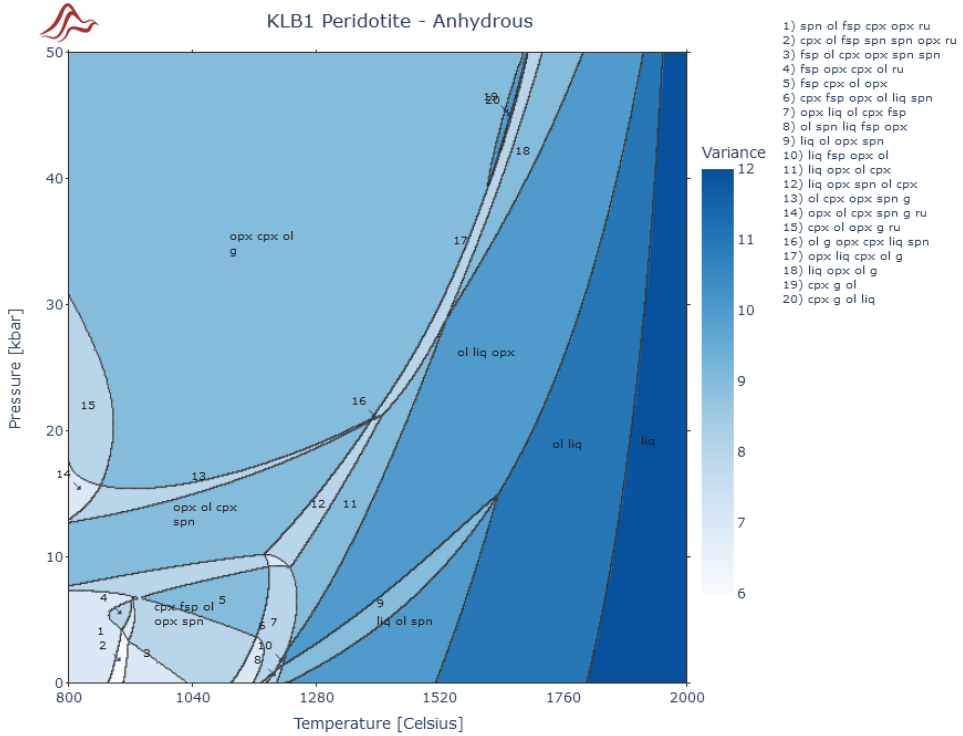
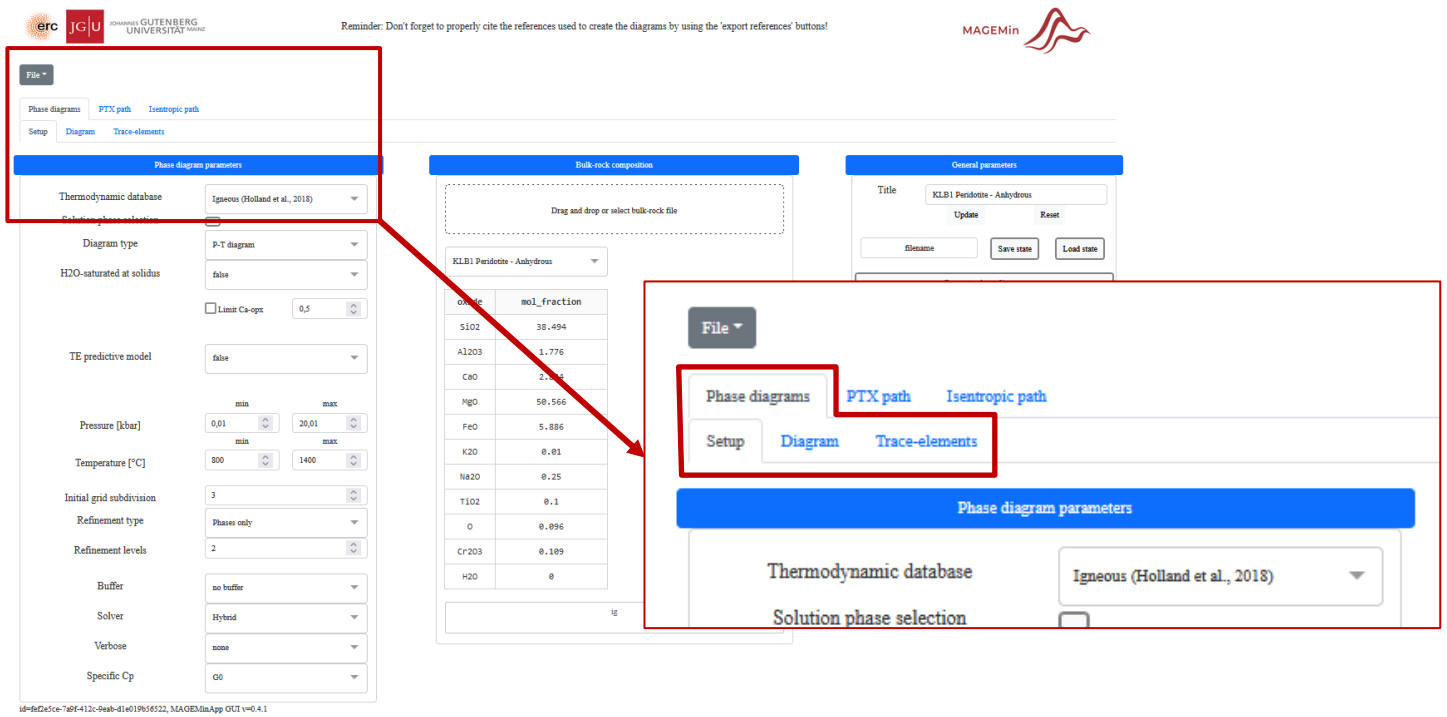
MAGEMinApp: phase diagrams tutorials

