MAGEMIN WORKSHOP

SGGMP 2025

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MY THANKS TO

Nicolas Riel & the MAGEMin team - Johannes Gutenberg University of Mainz

Tris Stuck

Alex Win

...and thanks for inviting us!

SHOW OF HANDS

- Who has downloaded Julia and MAGEMinApp already?
- Who has used MAGEMin before?

SCHEDULE

- Introduction to MAGEMin (first ~15 min):
  - What is MAGEMin and what can it do?
  - How to get started or find more advanced info
  - MAGEMin idiosyncrasies - some tips and tricks before you get going.
- Exercises: Start at the beginning, or jump in part way through if you've used MAGEMin before.
- Discussion (last ~15 min): the underlying thermodynamic models.

WHAT IS MAGEMIN?

Program for calculating most-stable phase geological equilibria under a variety of conditions.

Similar to THERMOCALC, Perple_X, Theriak, GeoPS, but:

- very fast;
- very wide range of automatic calculations available;
- designed to integrate into geodynamics calculations.

MAGEMIN DEVELOPMENT

Dr Nicolas Riel
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Originally funded by a European Research Council Consolidator grant to Prof Boris Kaus.

Currently supported by the Deutsche Forschungsgemeinschaft.

MAGEMIN DEVELOPMENT

Dr Nicolas Riel
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Riel N, Kaus BJP, Green ECR, Berlie N (2022). MAGEMin, an Efficient Gibbs Energy Minimizer: Application to Igneous Systems. *Geochemistry, Geophysics, Geosystems* 23, e2022GC010427

Riel N, Kaus BJP, de Montserrat A, Moulas E, Green ECR, Dominguez H (2025). A bound-constrained formulation for complex solution phase minimization. *Geoscientific Model Development* 18, 6951-6962

Ongoing development with help from many programmers and modellers.

USEFUL LINKS

Link for this workshop:

https://sggmp25.com/magemin-workshop

Link to MAGEMin website:

https://computationalthermodynamics.github.io/MAGEMin_C.jl/dev/

MAGEMIN VERSUS OTHER EQUILIBRIUM CALCULATORS

MAGEMin – Nico Riel et al	• Fastest, largest set of automated diagrams, including fractional melting/crystallization. • Julia-based integration into scripts for external control. • Any of the HP dataset-based thermodynamic models: metapelites, metabasites, igneous. • Web interface via Julia. • Extensive documentation.
GeoPS – Xiang Hua & Jamie Connolly	• Many types of automated phase diagram, including fractional melting/crystallization. • Simple web app.
Perple_X – Jamie Connolly	• The original most-stable equilibrium calculator. • Very wide range of thermodynamic models available.
THERMOCALC – Roger Powell, Tim Holland, Eleanor Green	• Calculates equilibria, not most-stable equilibria. Don't use for big pseudosection calculations! • Non-automated calculations in small chemical systems. • Learn to understand phase equilibria.

MAGEMIN: GETTING STARTED

Julia, MAGEMinApp, MAGEMin_C: what are they?

Julia	Programming language that facilitates parallel computing and visualization. Must be installed and run through PowerShell (Windows) or Terminal (Mac) to install and run MAGEMin. General Julia info at: https://julialang.org/ Julia: A Fresh Approach to Numerical Computing. Jeff Bezanson, Alan Edelman, Stefan Karpinski, Viral B. Shah. (2017) *SIAM Review*, 59: 65–98.
MAGEMinApp	Interactive interface for MAGEMin, viewed your web browser after you've activated it via Julia. Most users will access MAGEMin this way.
MAGEMin_C	The muscle behind MAGEMinApp: routines to do the phase diagram calculations. Access directly via Julia scripts.

The guided exercise will use MAGEMinApp. If you're already an expert, write a Julia script to do the same with MAGEMin_C!

Not online! – the web browser just displays SVG

MAGEMIN: GETTING STARTED

Overview of exercise

- Calculate a *P-T* pseudosection: a map of stable phase equilibria in *P-T* space for a single bulk rock composition.
- Explore the input, output, documentation.
- Explore variations on the calculation: isopleths, fixing fO2, T-X and P-X sections.
- Calculate instantaneous equilibria along a path in P-T-X space.
- Add trace elements into the calculation.

MAGEMIN: GETTING STARTED

If you're not already familiar with MAGEMin:

- Don't necessarily expect to get to the end.
- Should be easy to work to the end after the workshop.

If you are already familiar with MAGEMin:

- Several jump-in points throughout the exercise.
- Have you seen MAGEMin's latest capabilities?

MAGEMIN TIP: COMPOSITION

MAGEMin inherits its approach to composition (bulk composition and phase compositions) from THERMOCALC.

Underlying units:

- mol% oxides – for the bulk rock/system composition.
- mole fraction of end-members – for individual phases.

For Fe2+ versus Fe3+ in the bulk rock, MAGEMin's units are

- molar FeOt (all iron as FeO)
- molar O (oxygen).

Generally, user can control input and has a choice of output.

But I'll indicate where it's good to be aware of this behaviour.

MAGEMIN TIP: COMPOSITION

Quick reference: ferric and ferrous iron units

Equating numbers of moles:

FeO = FeOt – 2 O

Fe2O3 = O

thus, $Fe^{3+}/(Fe^{2+} + Fe^{3+})$ = 2 O/FeOt

where FeOt is all iron as FeO

DEMO

please cooperate, MAGEMin :-)

Starting point for beginners

EXERCISE 1

Work through the following, with help as needed from:

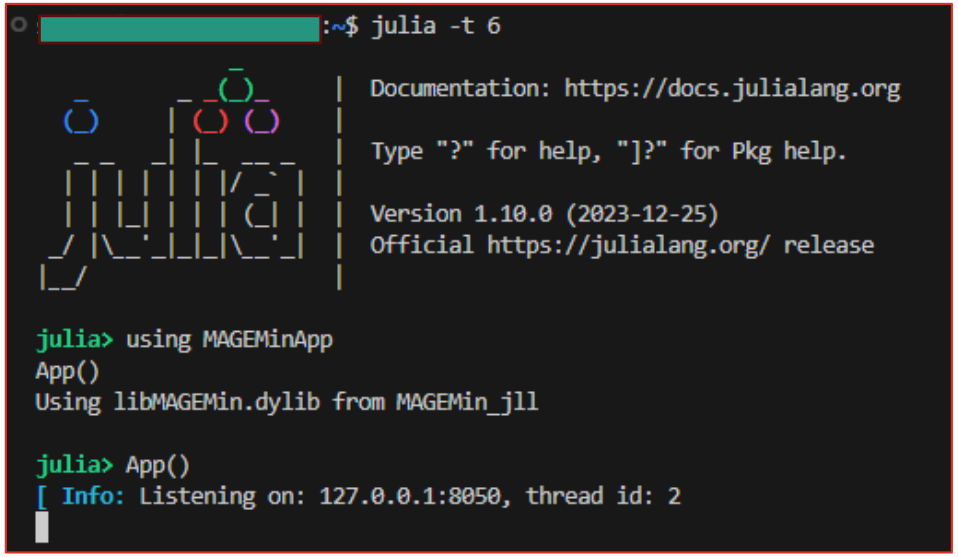
- The slides below
- Demonstrators
- The MAGEMin website at https://computationalthermodynamics.github.io/MAGEMin_C.jl/dev/MAGEMinApp/MAGEMinApp
- Tris Stuck's introductory video (no sound) available from https://sggmp25.com/magemin-workshop.

Starting point for beginners

EXERCISE 1

1. Start MAGEMinApp

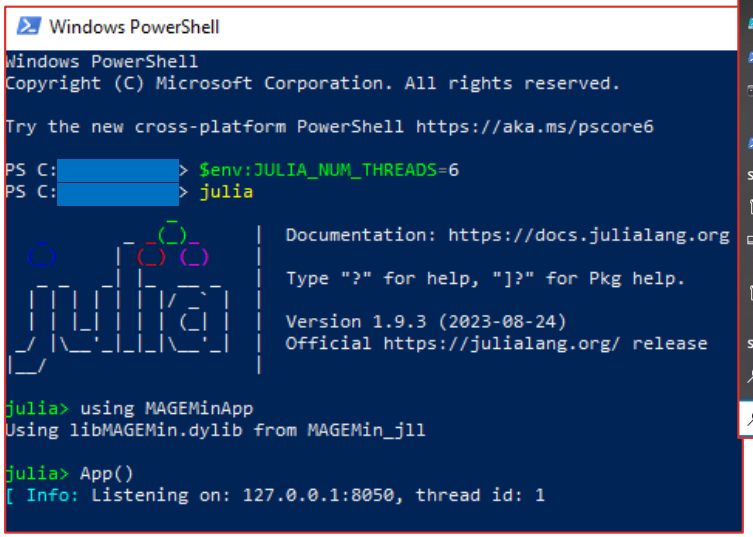
VISUAL STUDIO CODE / TERMINAL
MAC, LINUX

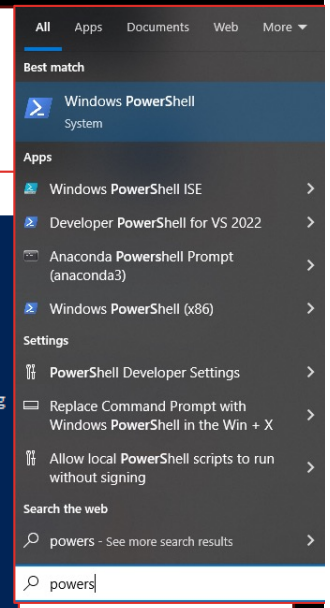


julia –t 6
using MAGEMinApp
App()

"-t 6" and "env:JULIA_NUM_THREADS=6" tell Julia to run on 6 processors. Modify or omit as preferred.

POWERSHELL
WINDOWS





$env:JULIA_NUM_THREADS=6
julia
using MAGEMinApp
App()

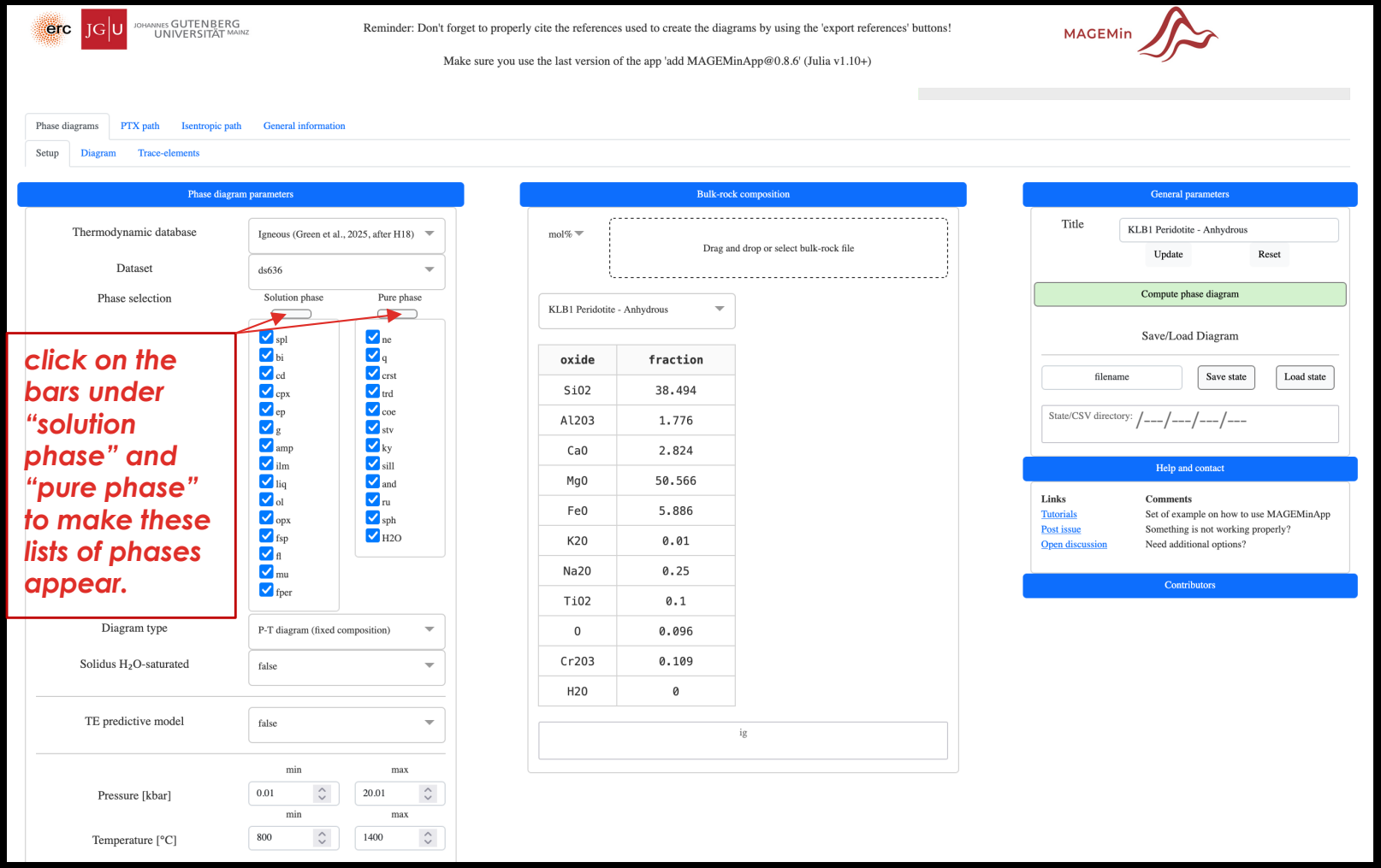
Now copy-paste 127.0.0.1:8050 into your internet browser's address bar. Julia is listening!

Starting point for beginners

EXERCISE 1

1. **Start MAGEMinApp**

Your browser should now be showing you:



EXERCISE 1

2. **Explore the MAGEMinApp interface**

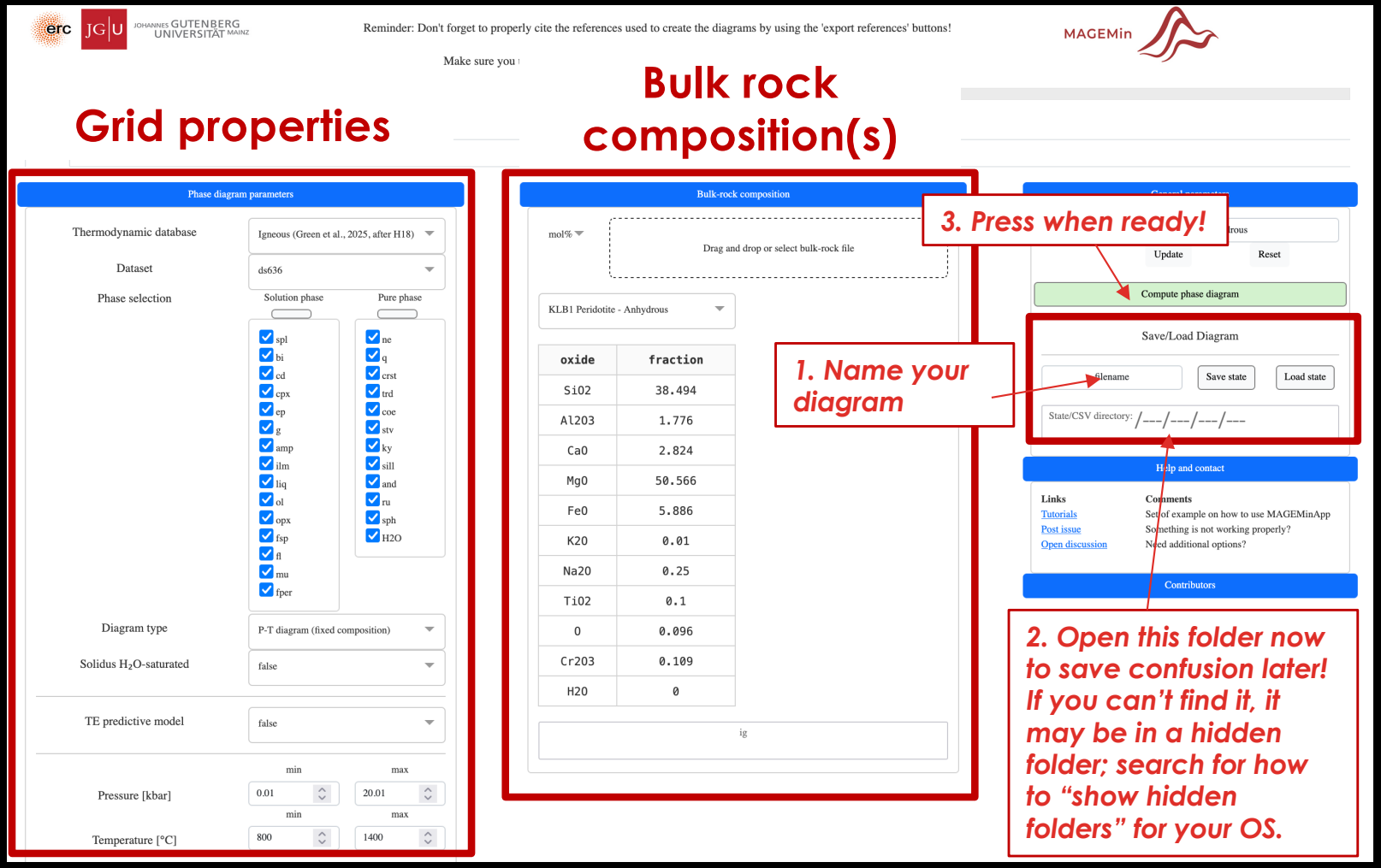
The default example that you see set up is:

- A *P-T* pseudosection calculation, for fixed bulk composition including fixed bulk FeO, Fe2O3;
- For the Kilbourne Hole peridotite composition KLB-1 as determined by Davis et al (2009); note this is displayed in mol% oxides;
- Calculations will use the underlying thermodynamic model called "igneous set" (Green et al 2025, following Holland et al 2018 – see discussion later).

