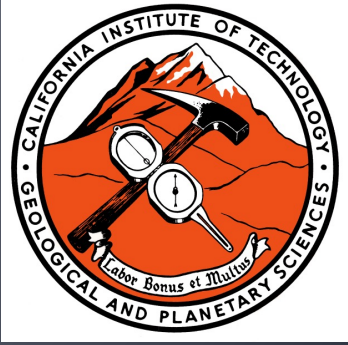
Paula Antoshechkina, Caltech
Paul D. Asimow, Caltech

alphaMELTS for MATLAB/Python

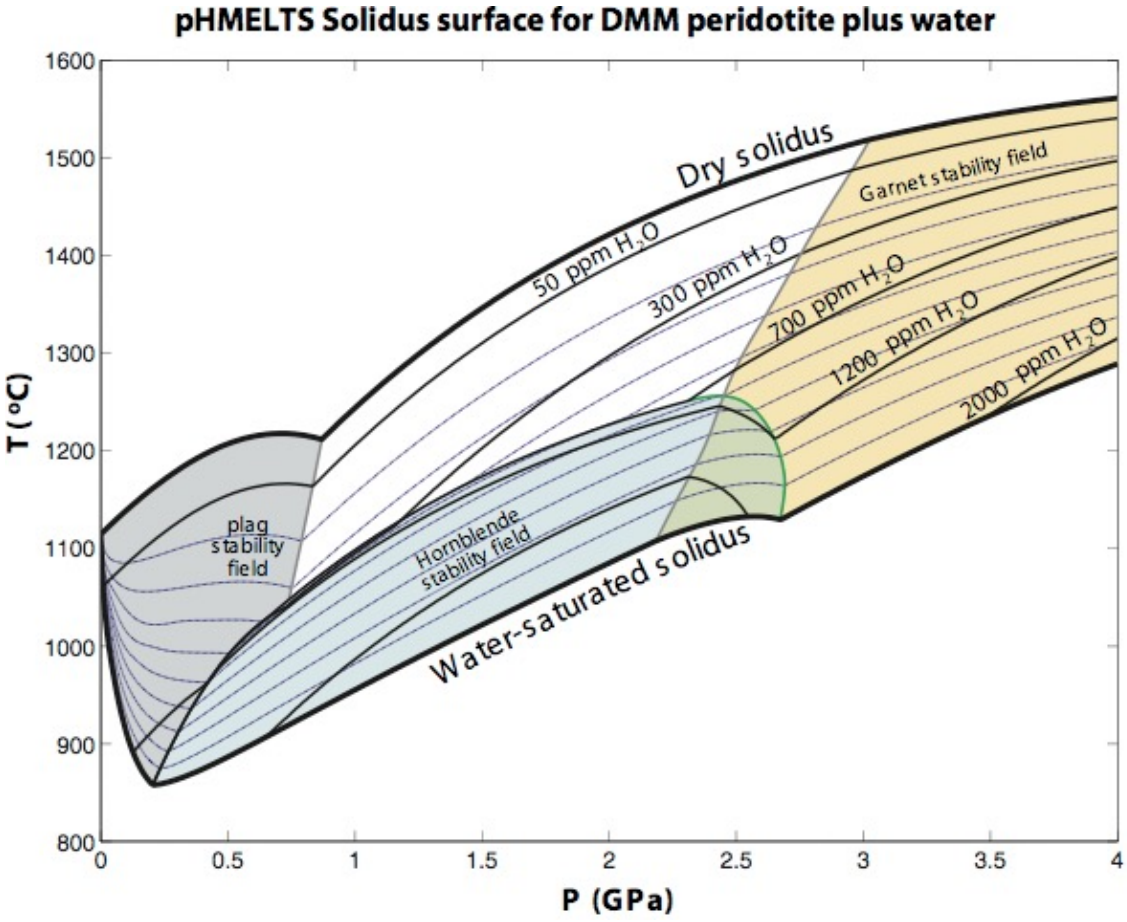
alphaMELTS2 workshop
Rotorua, NZ, January 28-29, 2023

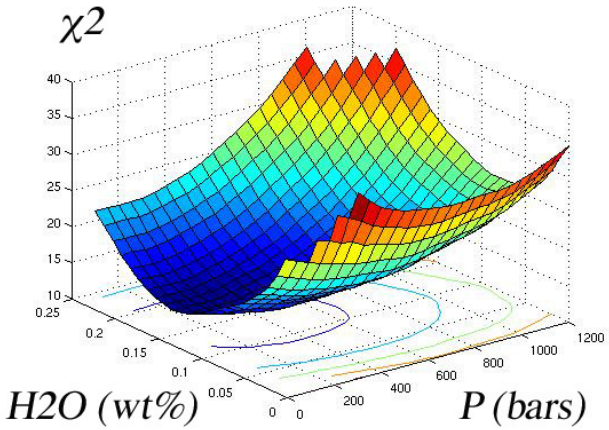
Caltech

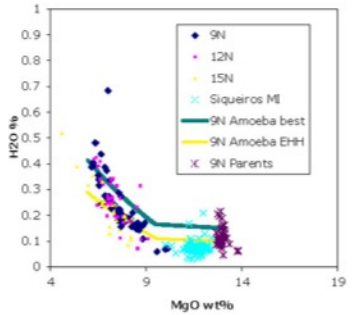


Early run-alphamelts.command

CAN RUN FROM MATLAB, PYTHON, R
- USE TEXT FILES FOR PLOTTING ETC.