Granulites & Granulites 2024

MAGEMin

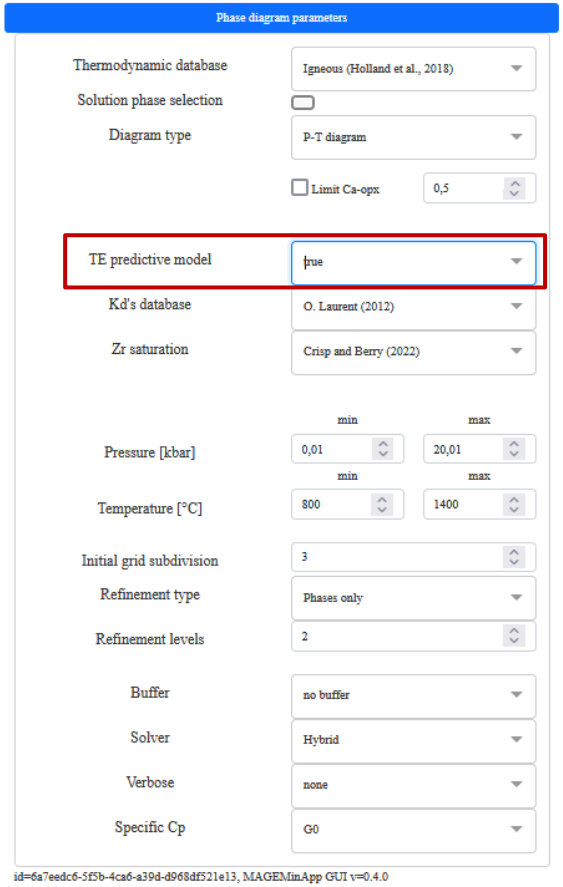


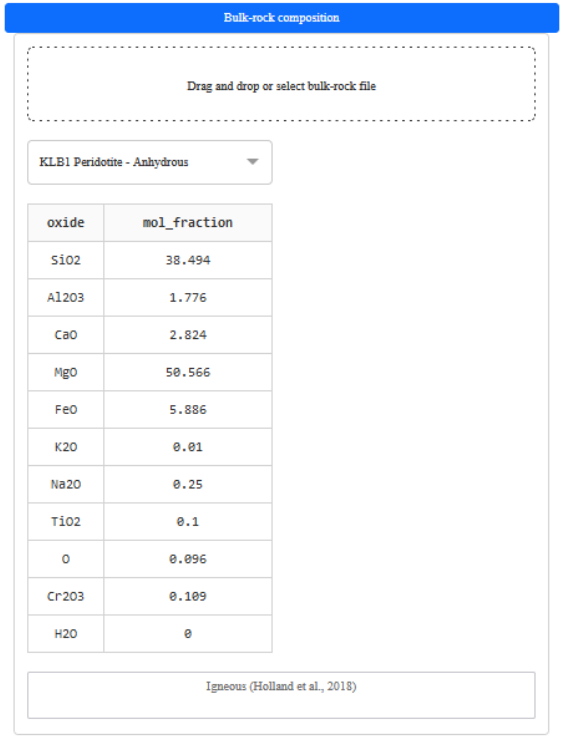
MAGEMinApp: phase diagrams interface

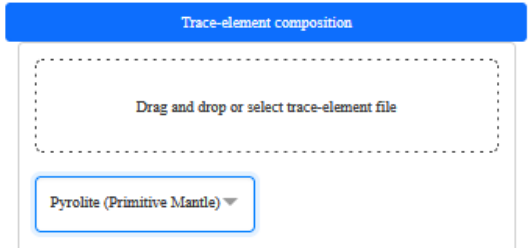


MAGEMinApp: first P-T phase diagram

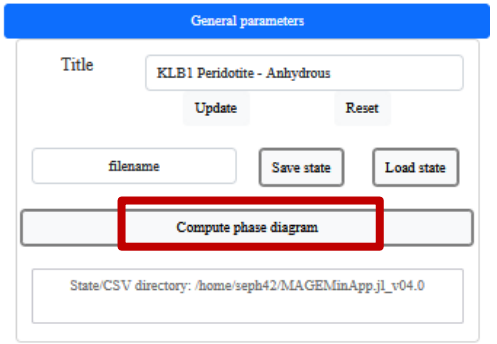
- **Select the following setup (nearly default)**