EXERCISE 1

2. **Explore the MAGEMinApp interface**

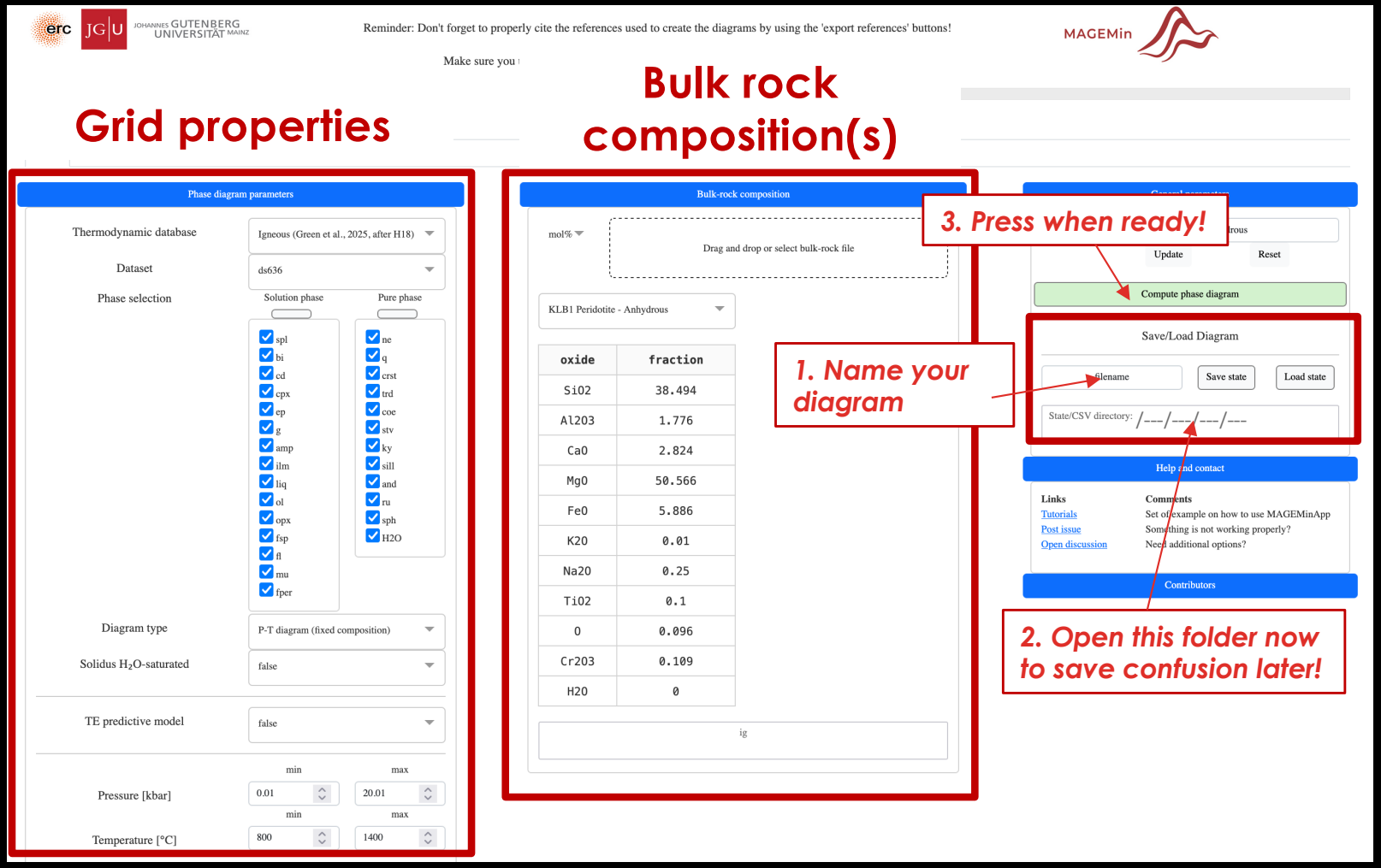
Inspect the settings, locate your save folder, and press the green Compute button when ready!



EXERCISE 1

2. **Explore the MAGEMinApp interface**

The calculation will take a few seconds, depending how many processors you are using. Follow progress in the Julia window…

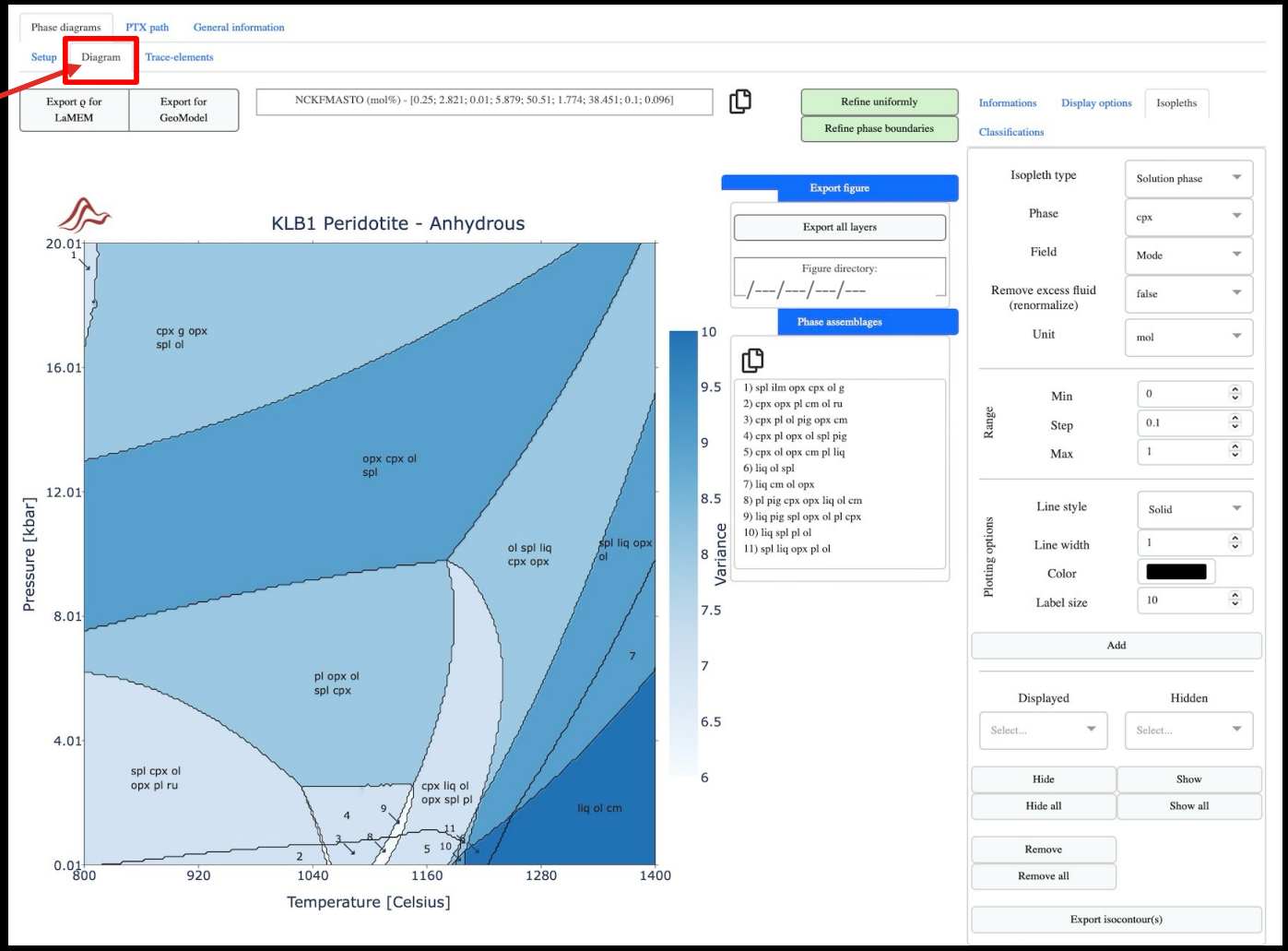


EXERCISE 1

3a. **Inspect your first MAGEMin phase diagram**

Click the "Diagram" tab.

We can already see the phase assemblage fields nicely.



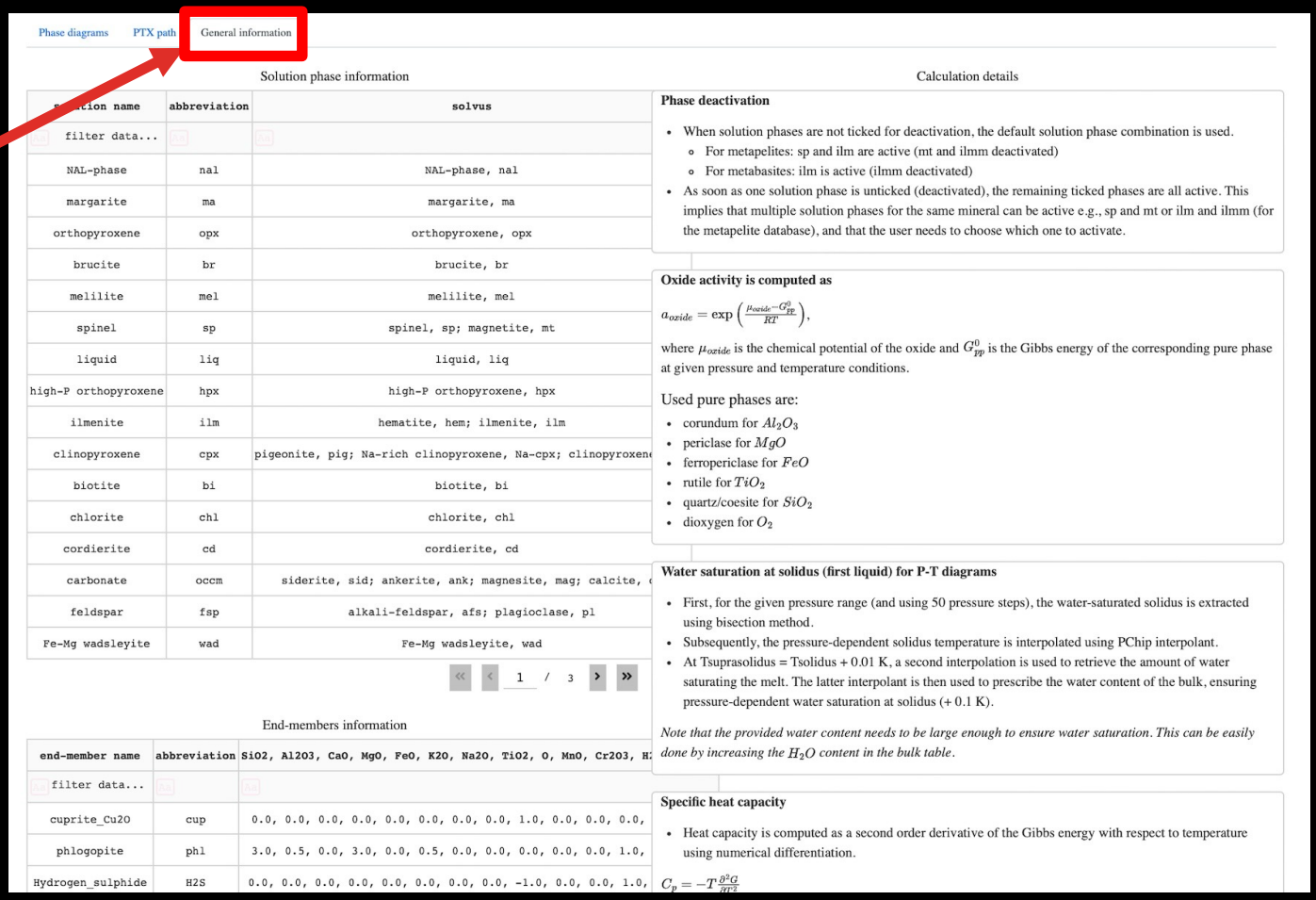
EXERCISE 1

3b. **Inspect your first MAGEMin phase diagram**

Confused by the mineral abbreviations?

Click on "General information"

Lots to read here....



Phase diagrams | PTX path | General information

Solution phase information

solution name	abbreviation	solvus
filter data...		
NAL-phase	nal	NAL-phase, nal
margarite	ma	margarite, ma
orthopyroxene	opx	orthopyroxene, opx
brucite	br	brucite, br
melilite	mel	melilite, mel
spinel	sp	spinel, sp; magnetite, mt
liquid	liq	liquid, liq
high-P orthopyroxene	hpx	high-P orthopyroxene, hpx
ilmenite	ilm	hematite, hem; ilmenite, ilm
clinopyroxene	cpx	pigeonite, pig; Na-rich clinopyroxene, Na-cpx; clinopyroxene
biotite	bi	biotite, bi
chlorite	chl	chlorite, chl
cordierite	cd	cordierite, cd
carbonate	occm	siderite, sid; ankerite, ank; magnesite, mag; calcite,
feldspar	fsp	alkali-feldspar, afs; plagioclase, pl
Fe-Mg wadsleyite	wad	Fe-Mg wadsleyite, wad

« ‹ 1 / 3 › »

End-members information

end-member name	abbreviation	SiO2, Al2O3, CaO, MgO, FeO, K2O, Na2O, TiO2, O, MnO, Cr2O3, H2
filter data...		
cuprite_Cu2O	cup	0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 1.0, 0.0, 0.0, 0.0,
phlogopite	phl	3.0, 0.5, 0.0, 3.0, 0.0, 0.5, 0.0, 0.0, 0.0, 0.0, 0.0, 1.0,
Hydrogen_sulphide	H2S	0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, -1.0, 0.0, 0.0, 1.0,

Calculation details

Phase deactivation

- When solution phases are not ticked for deactivation, the default solution phase combination is used.
  - For metapelites: sp and ilm are active (mt and ilmm deactivated)
  - For metabasites: ilm is active (ilmm deactivated)
- As soon as one solution phase is unticked (deactivated), the remaining ticked phases are all active. This implies that multiple solution phases for the same mineral can be active e.g., sp and mt or ilm and ilmm (for the metapelite database), and that the user needs to choose which one to activate.

Oxide activity is computed as

$a_{oxide} = \exp\left(\frac{\mu_{oxide} - G^0_{pp}}{RT}\right)$,

where μ_{oxide} is the chemical potential of the oxide and G^0_{pp} is the Gibbs energy of the corresponding pure phase at given pressure and temperature conditions.