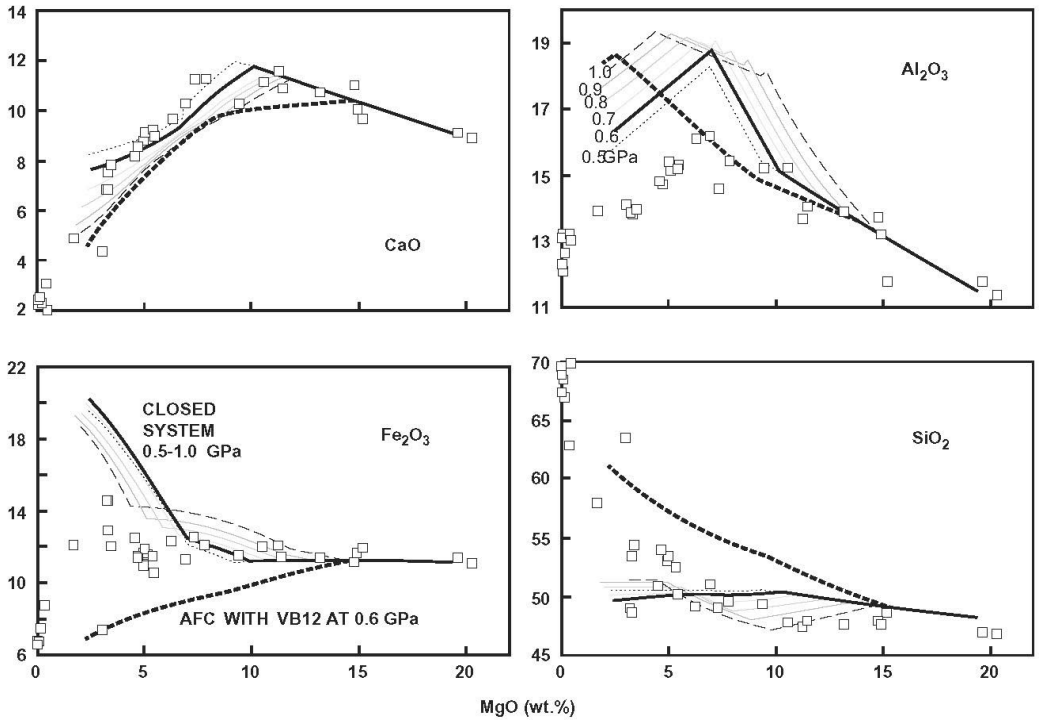


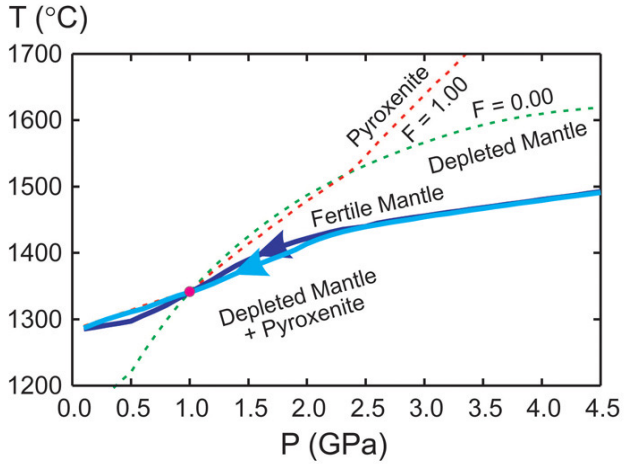


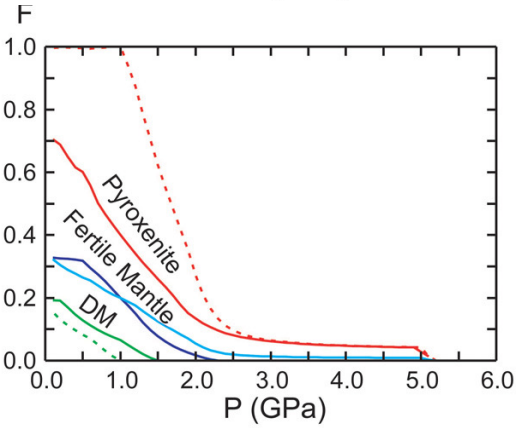


Assimilation / dual_adiabat

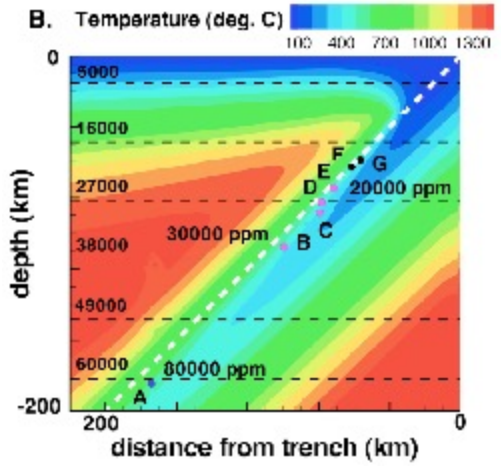
GUI REQUIRES "SUPPLEMENTAL CALCULATOR"
R.I.P. MELTS SUPPLEMENTAL CALCULATOR ~1995 - 2021

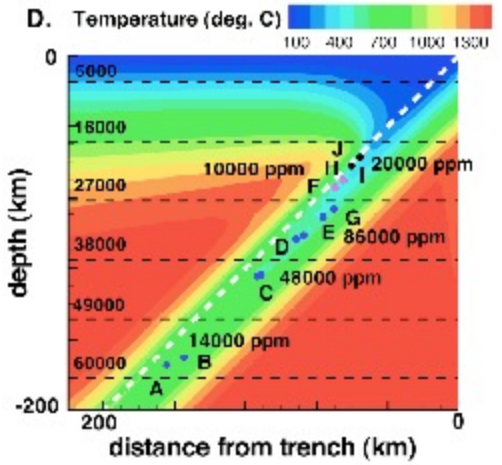


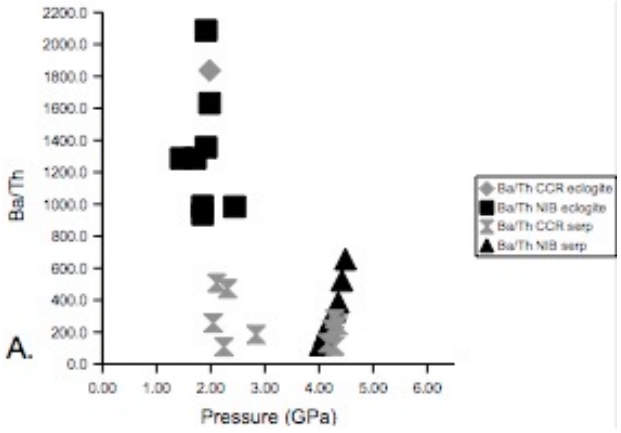


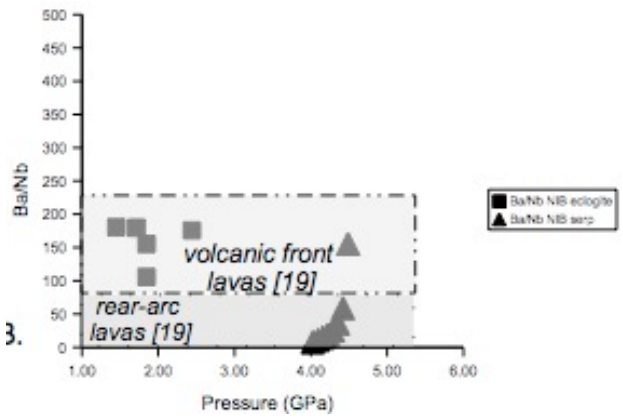


pHMELTS + Conman (text-based)