- **Select Pyrolite for trace-element composition**



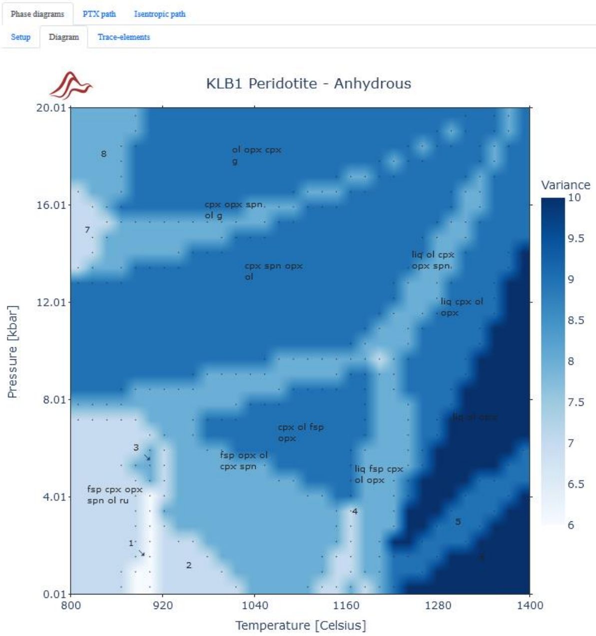
- **Click compute phase diagram**

MAGEMinApp: first phase diagram

- When computing you can see the progress in the Julia terminal

```
Computing 64 points... 100%|                                        | Time: 0:00:02
Computing 240 points... 100%|                                       | Time: 0:00:05
Computed 244 new points in 5.522367958 seconds
Computing 760 points... 100%|                                       | Time: 0:00:16
Computed 814 new points in 16.395254402 seconds
Interpolate data on grid 0.198 seconds
Get phase diagram labels 3.824 seconds
Computed trace element partitioning in 0.038169892 s
Updated plots in 0.91 seconds
```

- Once computed, the low-resolution diagram should look like this (the tab is changed to diagram automatically):



1) spn opx ol spn fsp cpx ru
2) spn fsp cpx ol spn opx
3) fsp opx ol cpx ru
4) fsp liq ol cpx opx spn
5) spn ol liq opx
6) liq spn ol
7) spn opx cpx g ol ru
8) cpx ol g opx ru

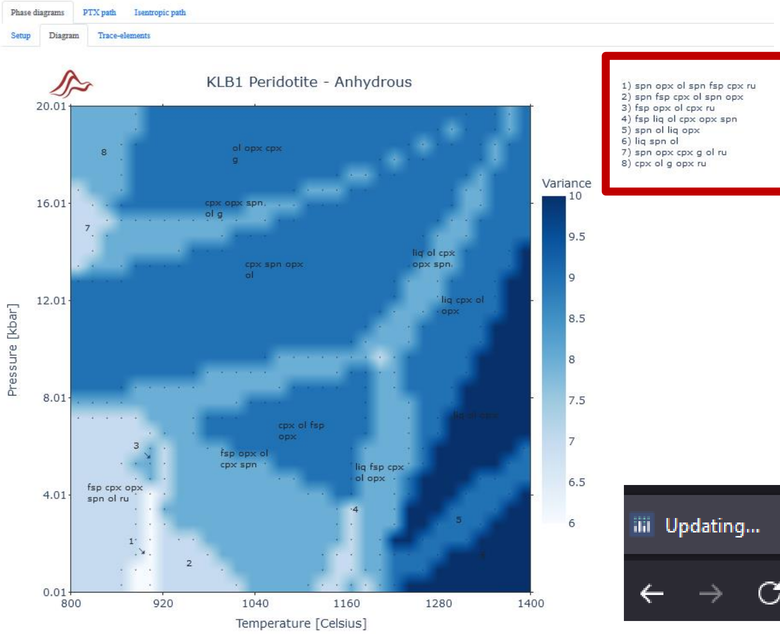
- **List of stable phase mineral assemblage that cannot fit the size of the field**

MAGEMinApp: first phase diagram

- When computing you can see the progress in the Julia terminal

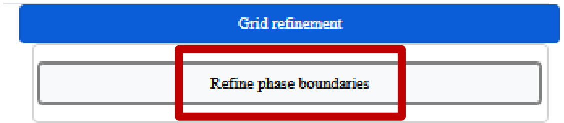
```
Computing 64 points... 100%|████████████████████████████████| Time: 0:00:02
Computing 240 points... 100%|███████████████████████████████| Time: 0:00:05
Computed 244 new points in 5.522367958 seconds
Computing 760 points... 100%|███████████████████████████████| Time: 0:00:16
Computed 814 new points in 16.395254402 seconds
Interpolate data on grid 0.198 seconds
Get phase diagram labels 3.824 seconds
Computed trace element partitioning in 0.038169892 s
Updated plots in 0.91 seconds
```