Used pure phases are:

- corundum for Al_2O_3
- periclase for MgO
- ferropericlase for FeO
- rutile for TiO_2
- quartz/coesite for SiO_2
- dioxygen for O_2

Water saturation at solidus (first liquid) for P-T diagrams

- First, for the given pressure range (and using 50 pressure steps), the water-saturated solidus is extracted using bisection method.
- Subsequently, the pressure-dependent solidus temperature is interpolated using PChip interpolant.
- At Tsuprasolidus = Tsolidus + 0.01 K, a second interpolation is used to retrieve the amount of water saturating the melt. The latter interpolant is then used to prescribe the water content of the bulk, ensuring pressure-dependent water saturation at solidus (+ 0.1 K).

Note that the provided water content needs to be large enough to ensure water saturation. This can be easily done by increasing the H_2O content in the bulk table.

Specific heat capacity

- Heat capacity is computed as a second order derivative of the Gibbs energy with respect to temperature using numerical differentiation.

$C_p = -T\frac{\partial^2 G}{\partial T^2}$

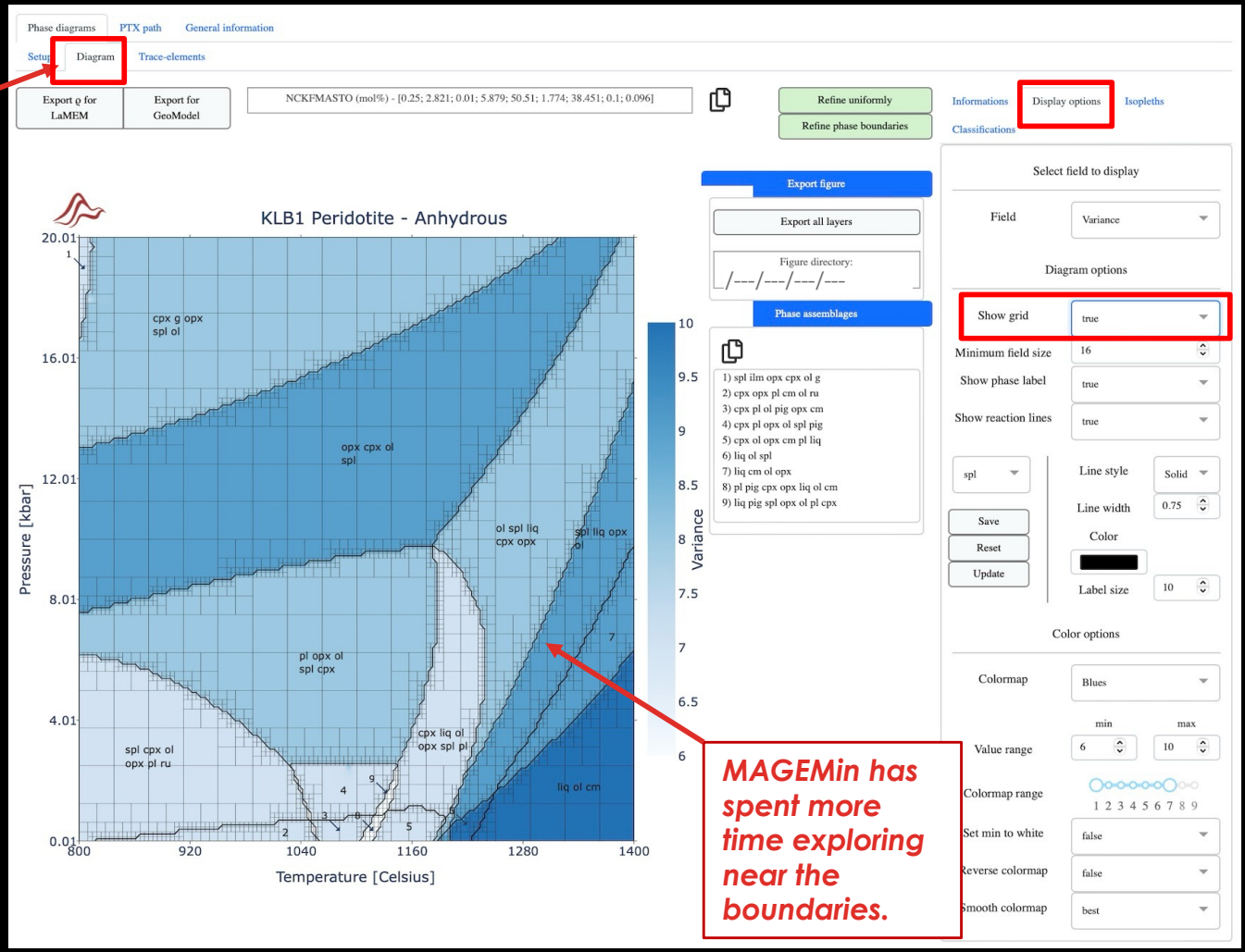
EXERCISE 1

3c. **Inspect your first MAGEMin phase diagram**

Click back on the "Diagram" tab.

We can already see the phase fields nicely, but the field boundaries are wobbly.

Where has MAGEMin spent its time? Find out by clicking "Display options" and setting "Show grid" to true.



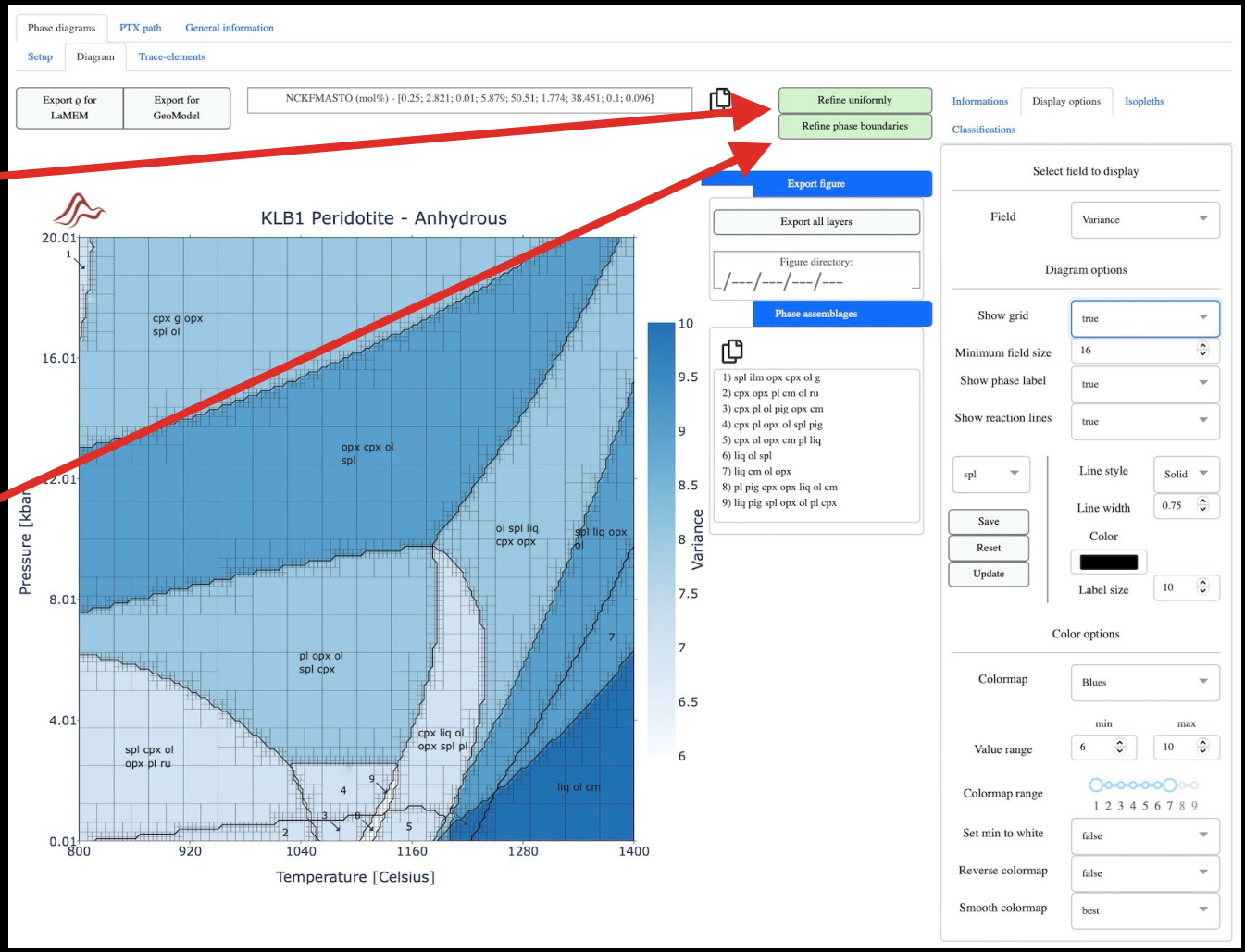
MAGEMin has spent more time exploring near the boundaries.

EXERCISE 1

4. **Refine the boundaries further**

Option 1: “Refine uniformly”. Refines the whole diagram. Takes longer.

Option 2: “Refine phase boundaries”. Cleans the boundaries with less effort, but won’t find any small fields that are currently missing.



EXERCISE 1

5a. **Calculate lines of constant mol% cpx**

Click “Isopleths” tab.

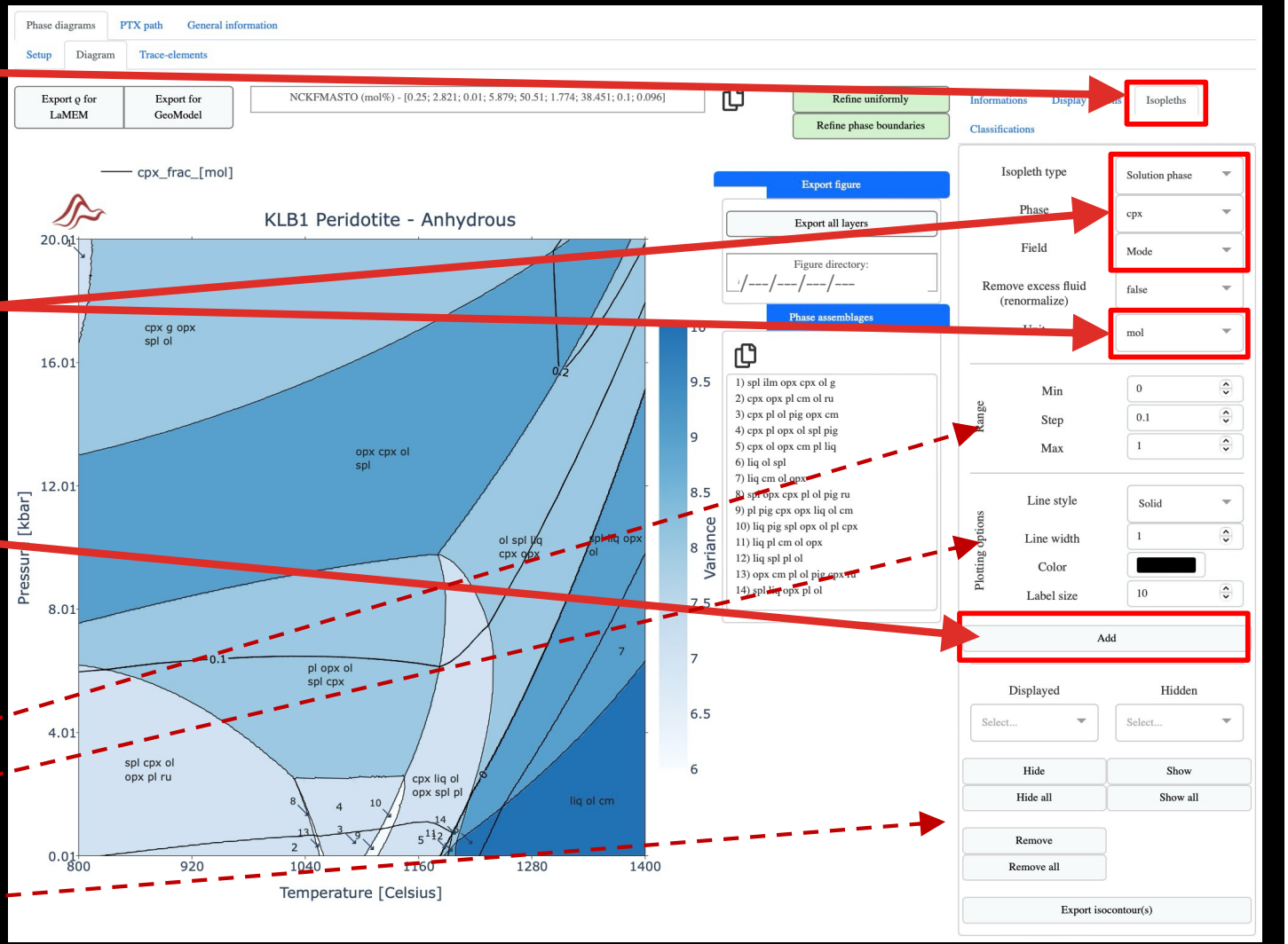
Cpx is a “solution phase” (variable composition).

Choose “mode” (proportion) and unit “mol”.

Click “Add”.

Try playing with the range and steps of the isopleths, and the display style.

You can show, hide and remove isopleths.

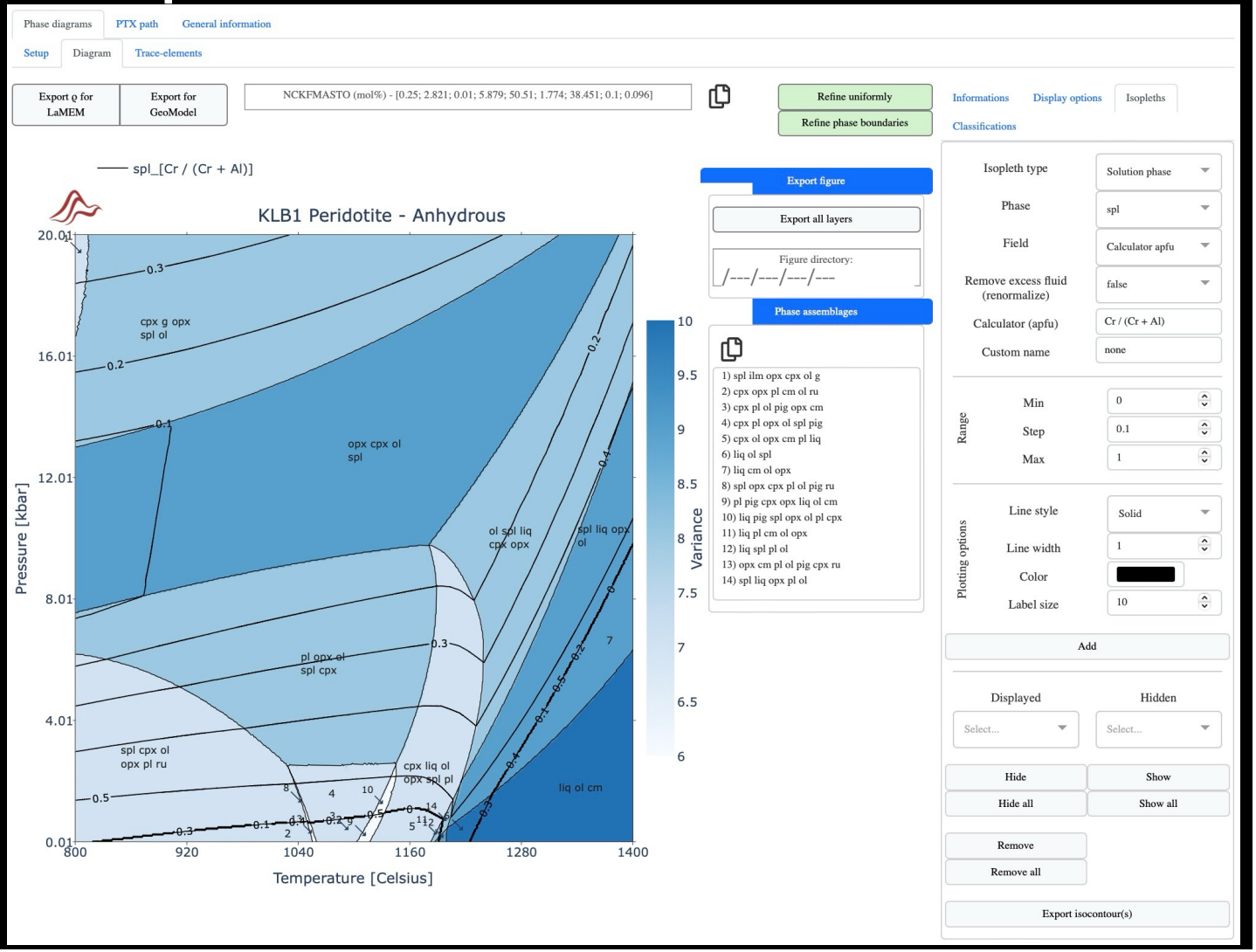


EXERCISE 1

5b. **Compositional isopleths**

Under "Field" you can choose different types of compositional isopleths, expressed as oxides, cation ratios, or end-members in the equation of state for the phase (see later).