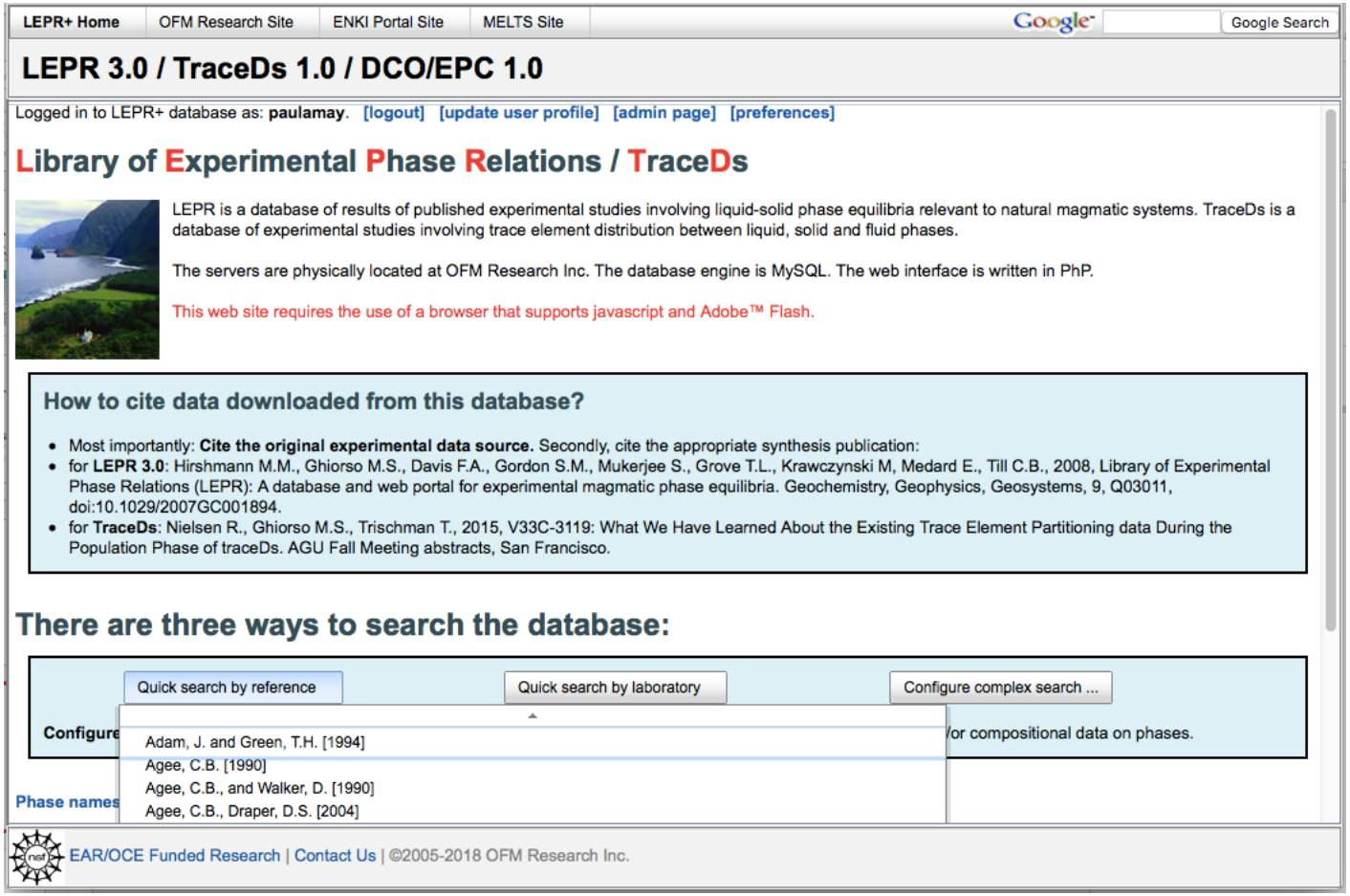




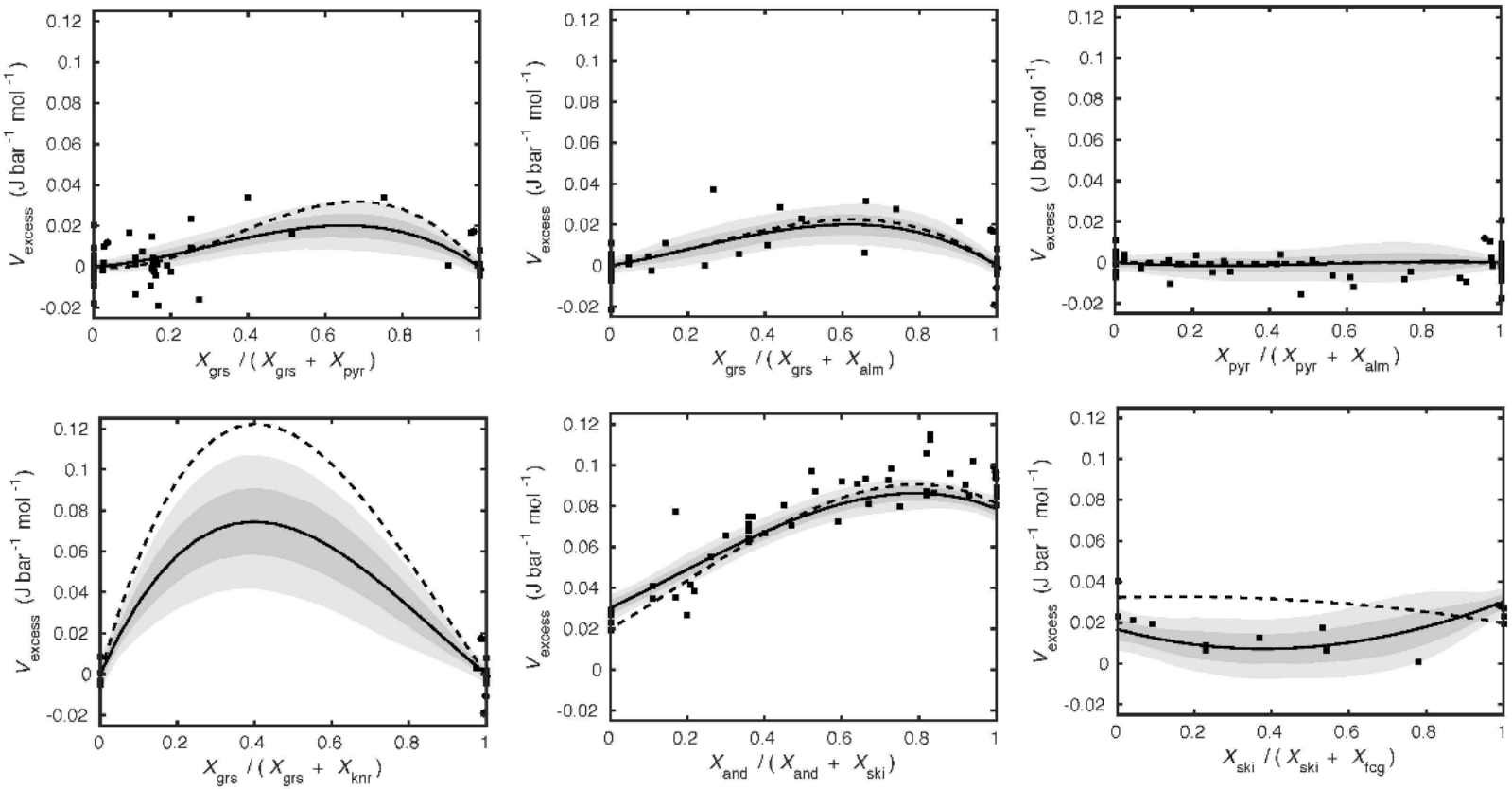




LEPR/traceDs: lepr.earthchem.org
Dev server at traceds.caltech.edu



Leprechaun + MELTS functions

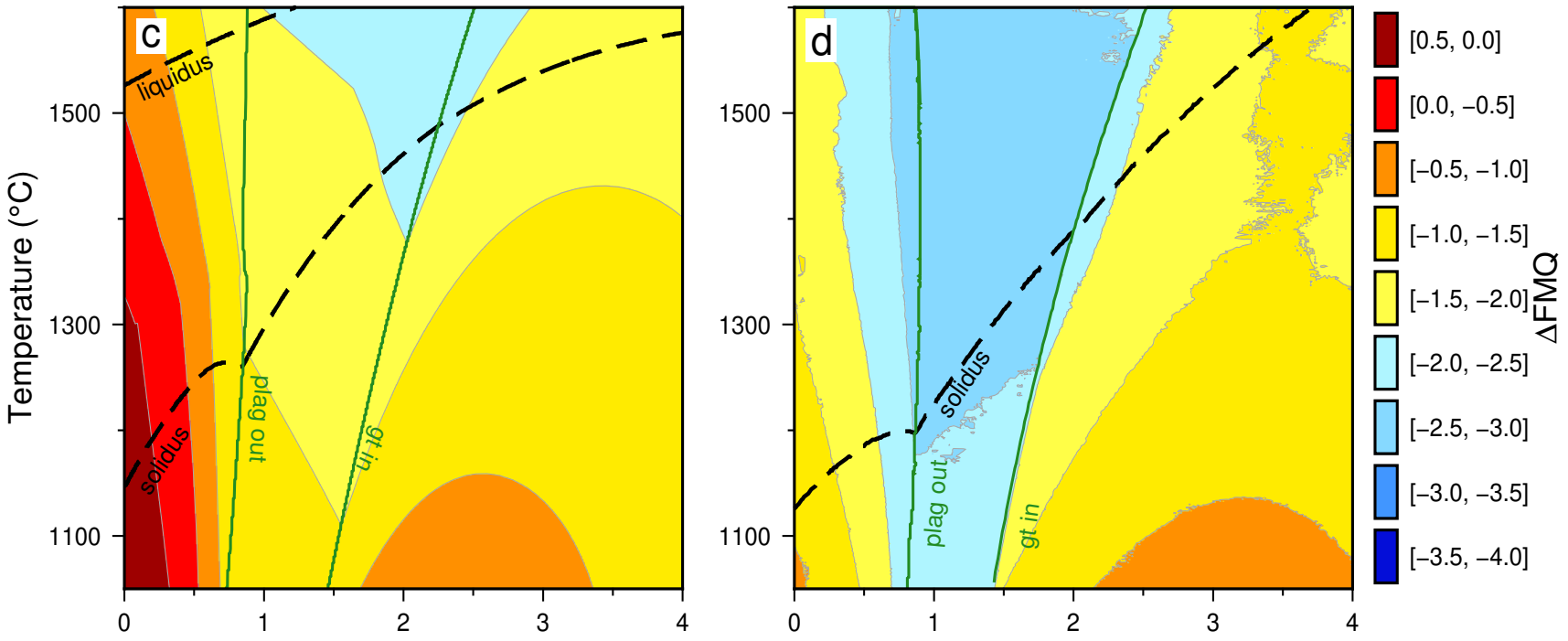


MATLAB/Python Outline

- Library of C functions, libalphaMELTS, that also underlies the alphaMELTS 2 executable
  - Some functions will mimic alphaMELTS 2 menu options