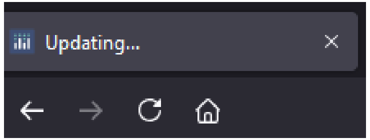
- Once computed, the low-resolution diagram should look like this (the tab is changed to diagram automatically):



1) spn opx ol spn fsp cpx ru
2) spn fsp cpx ol spn opx
3) fsp opx ol cpx ru
4) fsp liq ol cpx opx spn
5) spn ol liq opx
6) liq spn ol
7) spn opx cpx g ol ru
8) cpx ol g opx ru

- **List of stable mineral assemblage that cannot fit the size of the field**
- **Let's improve the resolution by clicking "refine phase boundaries" in the "Diagram Tab"**

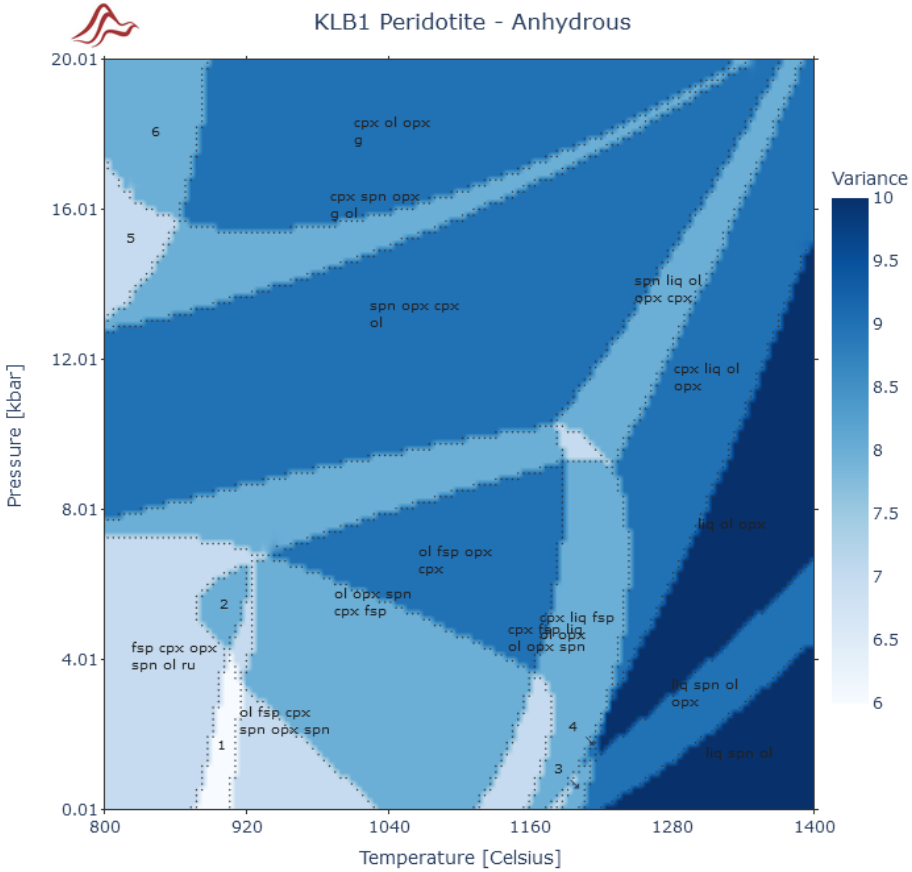




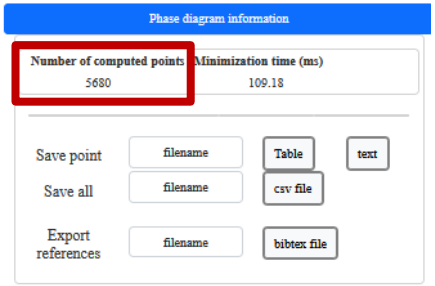
- Note that during any loading/calculation the title of your MAGEMinApp web-browser tab indicates "Updating…" **Wait until the message is gone before new actions!**

MAGEMinApp: first phase diagram

- After refining twice, the phase diagram starts to look better



1) fsp spn ol cpx opx spn ru
2) opx ol cpx fsp ru
3) liq spn fsp ol opx
4) fsp liq ol opx
5) opx ol g cpx spn ru
6) ol cpx g opx ru



- **In "Phase diagram information" the number of computed points is displayed.** Generally, the diagram looks clean when the number of points is > 30-40k

- **Clicking on any point will display some info about the equilibria**

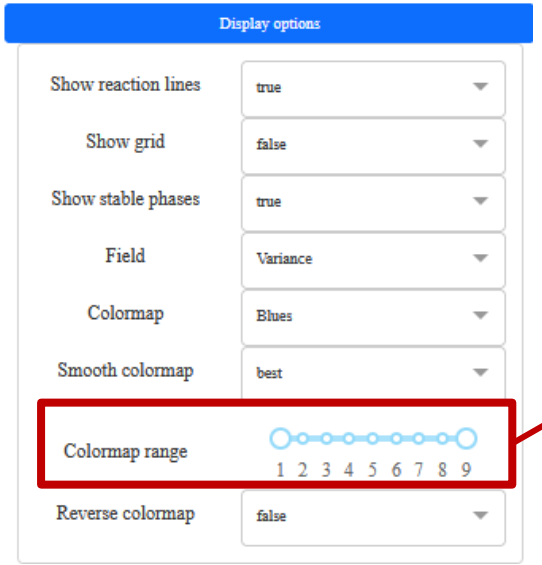
Variable	Value	Unit
P	8.604	kbar
T	982.813	°C
G	-816.909	kJ
ρ_sys	3245.7	kg/m³

