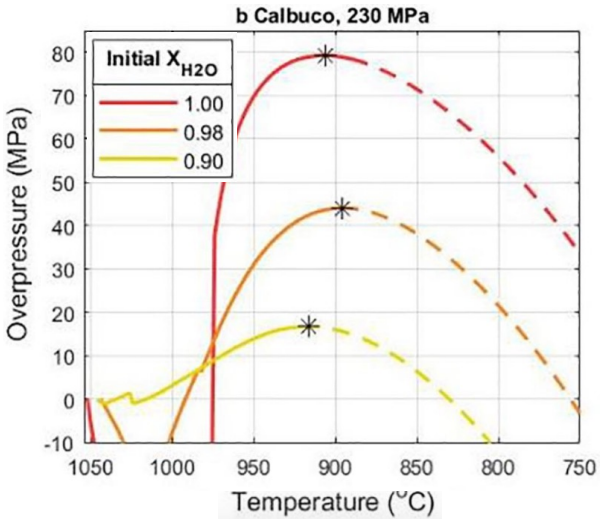
MELTS barometry

- MELTS geobarometry part 1 - quartz - 2-feldspar saturated rhyolites



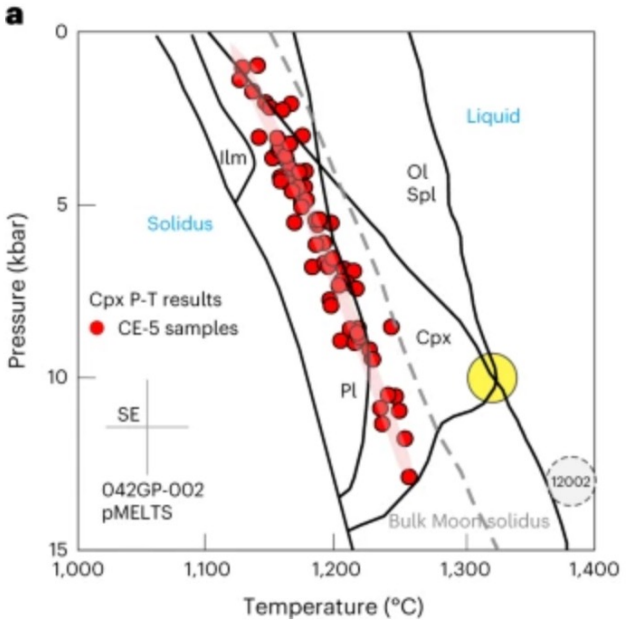
Thermodynamic models (& MELTS) underpin many scientific efforts

Eruption triggering mechanisms



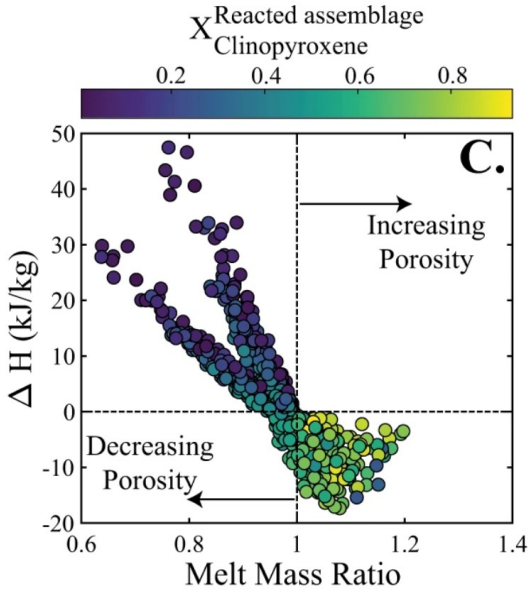
Brookfield et al. (2023)

Barometry of Lunar basalts



Luo et al. (2023)

Melt-mush reaction & mush porosity



Gleeson et al. (2023) & Boulanger & France (2023)