In this example I've plotted Cr/(Cr+Al) in spinel.



EXERCISE 1

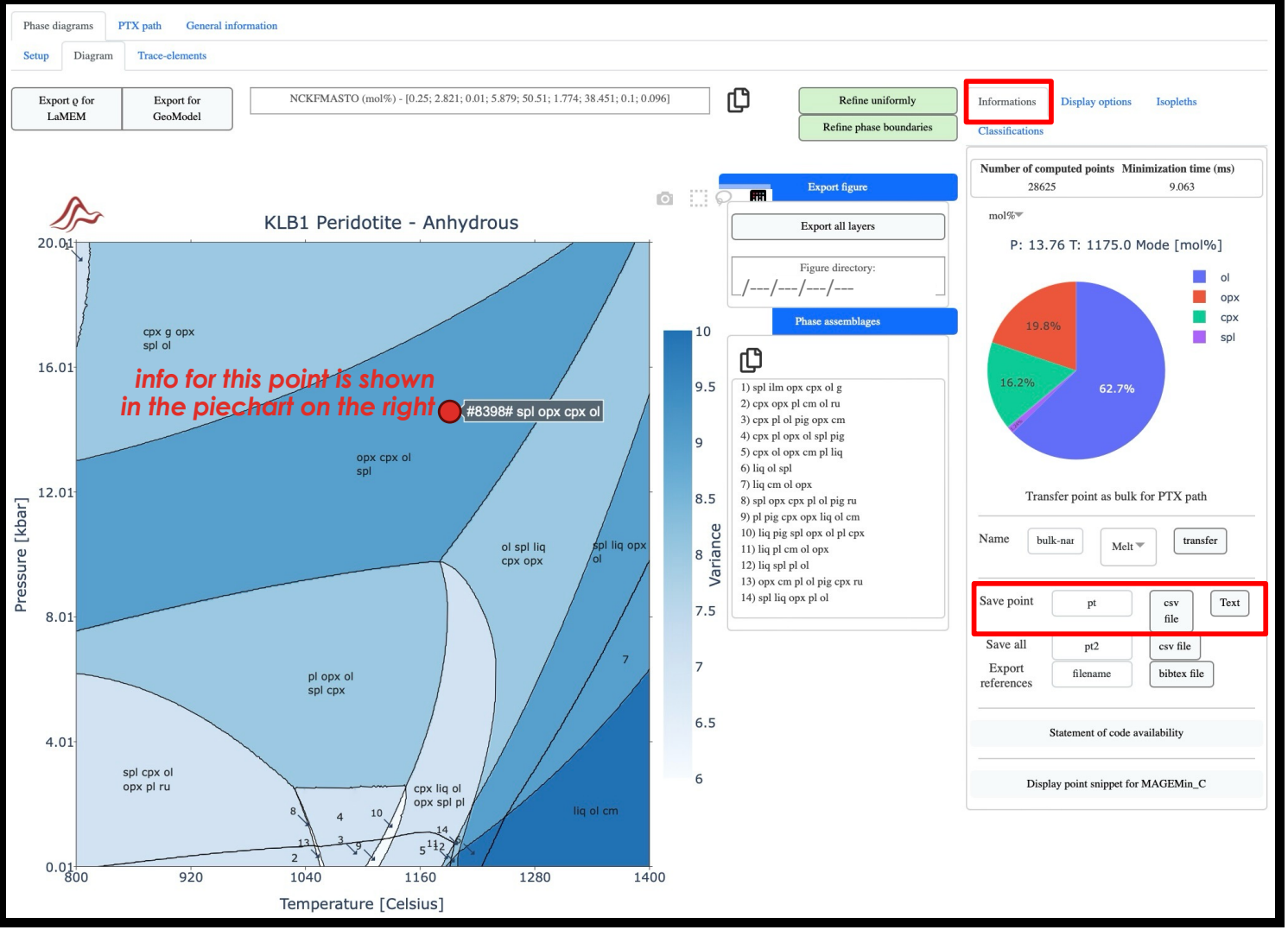
6a. **Saving your calculations: information at a point**

Click the "Informations" tab.

Click on diagram to display modal proportions of phases at that point.

"Save point": "csv file" saves all numerical info to the folder you noted in Step 2 (Excel will open csv).

"Save point": "Text" saves a THERMOCALC-style text file to Downloads.



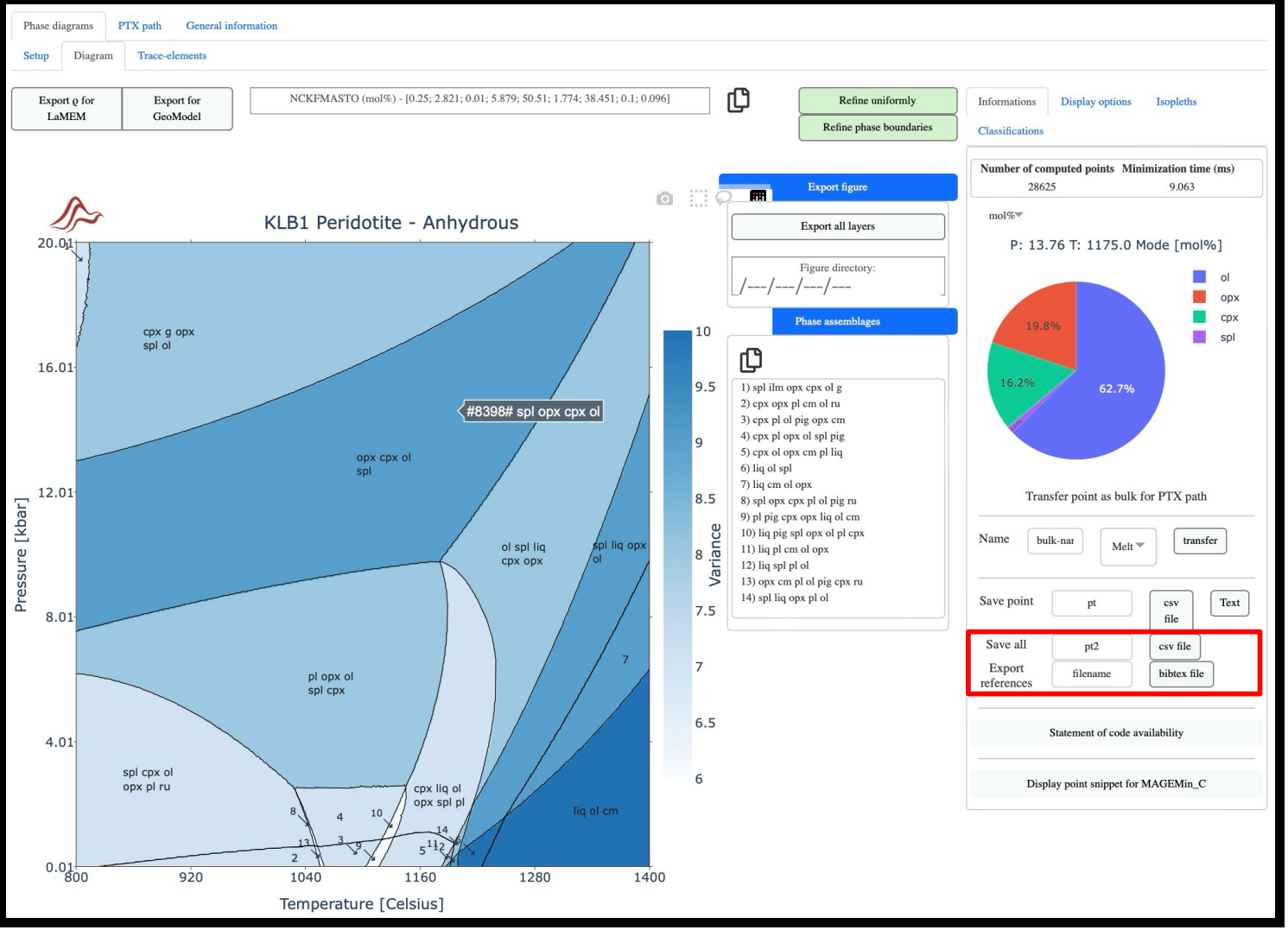
EXERCISE 1

6b. **Saving your calculations: all numerical info**

Save numerical output for all points, plus references, with "Save all" and "Export references".

Output goes in the folder you noted in Step 2, as a CSV file.

Find and inspect the CSV file, e.g. with Excel. Phase compositions are given in both wt% and mol%, with iron as FeOt and O.

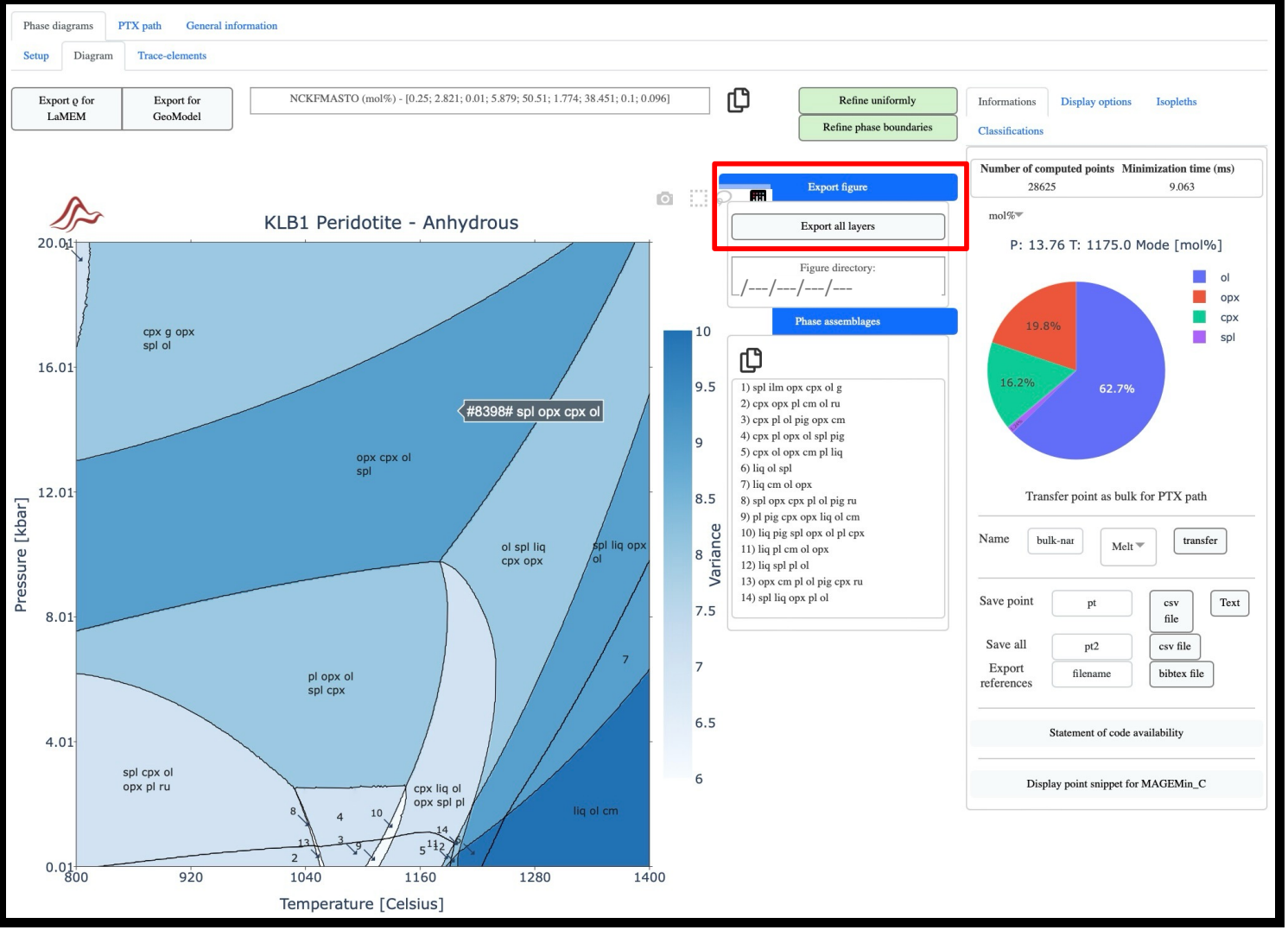


EXERCISE 1

6c. **Saving your calculations: the figure**

Use "Export figure" or "Export all layers" to export elements of the figure to your output folder, in the subfolder "output".

"Export all layers" sometimes crashes MAGEMin if you've been playing with lots of things beforehand.



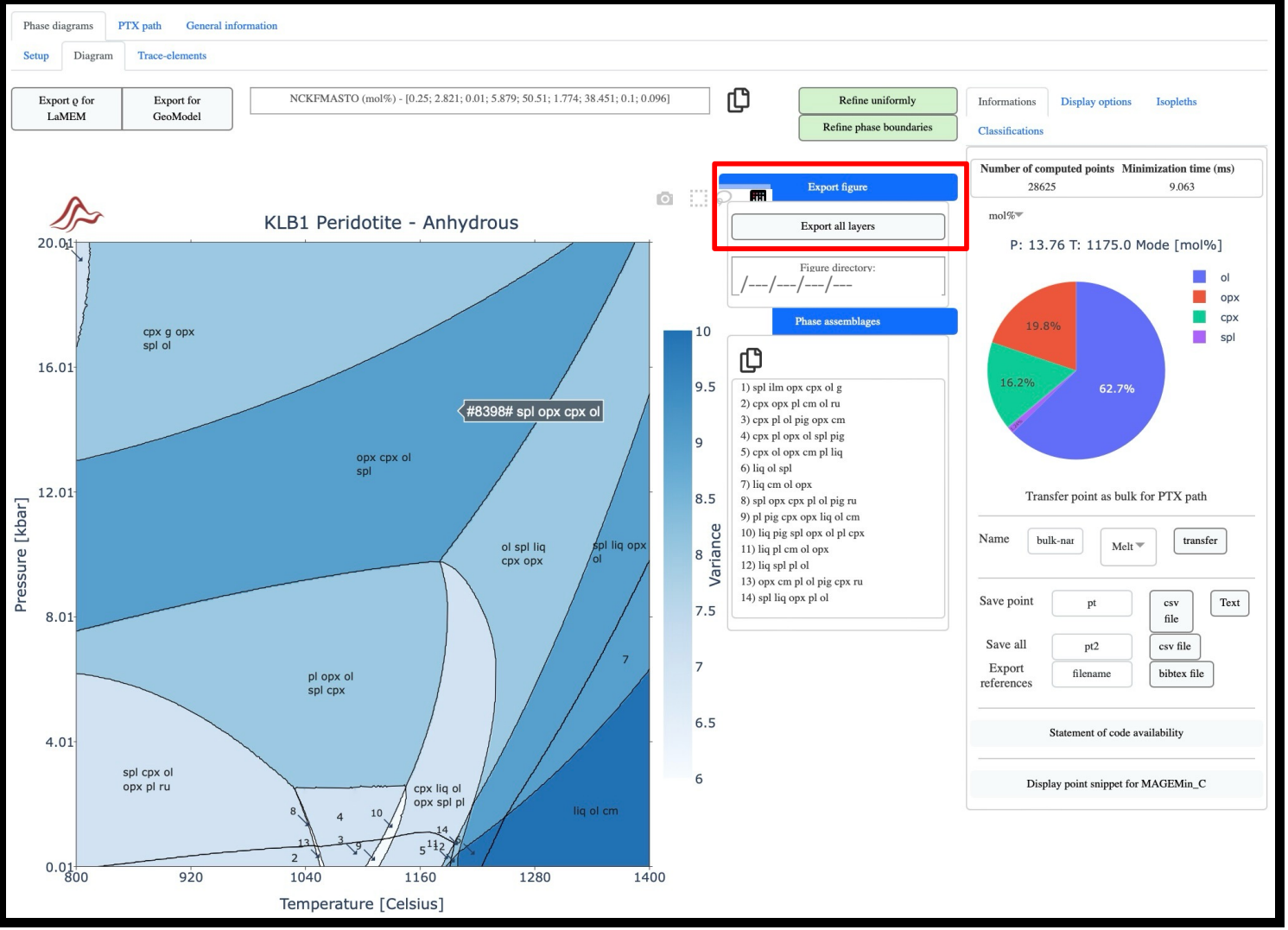
EXERCISE 1

6c. **Saving your calculations: the figure**

Figures are produced as svg.