  - Also lower level access so it is very flexible and moderately scalable
- MATLAB/Python wrappers
  - https://gitlab.com/magmasource/MELTS_Matlab
- Was originally called MELTS for MATLAB
  - Starting to integrate more alphaMELTS-specific features

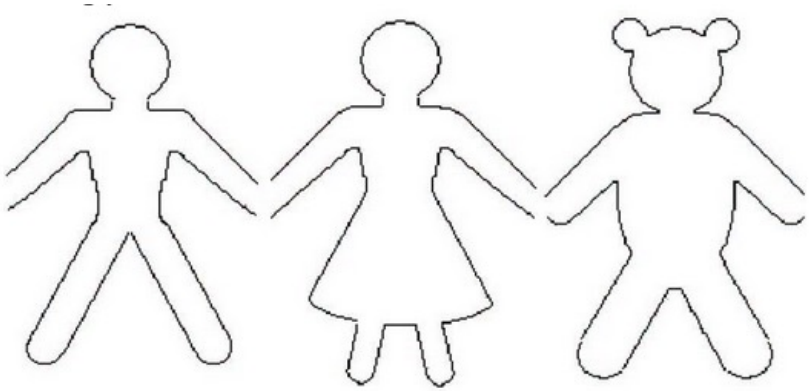
    https://agu2018fallmeeting-agu.ipostersessions.com/default.aspx?s=89-81-04-E9-EA-64-38-13-B4-11-17-CF-90-80-32-85&guestview=true