Phase	Mode
fsp	0.021
cpx	0.127
ol	0.616
opx	0.225
spn	0.012

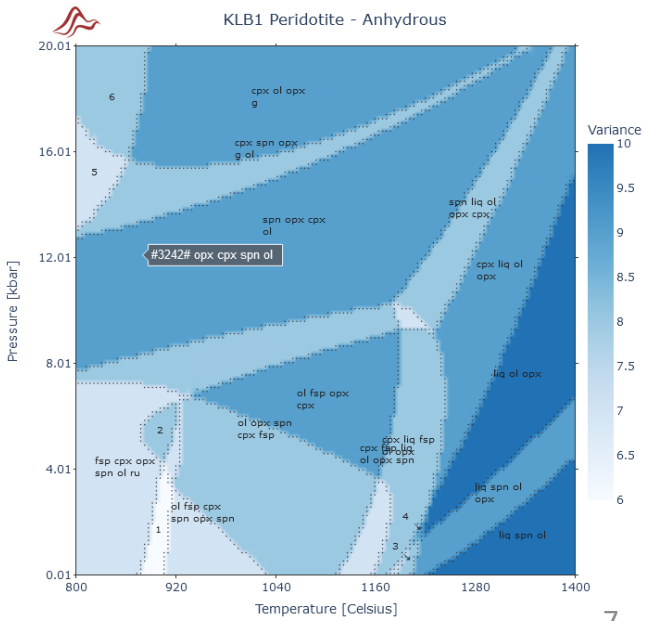
Oxide	mol
SiO2	0.385
Al2O3	0.018
CaO	0.028
MgO	0.505
FeO	0.059
K2O	0.0
Na2O	0.002
TiO2	0.001
O	0.001
Cr2O3	0.001
H2O	0.0