You can open them in your internet browser.

The free illustration software Inkscape is great for further editing (and is outstanding in general these days).



Possible starting point for not-beginners

EXERCISE 2

In Exercise 2 we will look at some calculations on synthetic metapelite compositions, discovering some new aspects of MAGEMin including:

- Entering bulk composition information from a datafile;
- T-X or P-X pseudosections;
- Water "in excess";
- What happens when things get too hard for even MAGEMin's solver.

We'll also get a chance to consider variables related to Fe^{2} and Fe^{3+} in action.

The exercise is based on calculations in: White RW, Powell R, Holland TJB, Johnson TE & Green ECR (2014) New mineral activity–composition relations for thermodynamic calculations in metapelitic systems. *Journal of Metamorphic Geology* 32, 261-286. doi:10.1111/jmg.12071

EXERCISE 2

First, reset MAGEMinApp ready for a new set of calculations. I like to:

1. Terminate Julia's current process in the Terminal window with cmd+. while leaving Julia itself still running (not sure if this is possible in Windows? you may need to close the PowerShell entirely and restart Julia).
2. Restart MAGEMinApp – if Julia is still running then repeating the App() command will do it.
3. Close my browser tab and open a new one.

Also a useful procedure when MAGEMinApp crashes!

EXERCISE 2

We want to load some bulk compositions from the file *bulk-rock_SGGMP.dat*

Note: The format of the bulk composition file has changed over time. However, current examples should always be downloaded when you update your MAGEMinApp through Julia. To see them, locate the folder that Julia created and populated with output files in Exercise 1. It should contain a subfolder called "examples" with various bulk-[...].dat files.

EXERCISE 2

1. **Inspect *bulk-rock_SGGMP.dat***

```
# Spaces before/after ";" do not matter
# make sure the header line "title; comments; db; sysUnit; oxide; frac; frac2" is provided as first unco
# column titles order in the header does not matter as long as the same order is respected for the bulk-
# Note that either [..., Fe2O3, FeO,...] or [..., FeO, O, ...] must be provided
# ------ *** Eleanor's note - this should really be [..., Fe2O3, FeO,...] or [..., FeOt, O, ...] ****
#
# Database to be used should be provided (ig, mp, mb, um)
#
# P,T-X bulk-rock composition:
#-----------------------------
# if you want to load two bulks for P-X or T-X diagrams simply add a second bulk after the first one (fi
# Once the bulk-rock composition file is loaded in MAGEMinApp, make sure you select your bulk for the le
#
# HEADER
title; comments; db; sysUnit; oxide; frac; frac2
# BULK-ROCK COMPOSITION

W14-Fig10a-x0;White et al., 2014;mp;wt;[H2O, SiO2, Al2O3, CaO, MgO, FeO, K2O, Na2O, TiO2, O];[1.8954, 67
W14-Fig10a-x1;White et al., 2014;mp;wt;[H2O, SiO2, Al2O3, CaO, MgO, FeO, K2O, Na2O, TiO2, O];[1.8911, 66
W14-Fig8a-x0;White et al., 2014;mp;wt;[H2O, SiO2, Al2O3, CaO, MgO, FeO, K2O, Na2O, TiO2, O];[5.2248, 64.
W14-Fig8a-x1;White et al., 2014;mp;wt;[H2O, SiO2, Al2O3, CaO, MgO, FeO, K2O, Na2O, TiO2, O];[5.2596, 64.
```

names for bulk compositions

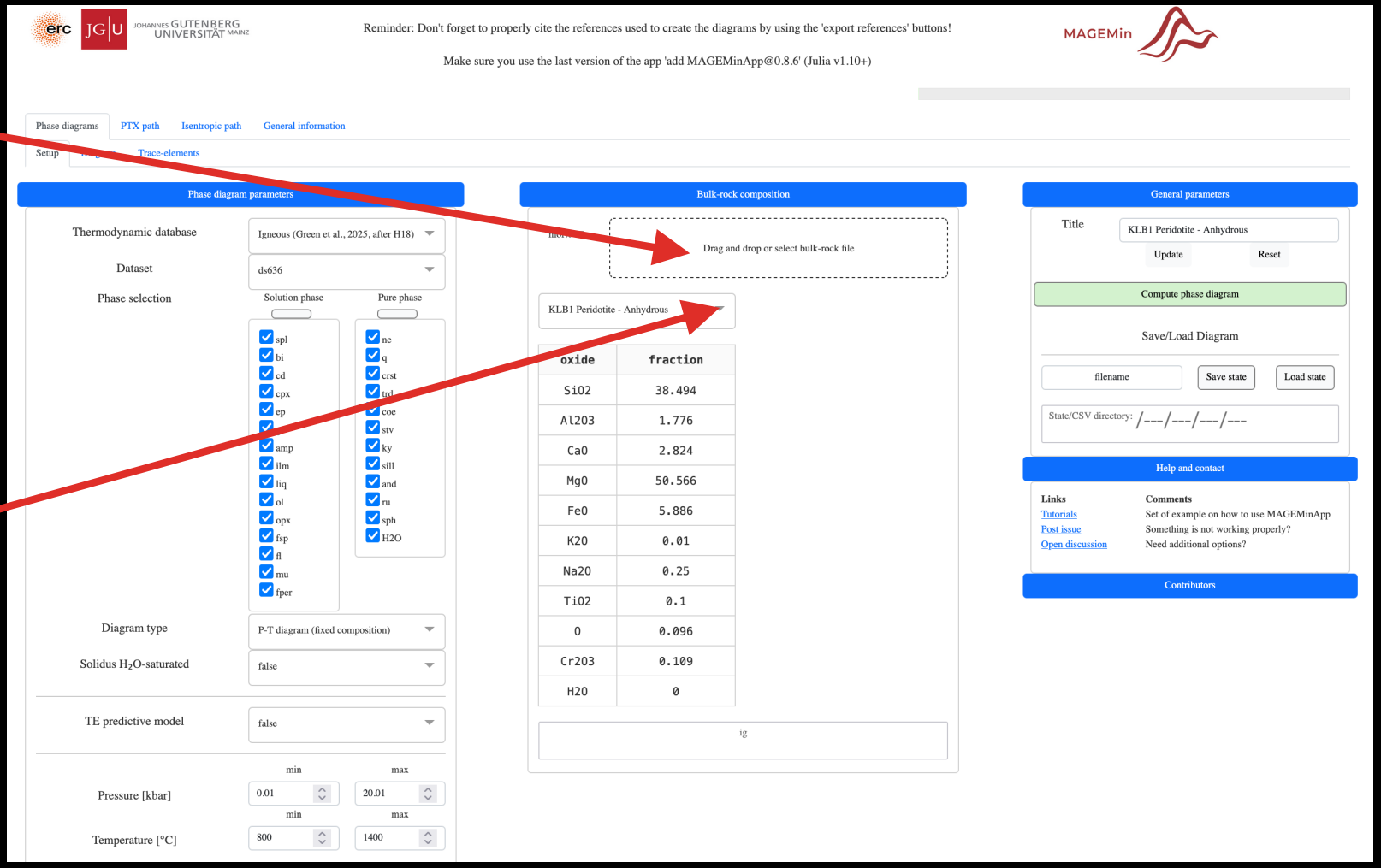
"mp": use with metapelite thermodynamic database
"wt": compositions are specified in wt%

EXERCISE 2

2a. **Load *bulk-rock_SGGMP.dat***

1. Drag and drop the file into the selection window

2. Click the dropdown box. There is no sign of our new bulk compositions...

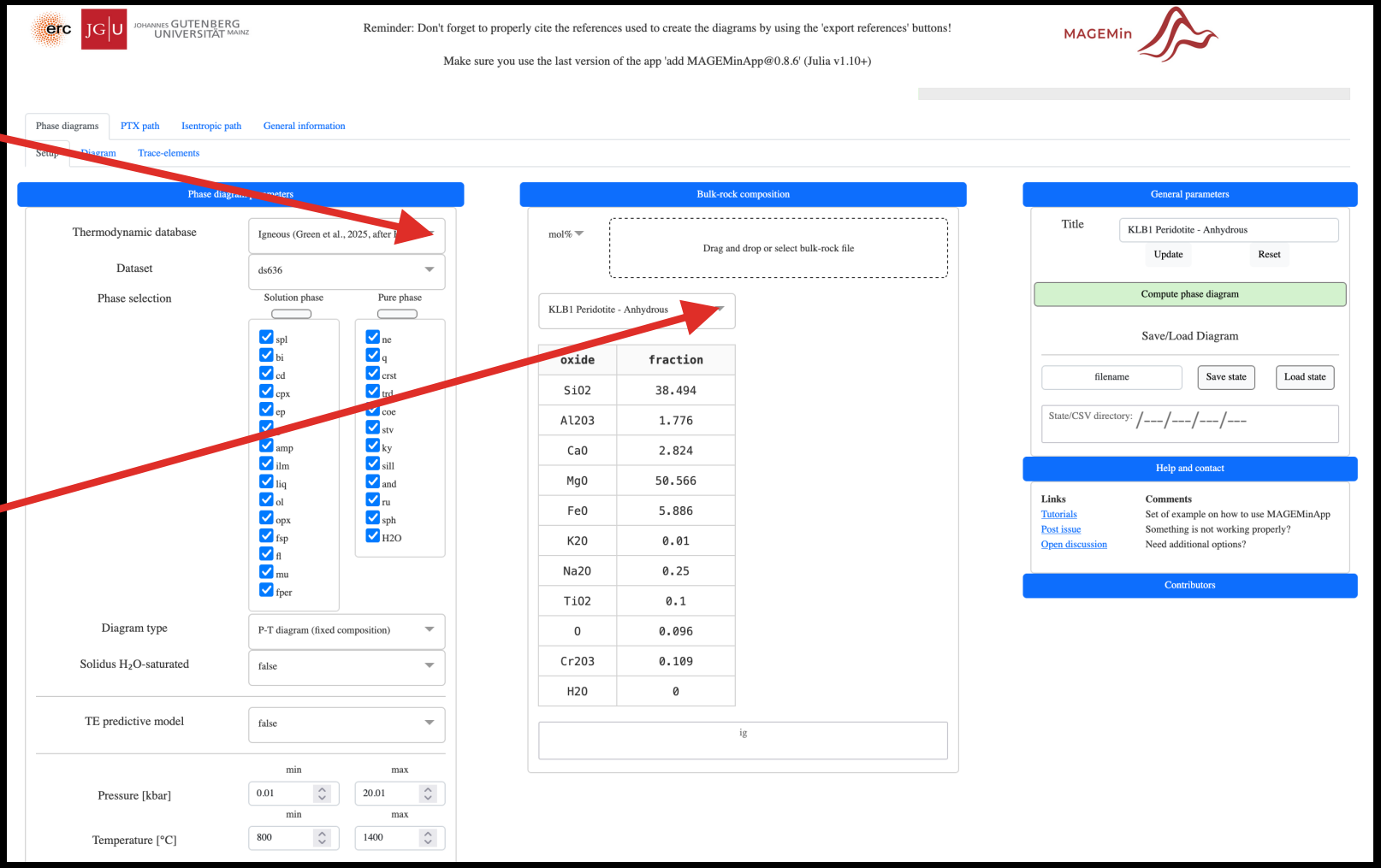


EXERCISE 2

2b. **Load *bulk-rock_SGGMP.dat***

3. Change "Thermodynamic database" to "metapelite"

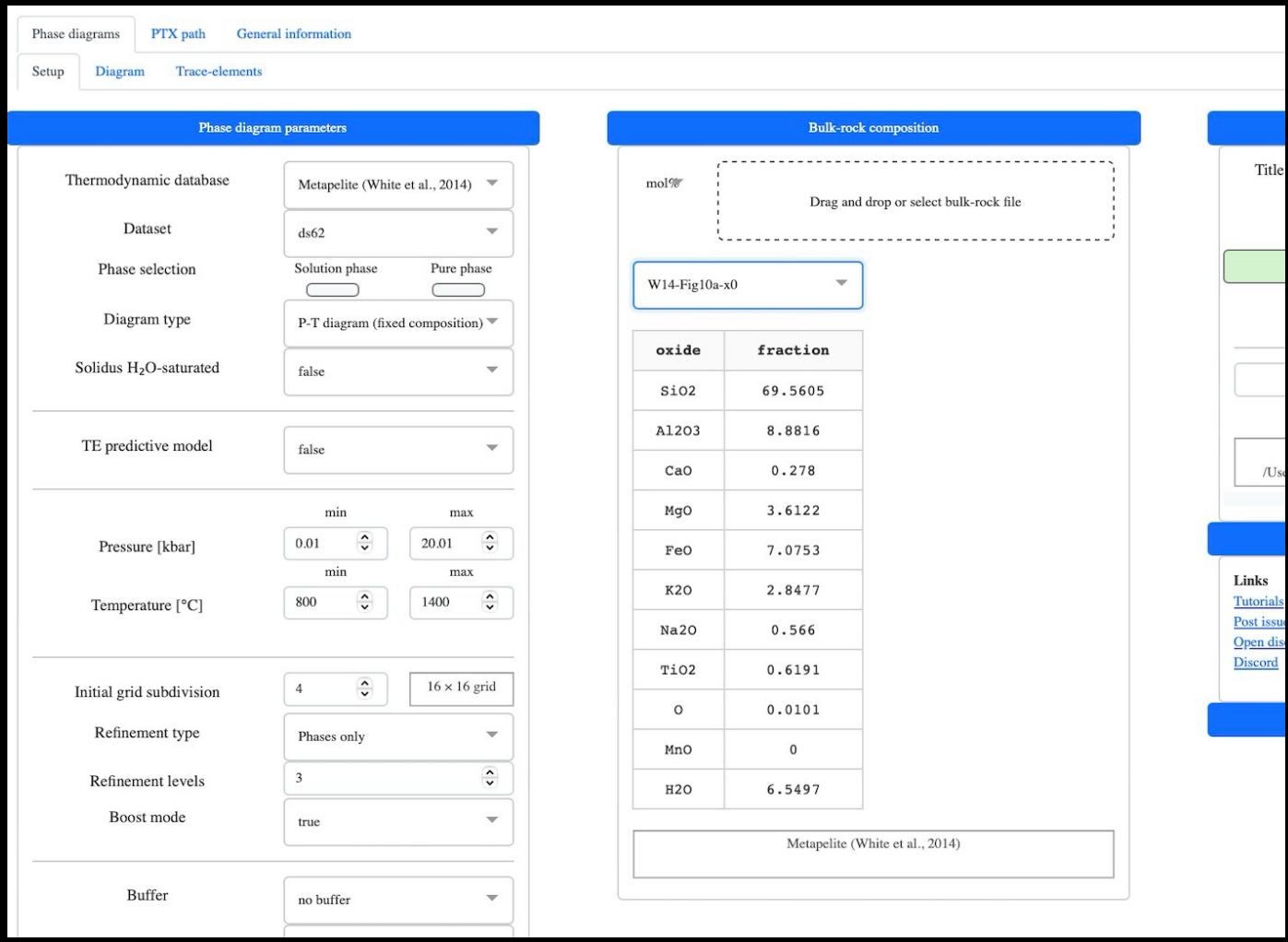
4. Now our new bulks should appear in the list.



EXERCISE 2

3. **Select bulk W14-Fig10a-x0**

Note the bulk composition is displayed in mole% here, even though we specified it in wt% in the input file.