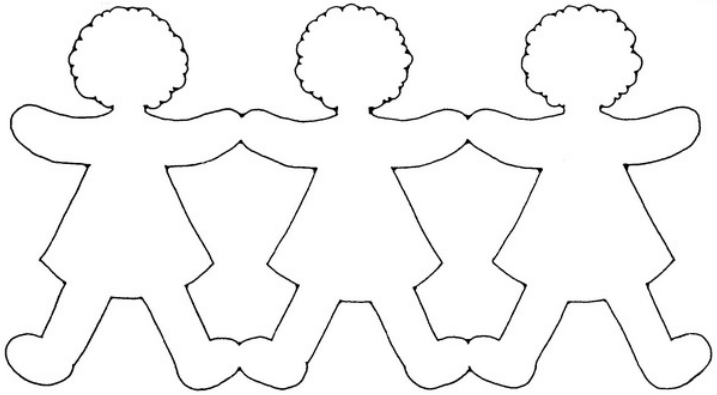
MELTS for MATLAB versus Perple_X



MATLAB/Python OOP

- Linked list of MELTS dynamic nodes
  - Each node can have GUI and 'Supplemental calculator'–like functionality
- Thermodynamic engine
  - ptpath = MELTSdynamic(4)
  - ptpath.engine
- Properties e.g.
  - ptpath.engine.temperature
- Methods include
  - ptpath.engine.findLiquidus
  - ptpath.engine.calcEquilibriumState





The paper doll analogy

- MATLAB is geared towards matrix operations, which makes for compact code for many applications but less so for MELTS calculations
  - The analogy we use in in-person workshops is how describing a group of people using separate lists for each of eye color, hair style etc. would be awkward; what we want is all the information about a particular person in one place
  - We do that by defining a "class"; properties of a particular instance of that class are accessed using the dot (.) operator (or '$' on R), which you can think of as a bit like "'s":

    paula.eyes.color = 'blue' paul.eyes.color = 'brown'
  - We can also add "methods" to the class, which are the things each instance of the class can do. The example we use in the in-person workshops is waving:

    paula.wave() paul.wave() thequeen.wave()
- In alphaMELTS for MATLAB/Python we take the analogy one step further
  - Each thermodynamic state (MELTSengine) is contained in a MELTSdynamic 'node' and the nodes are connected in a linked list
  - Each MELTSdynamic node contains information about which node is next, which node is first, which is the current node… sort of like a chain of paper dolls
  - When we add or delete nodes, join lists, or sort the list then the information about each node's place in the list is automatically updated… no scissors or tape required!
  - There are also tools to extract vectors and matrices of values from the MELTSdynamic list, as that's what we need for plotting

.melts file settings

- easyMelts / GUI
  - **Initial** Composition:
  - Log fO2 Path
  - Mode: fractionate solids
  - **Assimilant**: …
- alphaMELTS 2
  - The above plus …
  - Mode: fractionate olivine
  - Log fO2 Offset
  - **Set** min F:
- alphaMELTS for MATLAB/Python
  - **Initial** lines are all set another way
  - **Assimilant** lines will be set another way

    Not yet implemented
  - Other lines as strings

    .engine.set SystemProperties
  - **Set** lines (after workshop)

    (Set) Output: …

    Other **Set** lines

MATLAB/Python classes

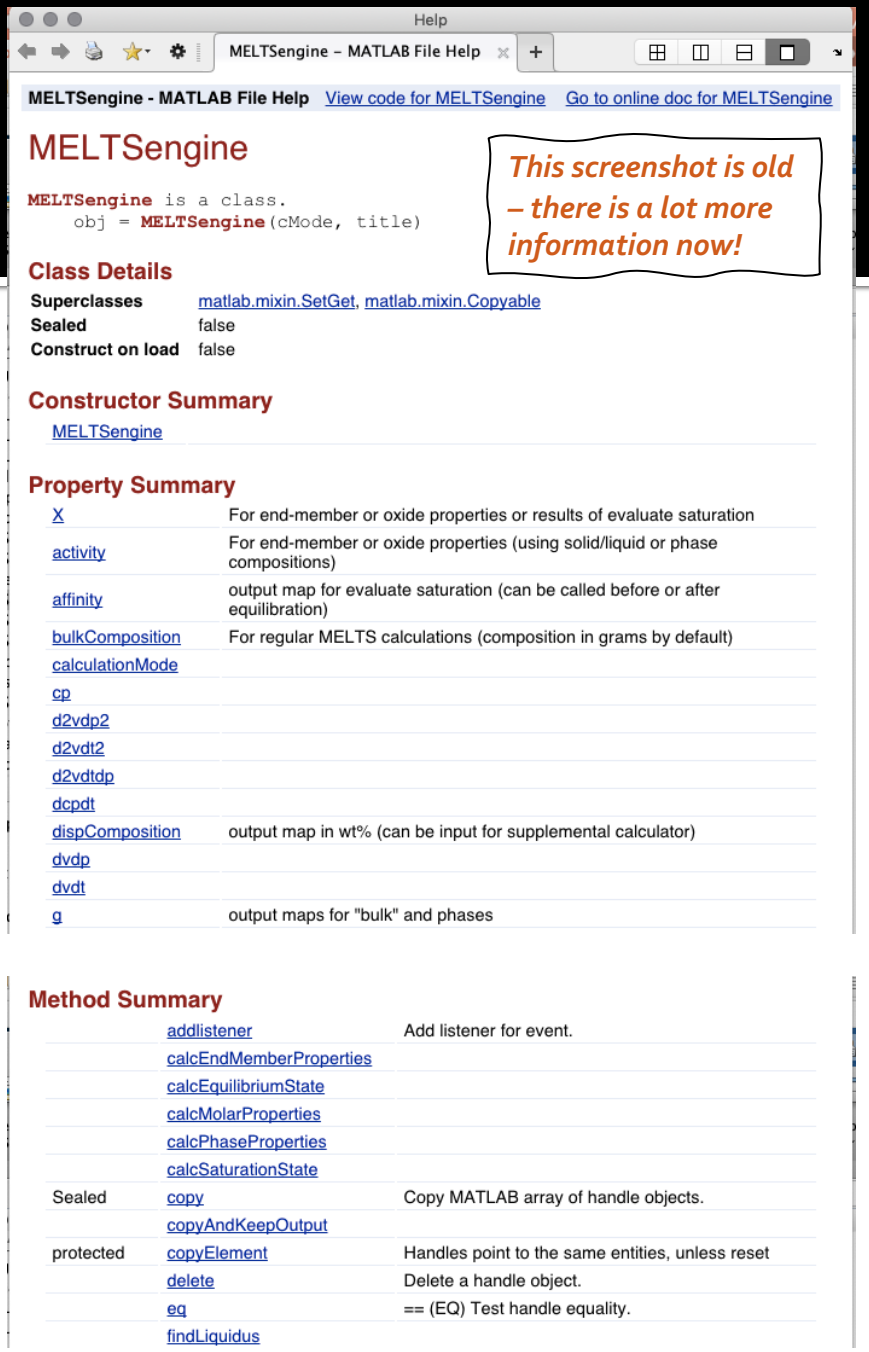
- MELTSdynamic handles linked list and system wide properties associated with choice of model (e.g. rhyolite-MELTS 1.2.0; pMELTS…)
  - E.g. what phases are available?
- All the hard work is done in MELTSengine
  - E.g. what phases are actually present?
- MELTSstatus (and MELTSevent) track interaction with the C library of MELTS functions
  - How many calculations have we done (line number in any output files)? Did something go wrong, can it clean up?
  - Console on Windows version