MAGEMinApp: colormap range

- The bottom right panel allow you to change the display options

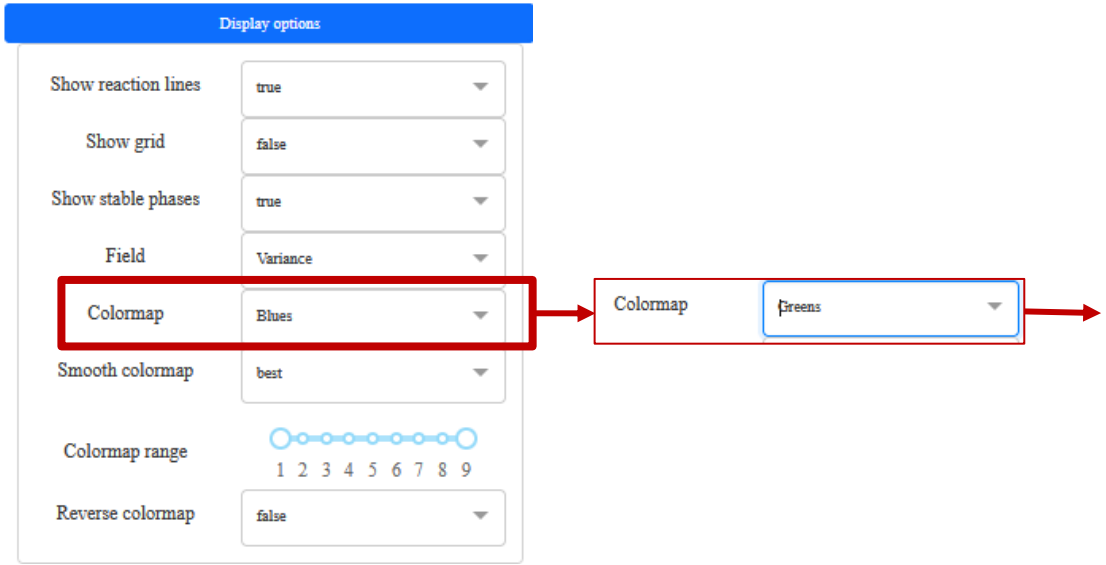


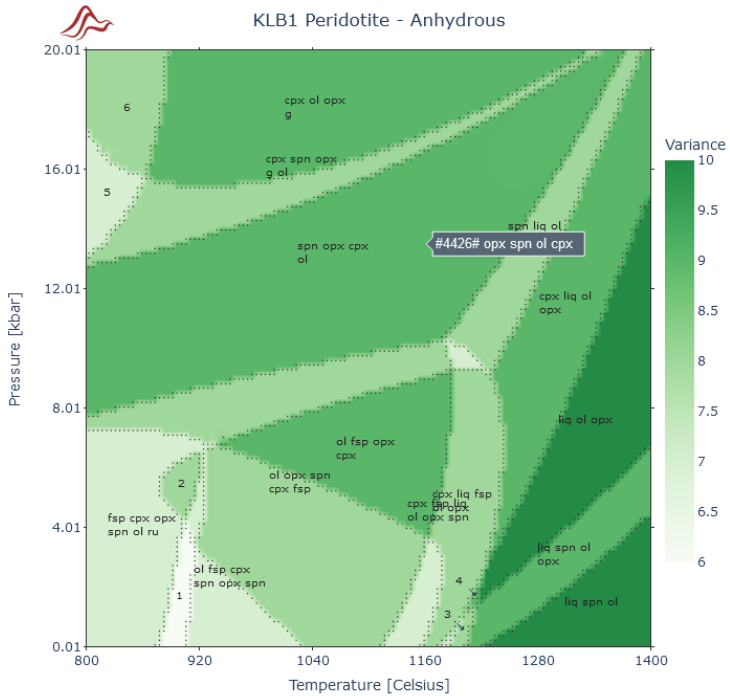
- Decreasing the colormap range allow the better visualize the high variance fields