EXERCISE 2

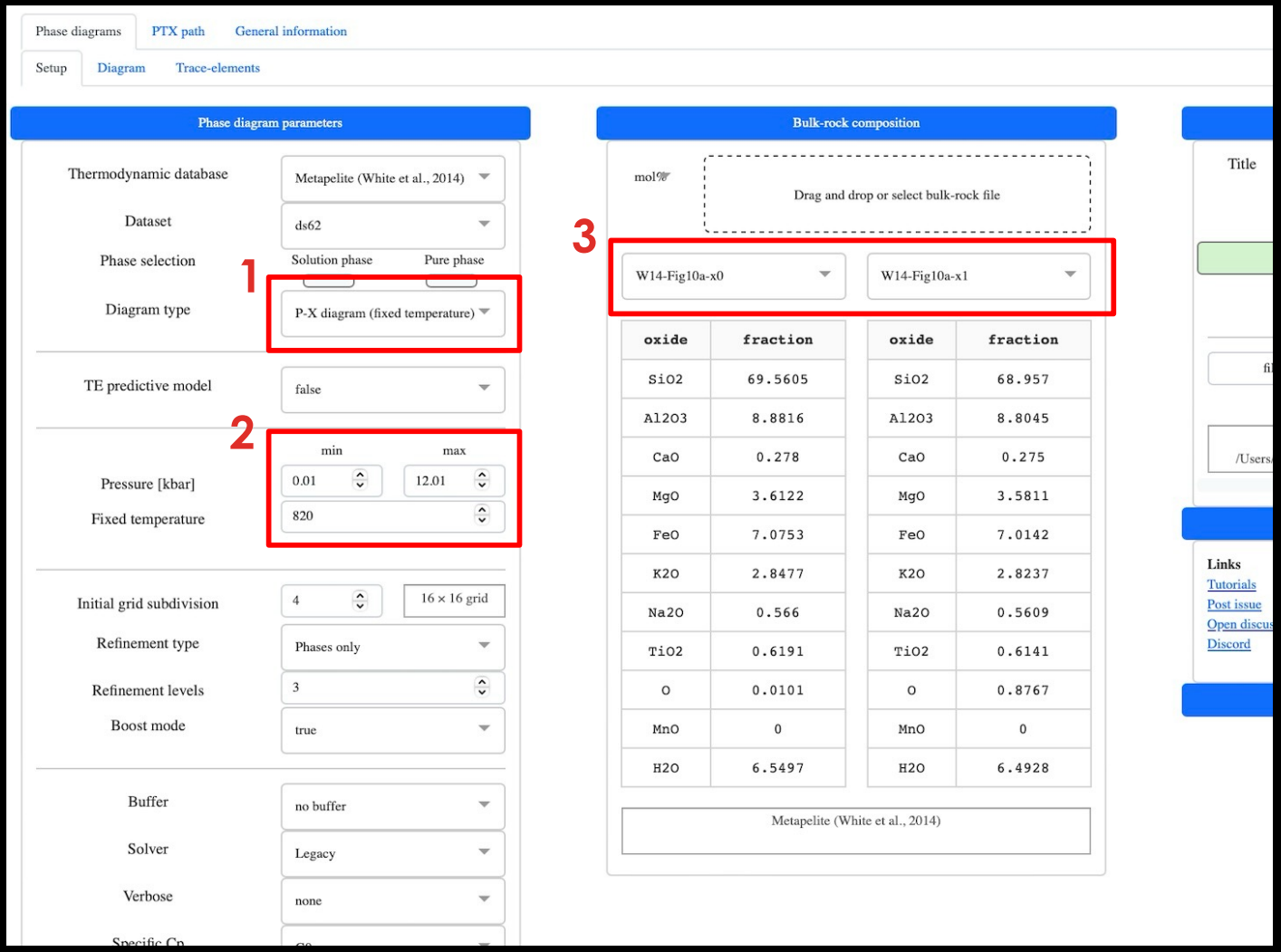
4. **Set up a supersolidus *P-X* diagram with variable $Fe^{3+}/(Fe^{3+} + Fe^{2+})$**

Set up a P-X diagram at 820°C between W14-Fig10a-x0 and W14-Fig10a-x1, for a pressure range of 0-12 kbar.

Looking at the two bulk compositions in moles, and using the formula on page 13, note we're exploring a range of

$Fe^{3+}/(Fe^{3+} + Fe^{2+})$

of 0 to 0.25



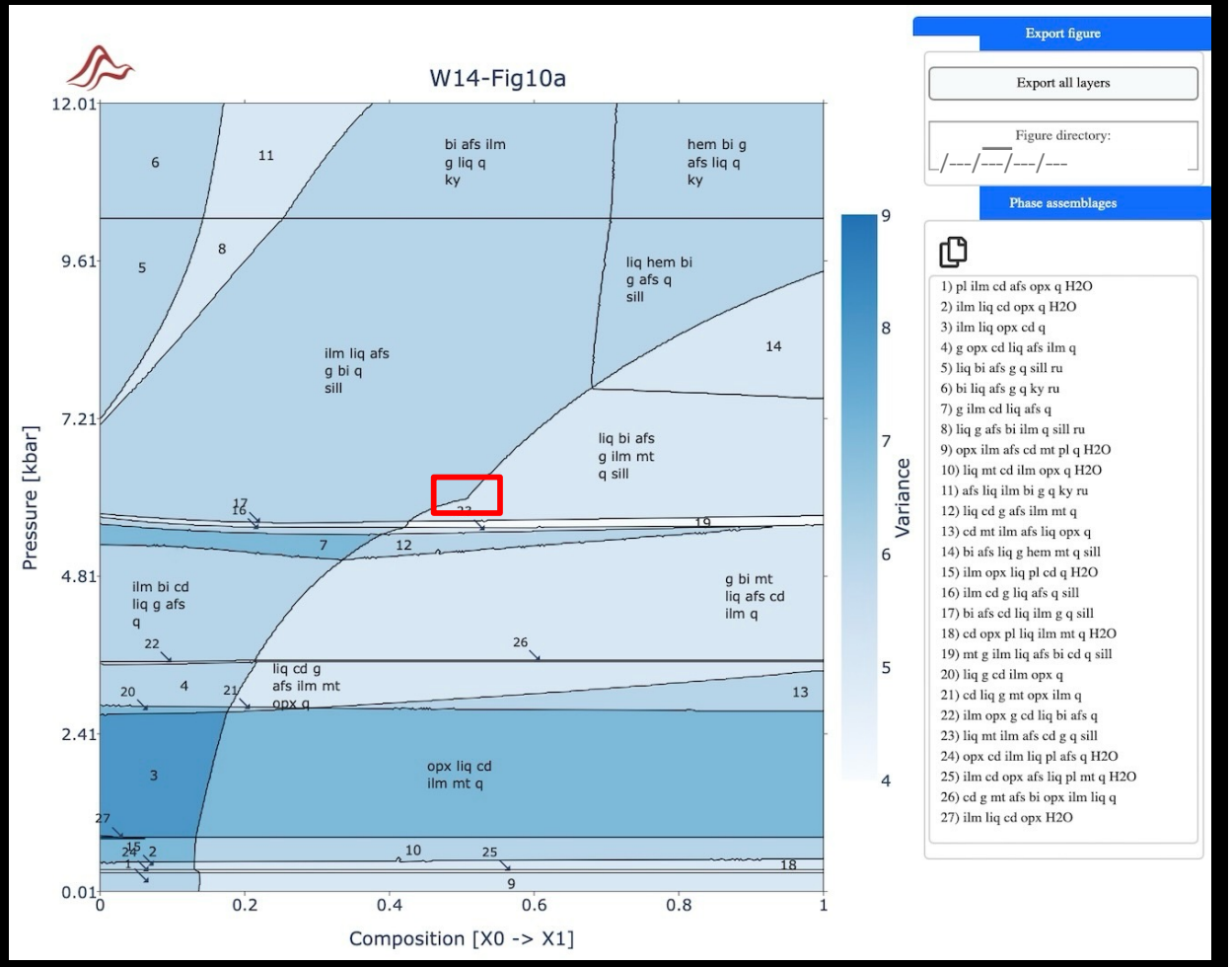
EXERCISE 2

5. **Inspect the resulting diagram**

After a few refinements, we arrive here.

Metapelite fans may note this is slightly different from the original diagram. This is due to a change to the most recent thermodynamic representation of ternary feldspar.

This cusp looks odd... We should follow it up, by plotting it at high resolution and plotting many isopleths, to make sure it is explained by e.g. proximity to a mineralogical solvus, rather than MAGEMinApp's solver failing or a broken thermodynamic representation.



An exercise for the reader...

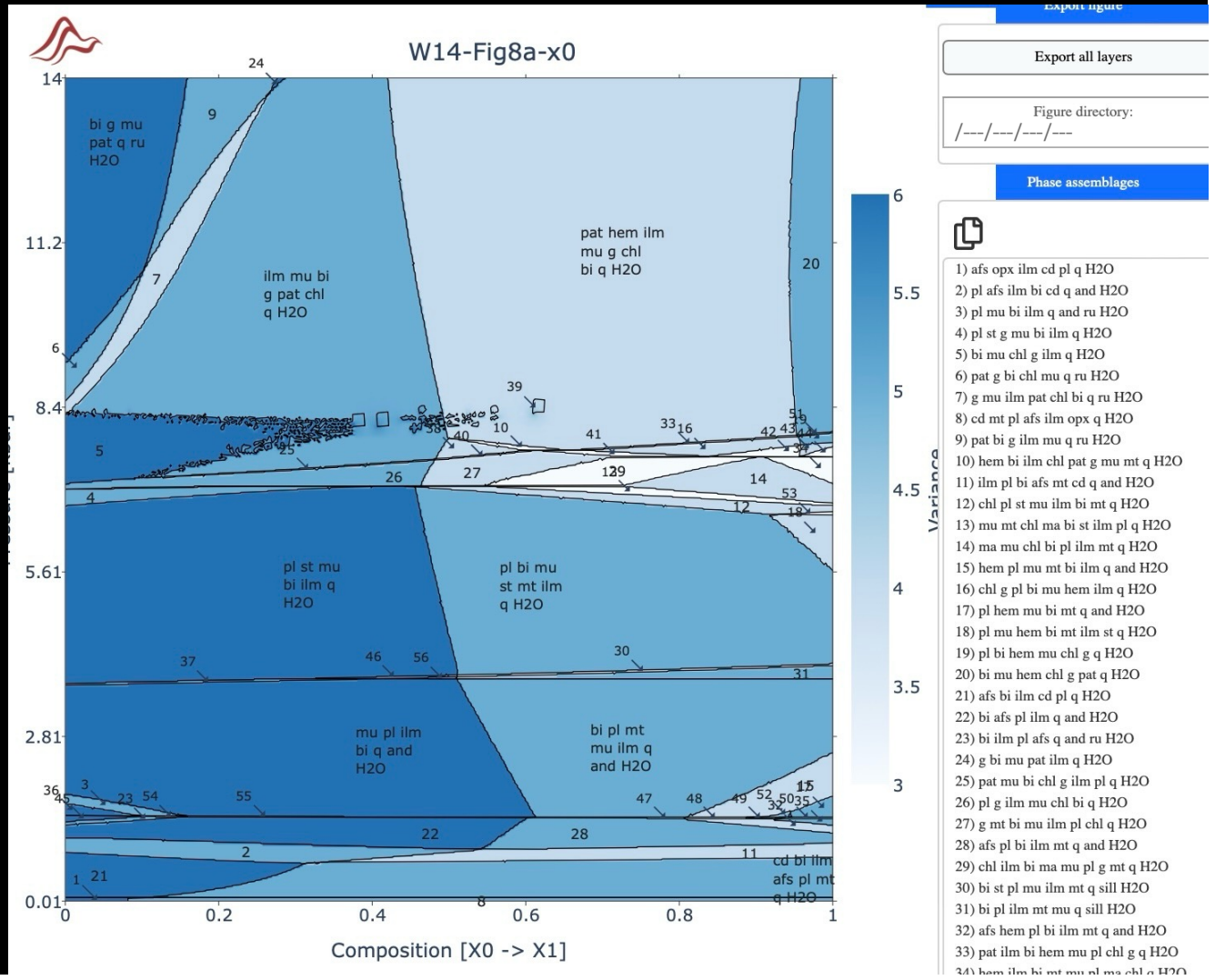
EXERCISE 2

6. **A P-X plot below the solidus**

Now set up a P-X diagram at 580°C between **W14-Fig8a-x0** and **W14-Fig8a-x1**, for a pressure range of 0-14 kbar.

In this plot, we are below the solidus. I have added an arbitrary large amount of H2O to ensure the mineral assemblages are H2O-saturated.

After several refinements, we obtain this:



EXERCISE 2

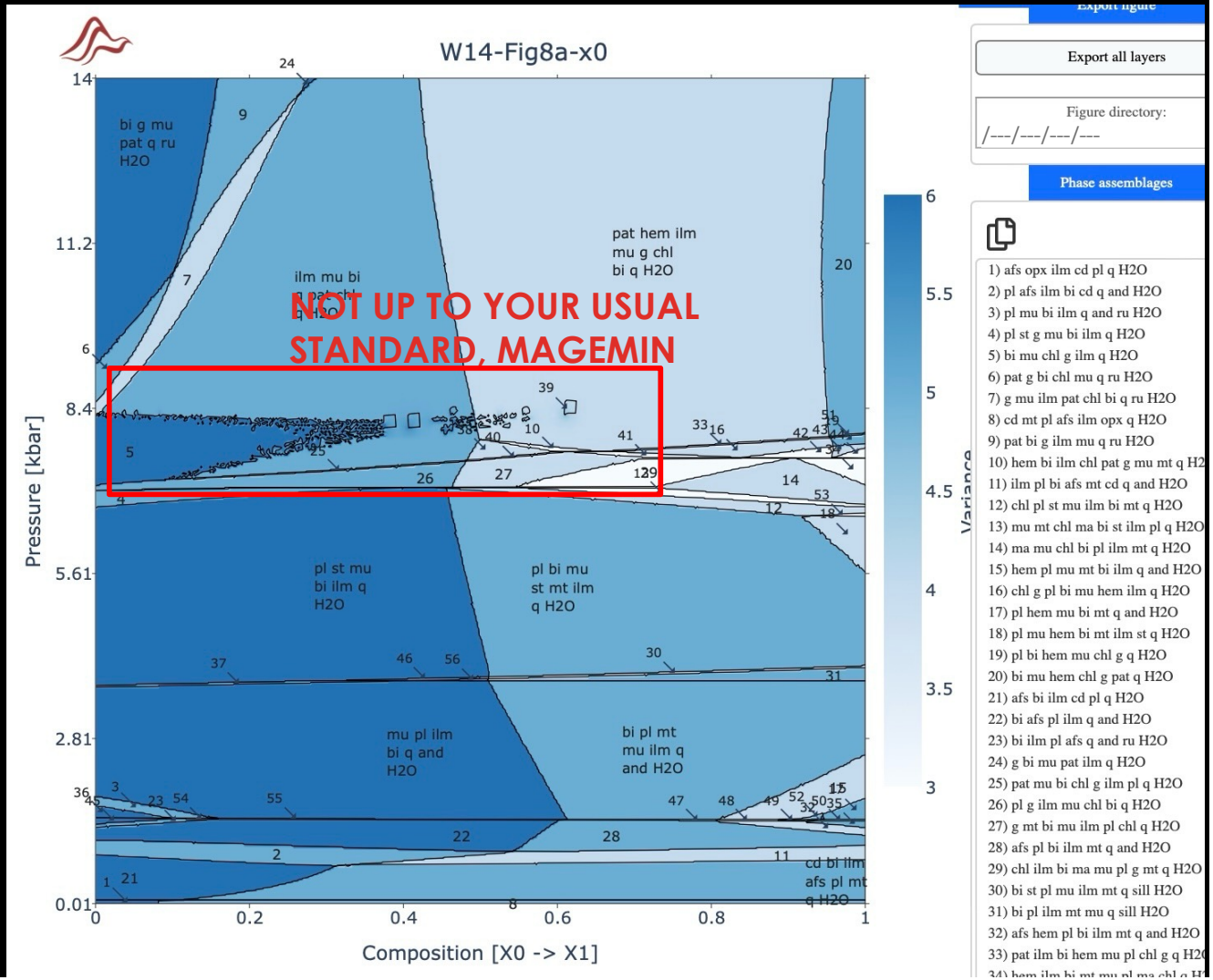
6. **A P-X plot below the solidus**

After several refinements, we obtain this:

This is the muscovite-paragonite solvus closing with increasing $Fe^{3+}/(Fe^{3+} + Fe^{2+})$.