More tools

- MELTSmap makes it easier to extract vectors and matrices of data from the 'paper doll'-like structures of properties needed for thermodynamic calculations
- Tools to join lists, add or remove nodes, sort lists of nodes
- Start a new MELTSdynamic list to switch between pMELTS and rhyolite-MELTS models
- Handles errors gracefully

Getting help

- MATLAB type e.g: "help MELTSengine"
  - Click on "Reference page for MELTSengine"
  - Explore the properties and methods
  - Will show how to call 'methods' (like functions), what output is like etc.
- Python (limited) type e.g: "help(MELTSdynamic())"
  - Also check .py source
- Coming soon: Doxygen docs for all platforms.



Examining alphaMELTS classes

- Can examine particular instance on MATLAB command line
  - Tab completion is your friend!

```
>> ptpath

ptpath =

  MELTSdynamic with properties:

      calculationMode: 4
           modeString: 'MELTSandCO2_H2O'
          systemNames: [1×46 string]
    endMemberFormulas: [46×1 MELTSmap]
     endMemberWeights: [46×1 MELTSmap]
        failureHandle: [1×1 event.listener]
            nodeIndex: 276
               engine: [1×1 MELTSengine]
                 Next: [0×0 MELTSdynamic]
                 Prev: [1×1 MELTSdynamic]
                First: [1×1 MELTSdynamic]
                 Last: [1×1 MELTSdynamic]
```

```
>> ptpath.engine

ans =

  MELTSengine with properties:

             status: [1×1 MELTSstatus]
    calculationMode: 4
              title: []
         meltsIndex: 275
            runMode: 1
           pressure: 250
        temperature: 1.1892e+03
          reference: -1.4584e+05
             logfO2: -13.2238
   systemProperties: [2×1 string]
    bulkComposition: [19×1 double]
       liquidNames: "liquid1"
        solidNames: ["olivine1"    "plagioclase1"    "fluid1"]
       phaseNames: [1×1052 string]
  phaseComposition: [19×1 double]
  molarComposition: []
                 g: [0×1 MELTSmap]
                 h: [0×1 MELTSmap]
                 s: [0×1 MELTSmap]
                 v: [0×1 MELTSmap]
                cp: [0×1 MELTSmap]
             dcpdt: [0×1 MELTSmap]
              dvdt: [0×1 MELTSmap]
              dvdp: [0×1 MELTSmap]
            d2vdt2: [0×1 MELTSmap]
           d2vdtdp: [0×1 MELTSmap]
            d2vdp2: [0×1 MELTSmap]
             molwt: [0×1 MELTSmap]
               rho: [0×1 MELTSmap]
              mass: [0×1 MELTSmap]
         viscosity: [0×1 MELTSmap]
    dispComposition: [0×1 MELTSmap]
          affinity: [0×1 MELTSmap]
                 X: [0×1 MELTSmap]
          activity: [0×1 MELTSmap]
               mu0: [0×1 MELTSmap]
                mu: [0×1 MELTSmap]
```

Features

- MATLAB
  - Able to change MELTS model during calculation
  - Also should scale
- Python
  - Not able to change MELTS model during run
  - Complements ENKI tools
- Both
  - Good for desktop applications
  - Can change system in between call to C library of functions

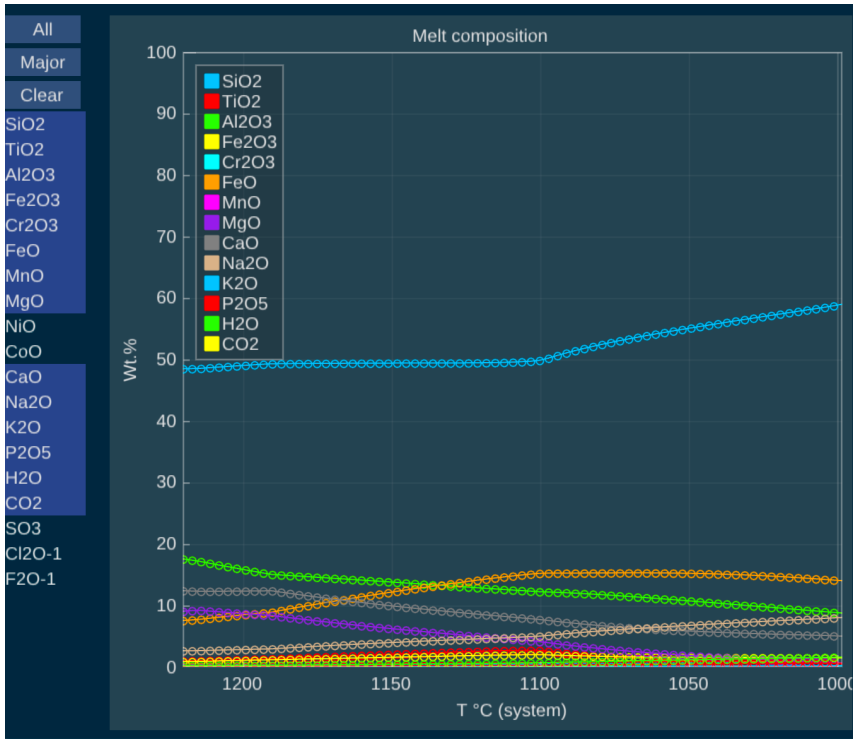
    Can in principle do (simple) MCS-like calculations and dual_adiabat-like calculations.
  - Can also output _tbl.txt and .tbl text files and process with "run_alphamelts.command –x"

Compare ENKI (enki-portal.org)