MAGEMinApp: colormap

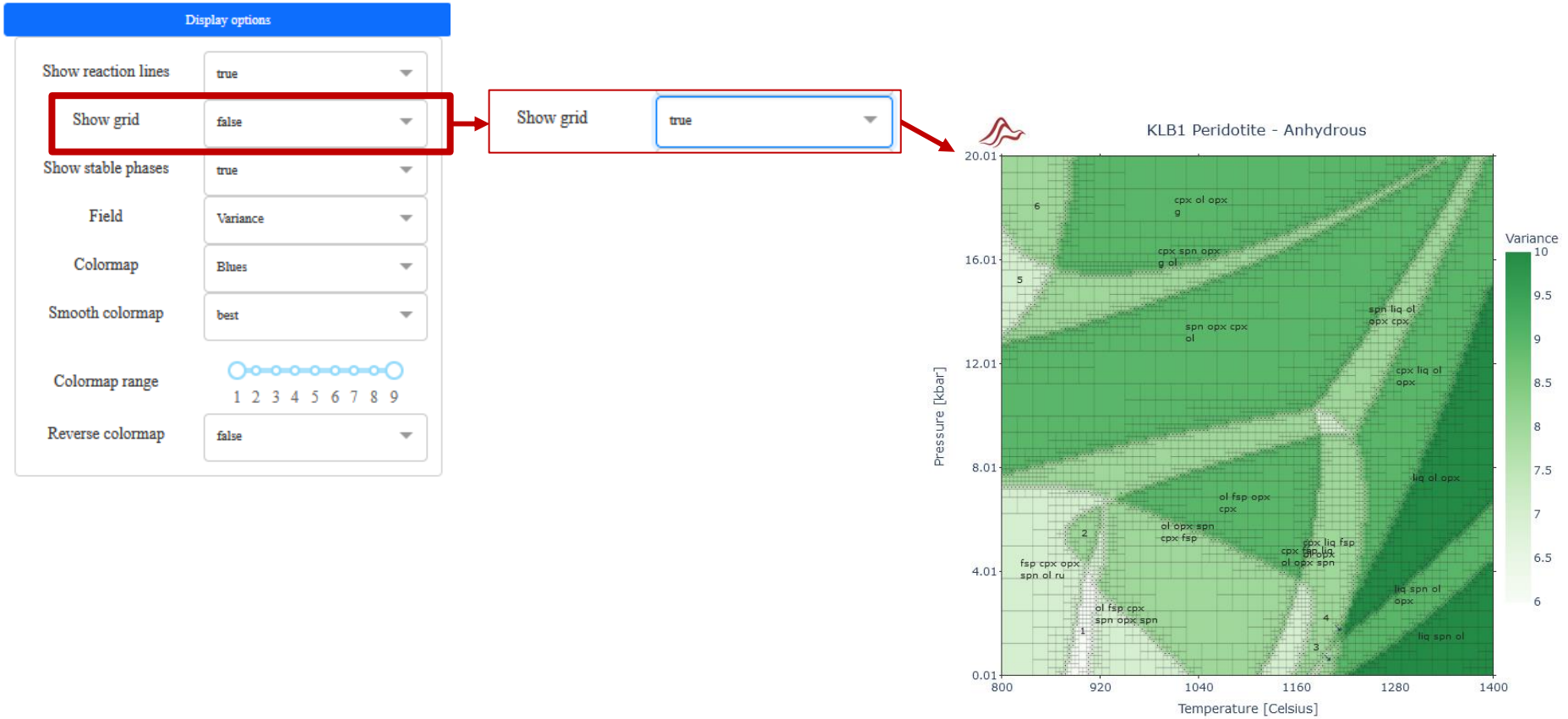
- You can of course change the colormap





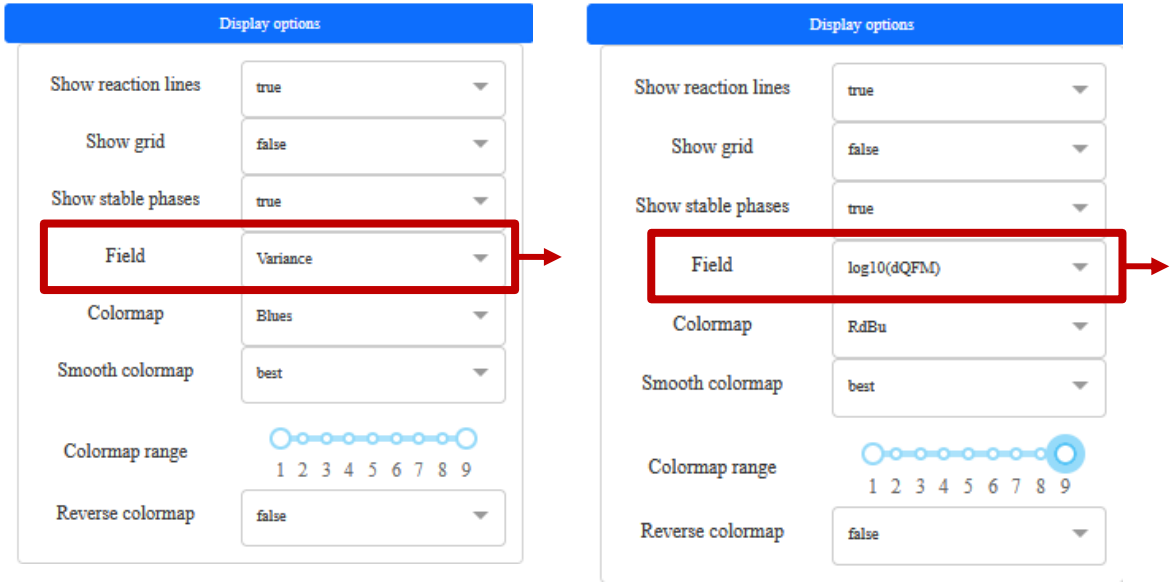
MAGEMinApp: grid display

- display the grid…

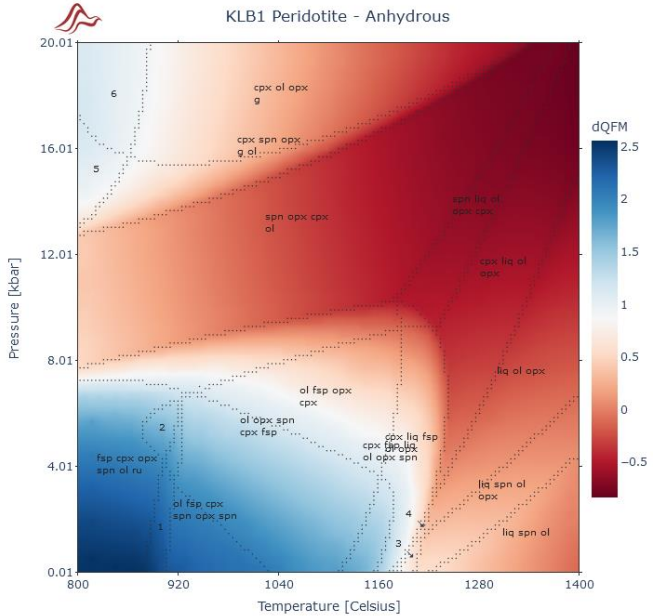


MAGEMinApp: field

- change the field to be displayed

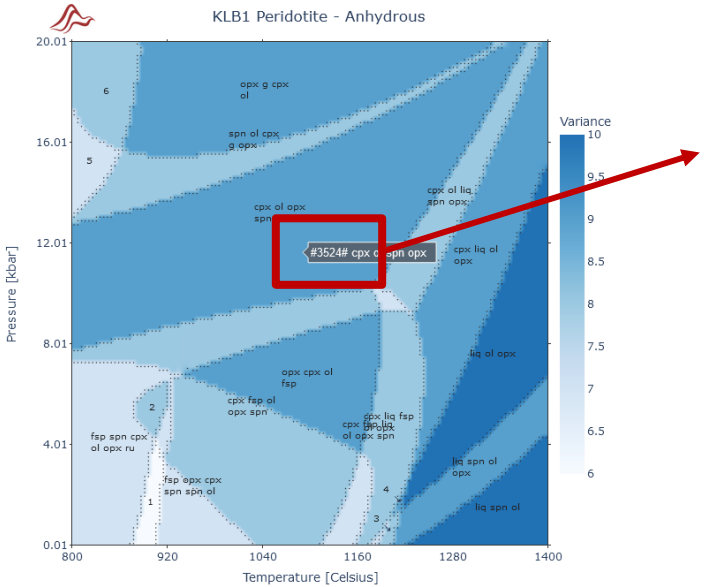


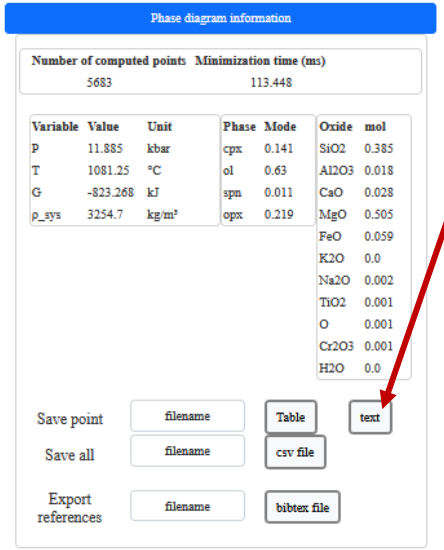
- For instance, dQFM using RdBu colormap



MAGEMinApp: saving data

- You can save point wise information or the whole diagram data using the right panel
- First, let's click on any grid point



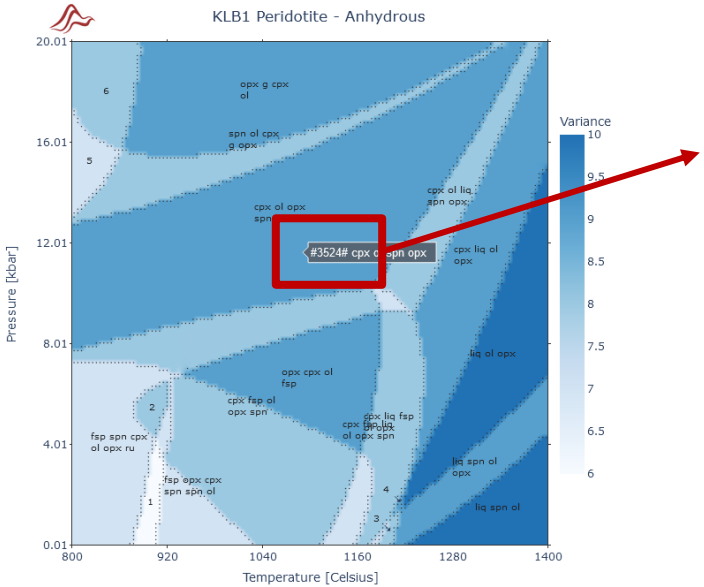


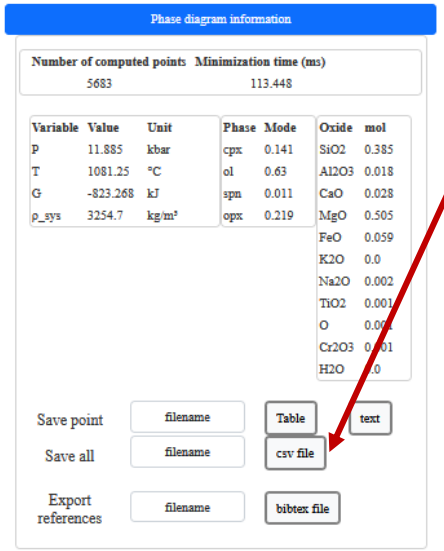
- **Change the filename to "test" and click "text"**
  this will save a file in your download directory
  e.g.,
  test_ig_Pkbar_11.885000000000002_TC_1081.25.txt

```
==========================================================
  cpx   ol   spn   opx  {11.8850 1081.2500} kbar/°C

End-members fractions[wt fr]:
      di      cfs     cats     crdi     cess     cbuf
 0.596337 0.066411 0.012233 0.017320 0.022295 0.032956
     mont       fa       fo      cfm
 0.003522 0.177025 0.819402 0.000051
      nsp      isp      nhc      ihc      nmt      imt