You can try zooming in to resolve the boundaries better, but you will never get very close.

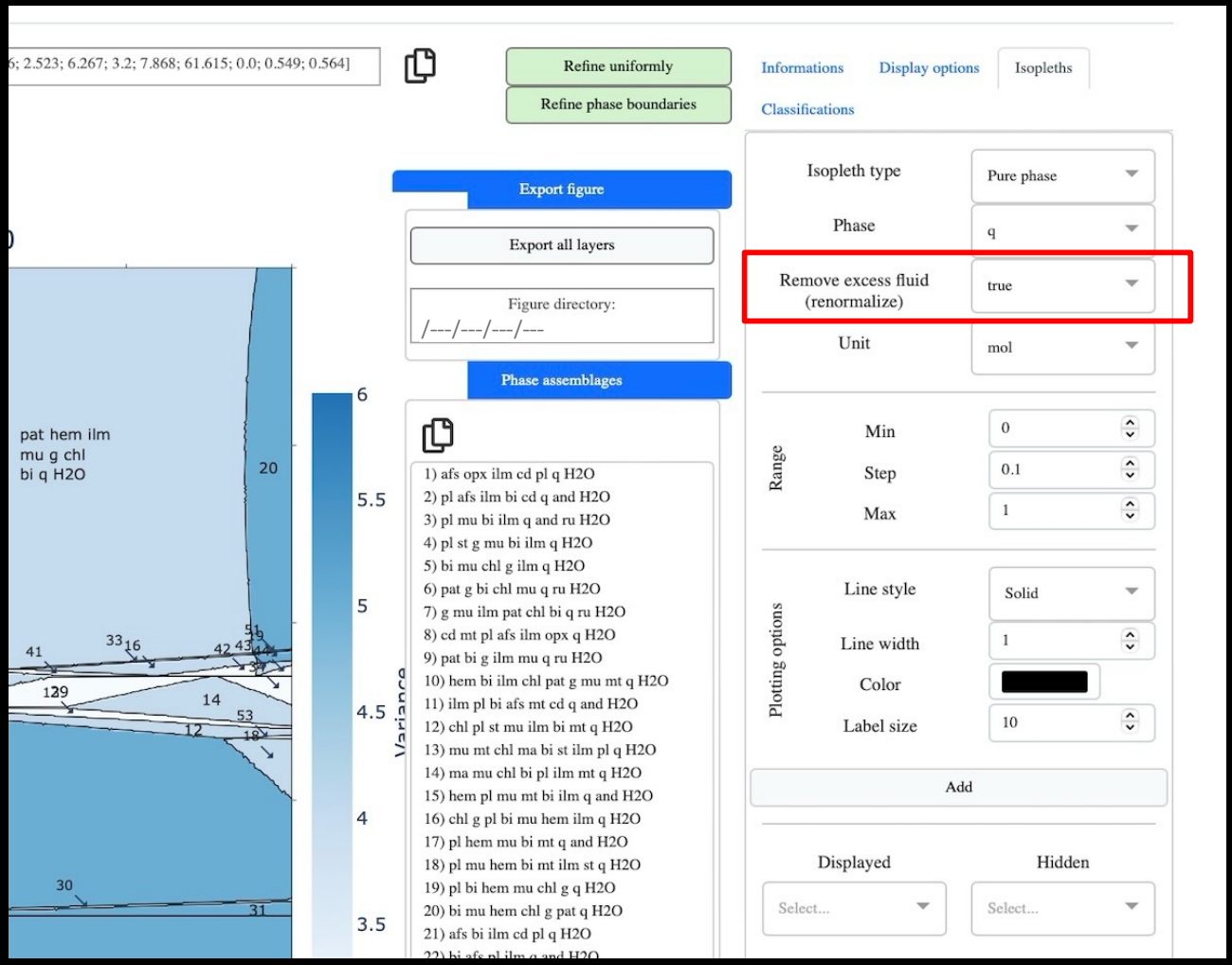
Even in Thermocalc, we used to have to fudge these a bit!



EXERCISE 2

6. **A P-X plot below the solidus: isopleths with excess H2O**

Finally: if we wanted to contour for constant modal proportions of phases, the presence of an arbitrary large amount of H2O in the bulk to saturate the assemblage would be misleading. Use "Remove excess fluid": "true" to renormalize the phase proportions without H2O.



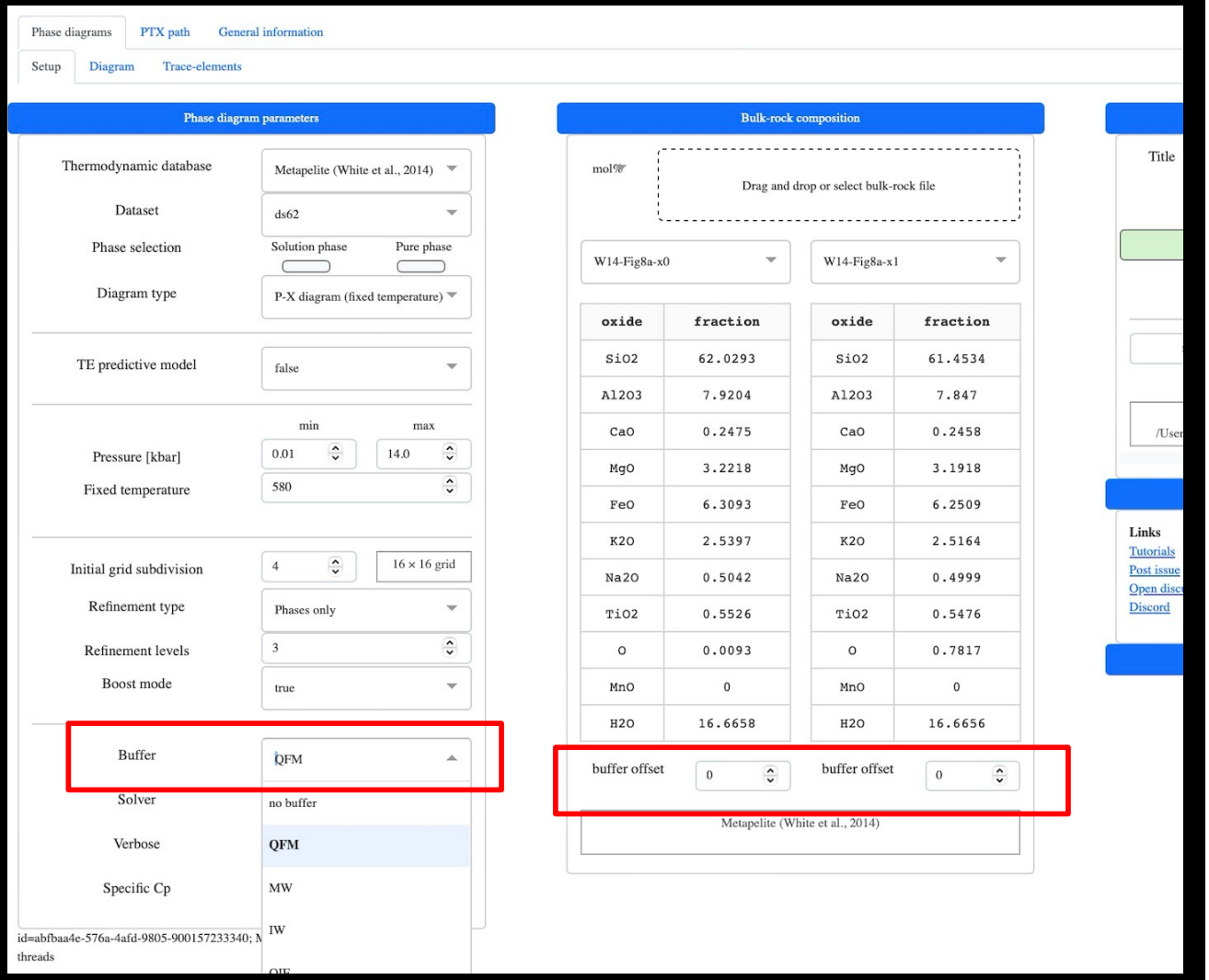
EXERCISE 2

7. **Buffering**

Before we leave the subject of Fe^{3+} vs Fe^{2+}:

What if we were modelling an experimental system, and had to buffer fO2 instead of fixing molar O?

Play around with this if you would like!



Possible starting point for not-beginners

EXERCISE 3

P-T-X paths

MAGEMinApp can automatically calculate equilibria at points along a *P-T* path, and, if required, treat this as an open-system problem in which the system composition evolves at each step via separation of phases.

Currently this is set up to simulate melting and crystallization, but not e.g. sequestration of elements in garnet (though you could write a script to do this with MAGEMin_C).

Batch melting/crystallization is simulated if a constant bulk composition is maintained throughout, with no separation of phases.

Fractional melting or crystallization is approximated if the melt and solids are separated at each step, as long as melt/crystallization increment is small.

EXERCISE 3

P-T-X paths

The output from melting and crystallization calculations can be displayed using a variety of diagrams including:

- phase composition versus *P-T* step plots
- phase compositions plotted on standard igneous classification diagrams such as the TAS plot
- "mode boxes" representing the changing proportions of phases in the system.

Try the tutorial at:

https://computationalthermodynamics.github.io/MAGEMin_C.jl/dev/MAGEMinApp/PTX_tutorials

Possible starting point for not-beginners

EXERCISE 4

Trace elements

MAGEMin models trace element partitioning using any database of kD values that the user provides.

By default it uses the Laurent (2012) database. This assigns kD values to a very large array of trace elements in phases. It uses three different constant values for the kD of an element in a phase, depending on the bulk SiO2 range. The partition coefficients can be found at the bottom of MAGEMinApp's General Information tab after calculating a relevant phase diagram.

You can display the trace element calculations in various ways, and normalize them in various ways. Note, I'm not sure which "chondrite" value has been used, or what "bulk" is. I will ask for this to be added to the "General information" tab.

EXERCISE 4

Trace elements

MAGEMin's tutorial on modelling trace elements is at
https://computationalthermodynamics.github.io/MAGEMin_C.jl/dev/MAGEMinApp/PD_tutorials#8.-Trace-element-modelling

To set up for this tutorial:

- Terminate and restart your MAGEMinApp session in Julia;
- Set "Thermodynamic database" to "Metapelite (White et al 2014)", which gives you the correct bulk composition by default;
- Set "Temperature" to 300.0 to 1000.0 °C, "TE predictive model" to true (this turns on the trace elements), and "Refinement levels" to 4.

This should match the required setup for the tutorial. Press "Compute phase diagram" and use the tutorial to interpret the results.

Starting point if you know it all already!

EXERCISE 5

MAGEMin_C

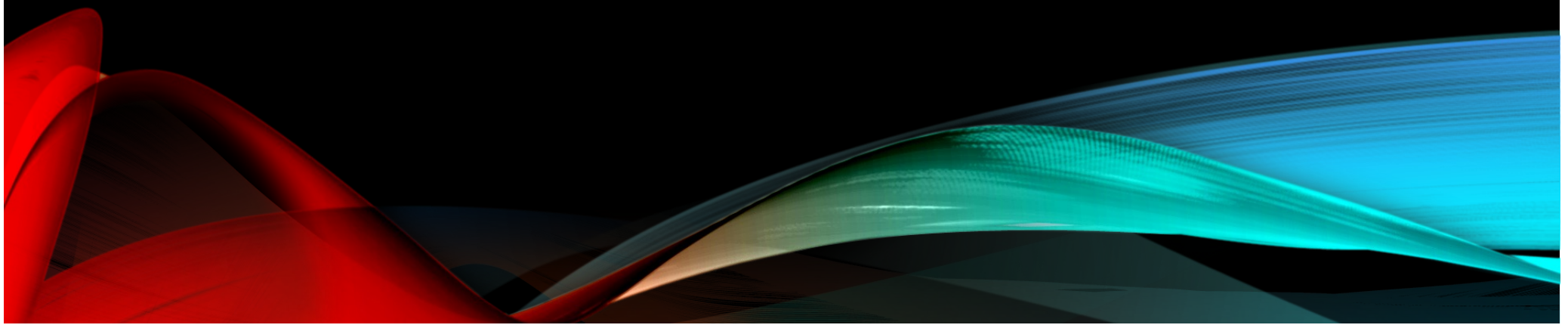
If you're happy with MAGEMinApp, how about MAGEMin_C?

Info for incorporating MAGEMin functionality into your larger code can be found at:

https://computationalthermodynamics.github.io/MAGEMin_C.jl/dev/MAGEMin_C/MAGEMin_C

DISCUSSION

The thermodynamic models underlying MAGEMin & friends



EQUILIBRIUM CALCULATORS *vs.* EQUATIONS OF STATE

- MAGEMin is software that does thermodynamic calculations:
  - Can thermodynamic equilibrium exist between a set of phases?
  - If so, what are the compositions of those phases in the equilibrium?
  - Is an equilibrium possible among a *different* set of phases that is *more stable*?
- To calculate this, MAGEMin must represent the thermodynamic properties of each phase using an **equation of state**.

EQUILIBRIUM CALCULATORS *vs.* EQUATIONS OF STATE

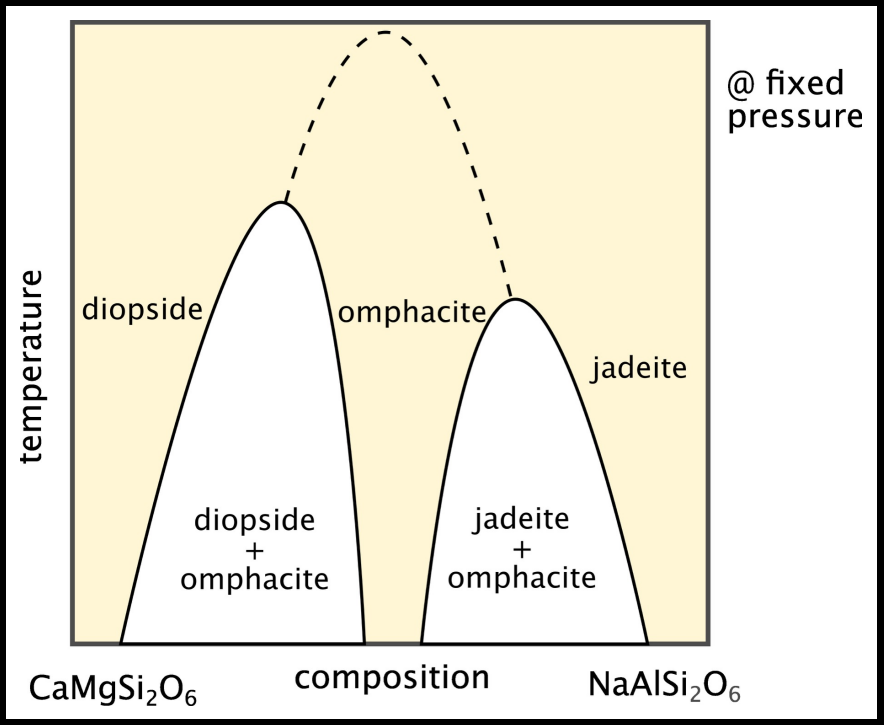
If you use **different software** to do calculations with the **same equations of state**, you should get the **same answer**.

If you use **different equations of state** to represent the phases, you will get **different answers**.

EQUATIONS OF STATE

Example:

- Equation of state (EoS) for low-temperature Ca-Na clinopyroxene (cpx).
- It's really 3 cpxs: jadeite, ordered omphacite, diopside (augite).
- The EoS has to represent how all of them respond to being squashed or heated.