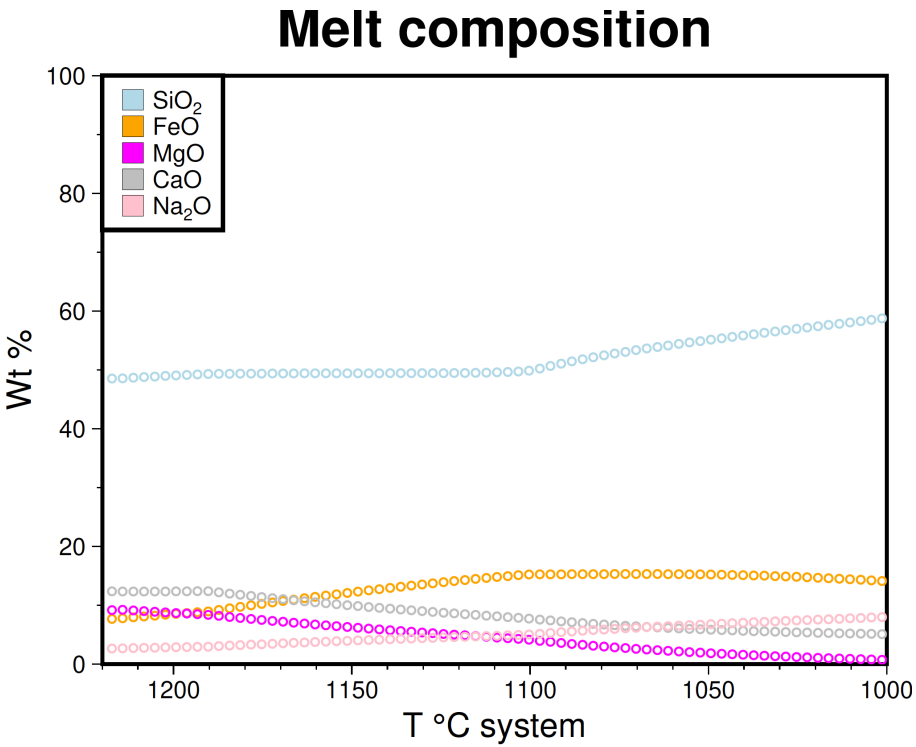
- alphaMELTS for Python
  - Based on "xMelts" C code (gitlab.com/ENKI-portal)
    - Codebase for rhyolite-MELTS GUI and Magma Chamber Simulator's MELTS-batch
    - Adapted for alphaMELTS 2 and alphaMELTS for MATLAB/Python
  - Relatively small and easy local installation
  - Classes and methods make automating typical tasks and plotting results easy
  - Will have higher level alphaMELTS menu-like functions
  - Will have trace elements and pHMELTS eventually
- ENKI Thermoengine
  - Uses "Thermoengine" ObjectiveC and Python code
  - Run online or locally via Docker
  - Low level methods allow for more flexibility than alphaMELTS for Python, but with a steeper learning curve
  - Best way to get started is with Workshop Jupyter Notebooks
  - Will have highly optimised "coder" module-generated C code eventually
  - Will scale efficiently and is recommended for larger coupled thermodynamic and fluid-dynamic simulations

Comparisons of the 'tutorial'

- Compare standalone alphaMELTS to easyMelts
  - Also very useful for debugging (+console)



- Also Compare MATLAB and Python with GMT
- Compare R (next slide)



More 'tutorial' comparisons

- Compare ENKI's Thermoengine
  - Steeper learning curve (e.g. no "Find Liquidus" unless you code it yourself)
  - Current code is fast but takes time to get files from ENKI server in the cloud or from the docker image
  - Future Thermoengine code will be ~10x faster so more scalable than alphaMELTS for Python

Initialize tools and packages that are required

[12]:
```
from thermoengine import equilibrate
import matplotlib.pyplot as plt
import numpy as np
%matplotlib inline
```

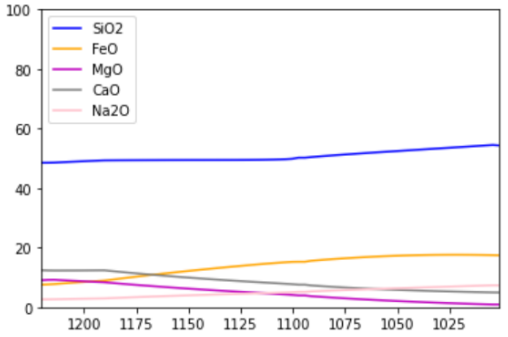
• • •

Create a MELTS v 1.0.2 instance.

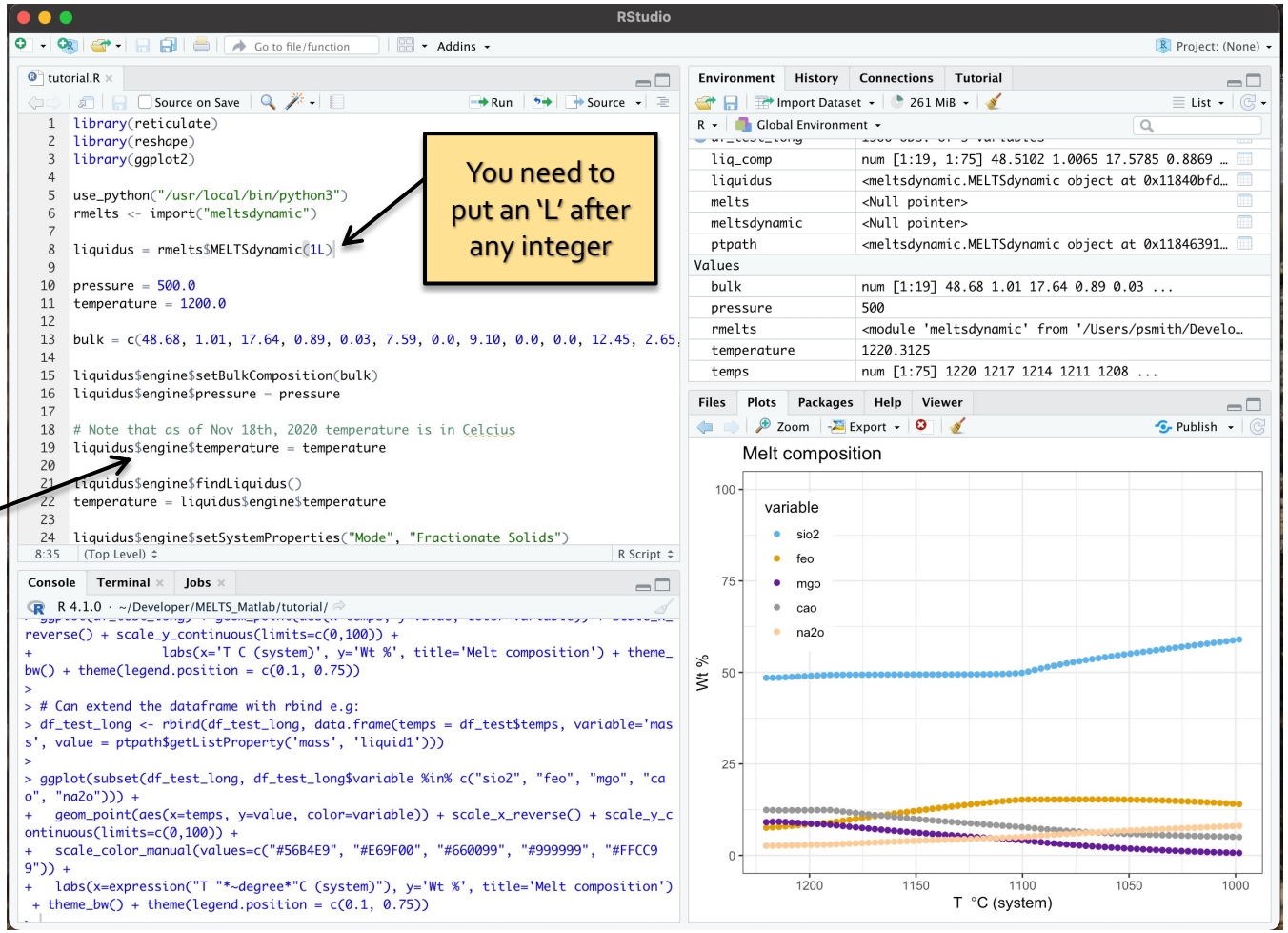
Rhyolite-MELTS version 1.0.2 is the default model.