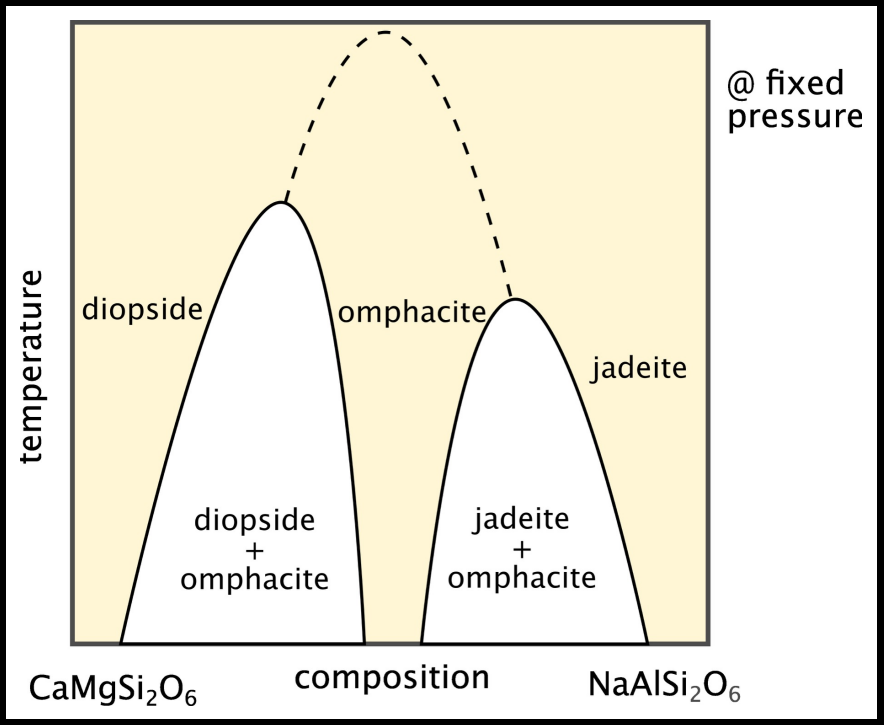


Phase relations in the diopside-jadeite system (a lot fewer oxides than in a natural cpx!).

EQUATIONS OF STATE

Example:

- The EoS has to represent how all of them respond to being squashed or heated.
- And, because Geology is harder than Physics or Chemistry, the EoS has to capture how these behaviours depend on composition (x) and state of order.
- Hence, x-eos rather than EoS.
- ...see also Tris Stuck's talk earlier on carbonates and scapolites.

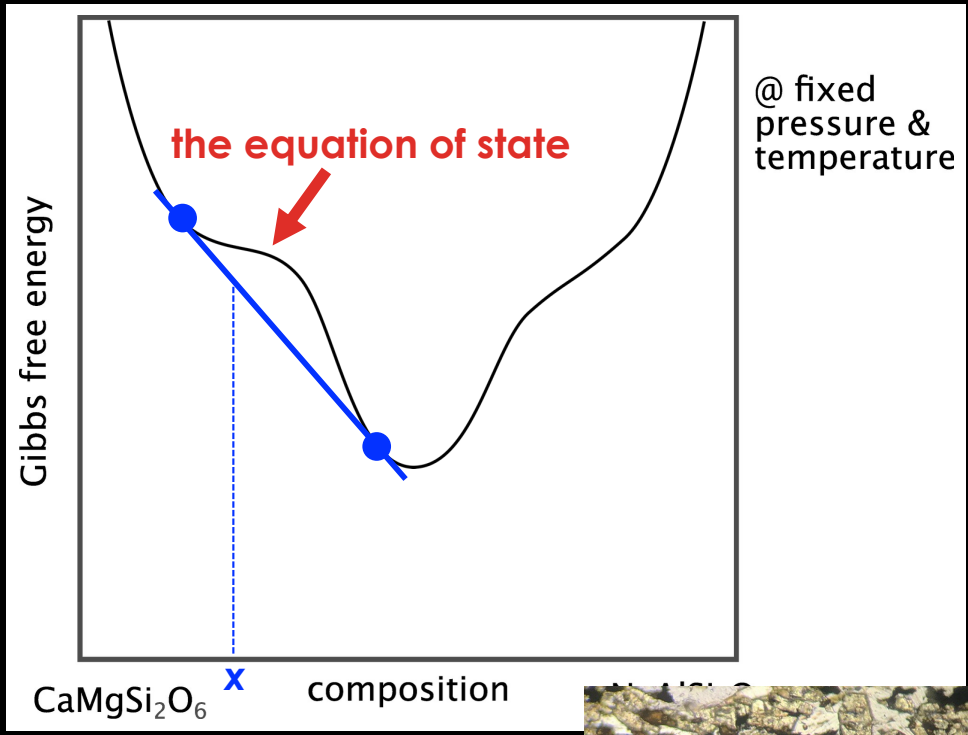


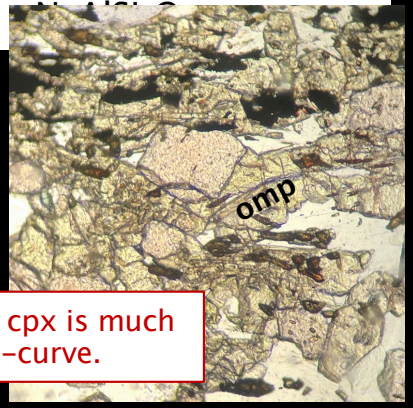
Phase relations in the diopside-jadeite system (a lot fewer oxides than in a natural cpx!).

EQUATIONS OF STATE

That low-T cpx x-eos in MAGEMin...

- Think of each x-eos as a Gibbs free energy (G) surface in pressure, temperature, composition and order space.
- MAGEMin's job is to find the equilibria (common tangents) accurately and precisely.
- ...but if the G-surface is wrong, MAGEMin's calc still won't be realistic.





...of course, real cpx is much prettier than a G-curve.

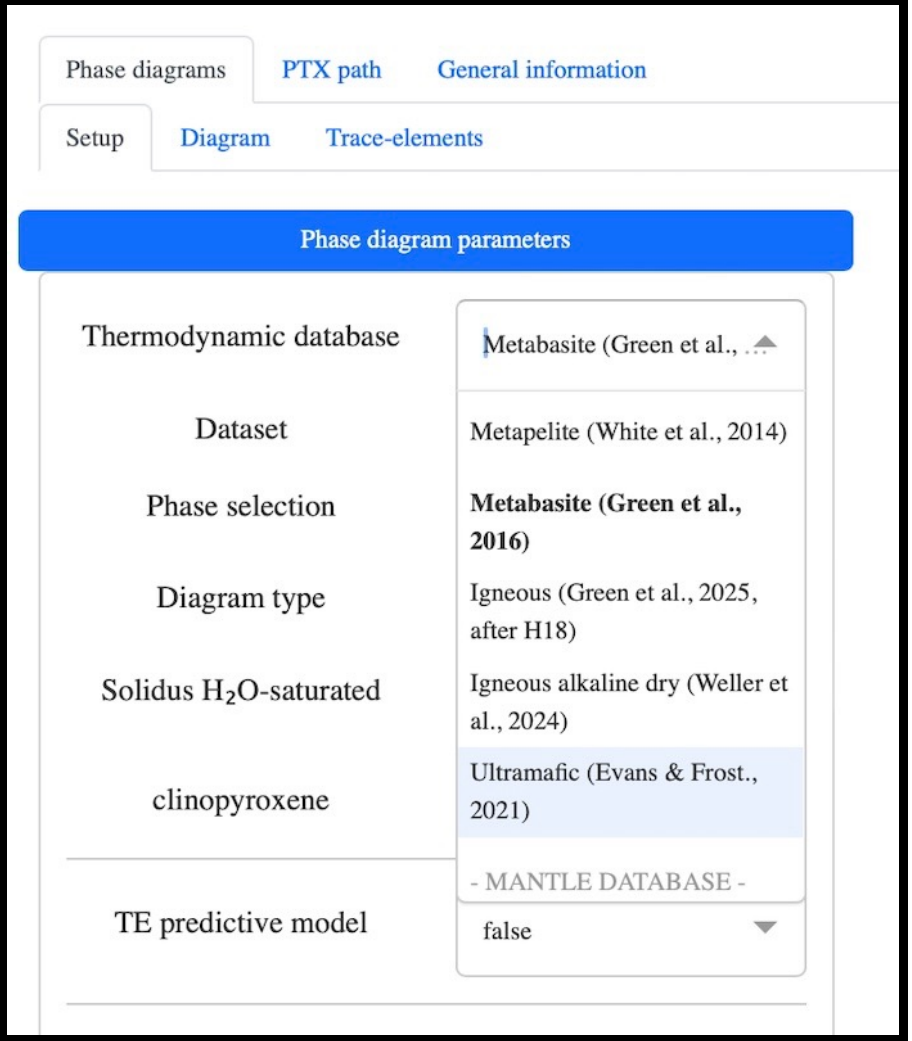
WHOSE FAULT IS IT ANYWAY?

So, if you get nonsense answers out of MAGEMin, it's probably not MAGEMin's fault...

- It *may* mean that your mineral assemblage is too far from equilibrium to model usefully.
- It *could easily* mean the x-eos are not working well enough, especially if you're using them far from the calibration conditions described in the papers.

YOU CAN HELP MAGEMIN BY…

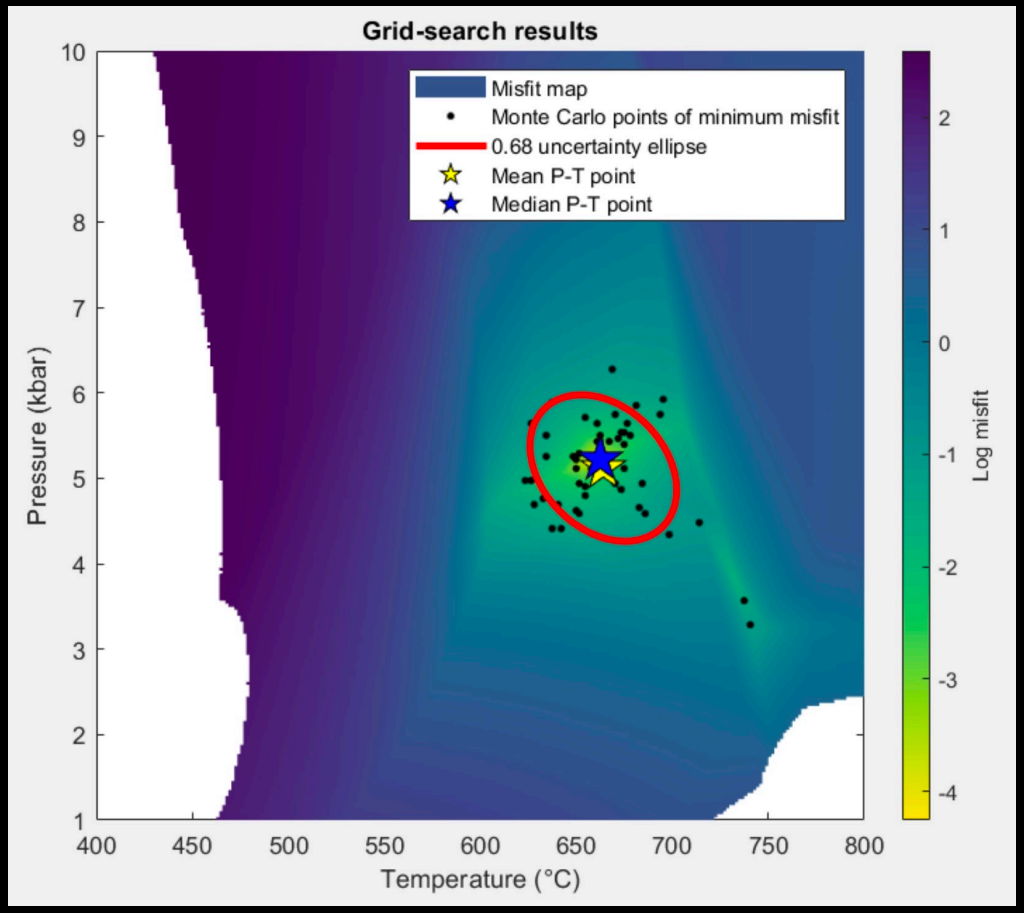
- Using the x-eos in the sets MAGEMin offers.
- Selecting the best set for the rock type you have.
- Not assuming that adding more oxides improves the modelling.
- Always being sceptical of your results and checking them for sense.
- Being especially wary about cumulative error along paths.



UNCERTAINTY ESTIMATION

Software like Lina Forma (McKay-Champion & Cawood, 2025) illuminate mismatch between observations & calculations.

The answer may be

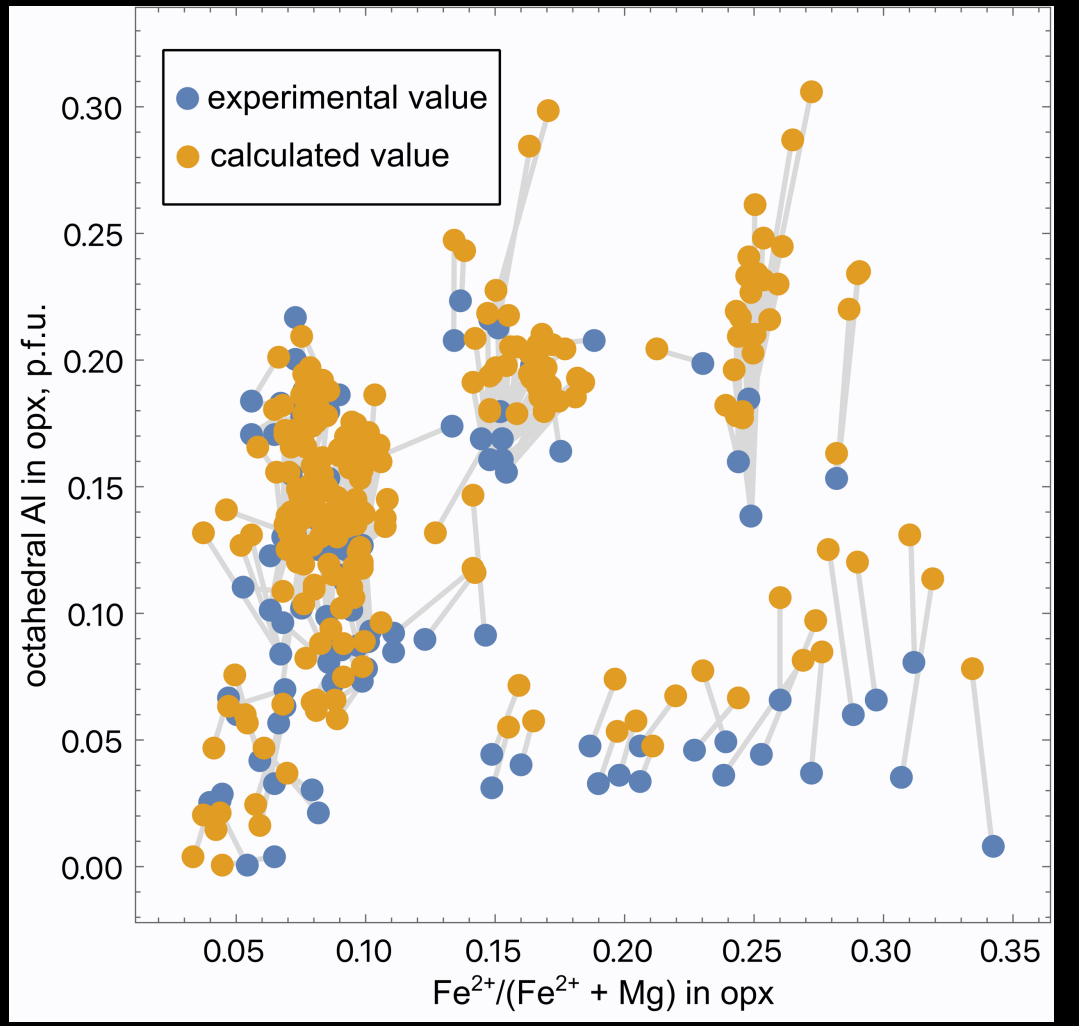


Example of the application of Lina Forma (McKay-Champion & Cawood, 2025), from the Masters thesis of Yi Mu, University of Melbourne.

IMPROVING THE EQUATIONS OF STATE

The Calaxeos project

A new generation of equations of state is on the way!



THANK YOU!

Questions?