[13]:
```
melts = equilibrate.MELTSmodel()
```

```
success, Minimal energy computed.  1022.30    50.00
success, Optimal residual norm.  1019.30    50.00
success, Optimal residual norm.  1016.30    50.00
success, Optimal residual norm.  1013.30    50.00
success, Optimal residual norm.  1010.30    50.00
success, Optimal residual norm.  1007.30    50.00
success, Optimal residual norm.  1004.30    50.00
```



R with alphaMELTS for Python



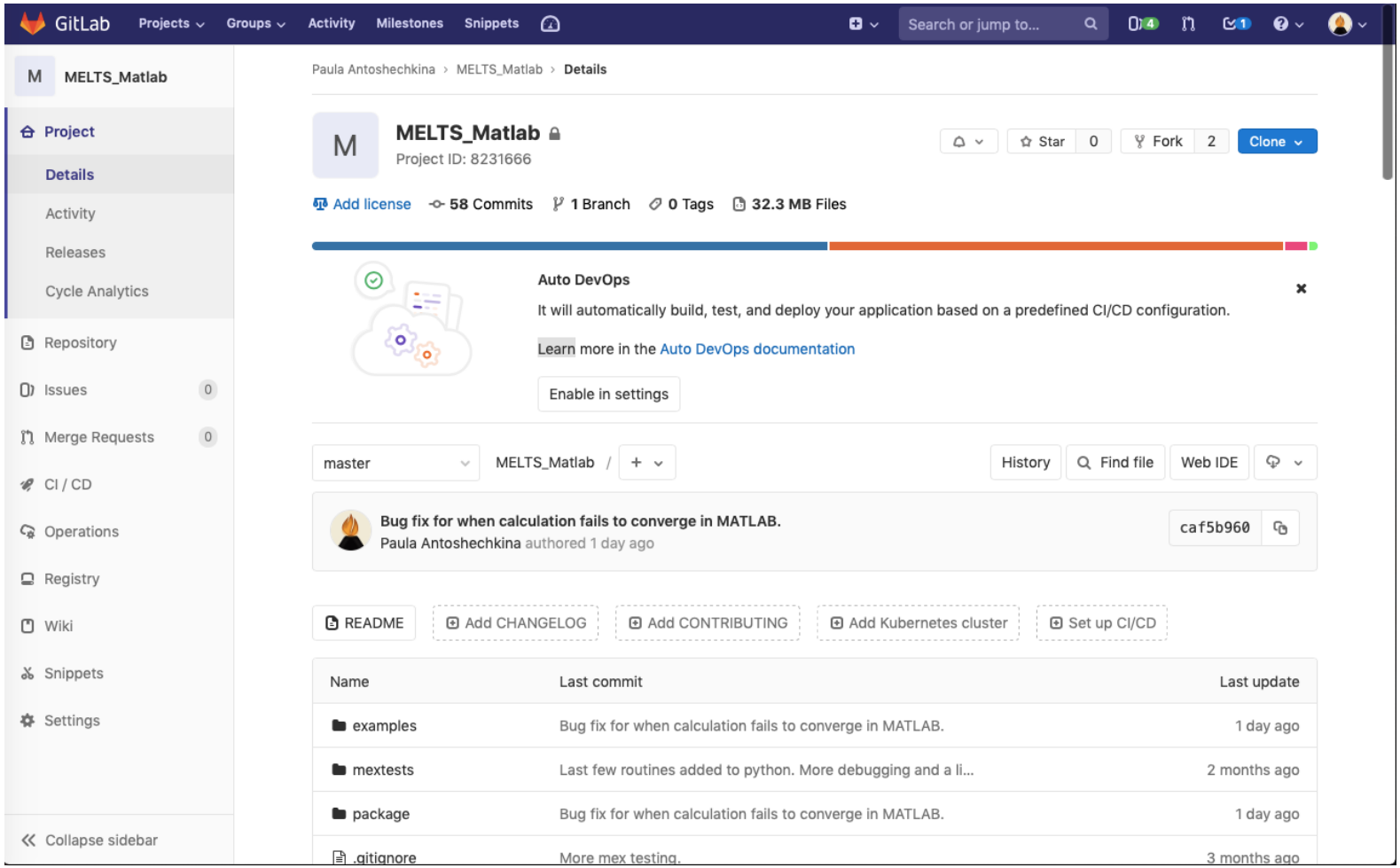
Python / R version

- Python version requires tinynumpy
  - pip install tinynumpy
  - pip3 install tinynumpy
- Running in Rstudio
  - reticulate::install_miniconda()
  - reticulate::py_install("tinynumpy", method="pip")
  - reticulate::repl_python()

Future work and links

- alphaMELTS@CIT
  - alphamelts.caltech.edu
  - 'Wiki' or similar documentation
- MAGMA@Caltech
  - magmasource.caltech.edu
  - For alphaMELTS 1.9 and all other MELTS interfaces
- DACITE
  - Database of AlphaMELTS at CIT Examples
  - Standalone, MATLAB, Python, Jupyter, R
- Trace Elements
- Code will eventually be Open Source on Github

alphaMELTS temp home on GitLab



alphaMELTS temp home on GitLab

- Sign up at gitlab.com
  - Send your username
  - Sign up for notifications
- Watch this space!
  - XML output that can be fed into GCDkit
  - fO_2 alternative
  - Different ways to do assimilation
  - Phase diagram mode
  - Integrated output file
  - Integration with pyrolite
  - Trace elements and pHMELTS