 0.553107 0.231982 0.141464 0.021306 -0.013429 0.02323
       en       fs       fm      odi     mgts     crer
 0.639219 0.053216 0.082200 0.045373 0.118856 0.023216

Oxide compositions [wt fr]:
            SiO2     Al2O3      CaO      MgO      FeO
   SYS 0.448600 0.035124 0.030719 0.395275 0.082032
   cpx 0.531572 0.054166 0.175962 0.168373 0.038439
    ol 0.408187 0.000000 0.000952 0.490787 0.100073
   spn 0.000000 0.636768 0.000000 0.230242 0.083187
   opx 0.527534 0.074349 0.012709 0.309750 0.064255

Stable mineral assemblage:
 phase   fraction[wt]        G[kJ]  V_molar[cm3/mol]
   cpx      +0.14461   -3457.26908         +66.64026
    ol      +0.62836   -2339.30393         +45.23134
   spn      +0.01071   -2446.84718         +41.03734
   opx      +0.21632   -3373.92842         +64.14469
```

MAGEMinApp: saving data

- You can save point wise information or the whole diagram data using the right panel
- First, let's click on any grid point





- **Change the filename to "test" and click "csv file"**
  this will save all data to an csv file

- Check Julia terminal. Here the file is saved in a different directory (not through the browser) because it can become very big!

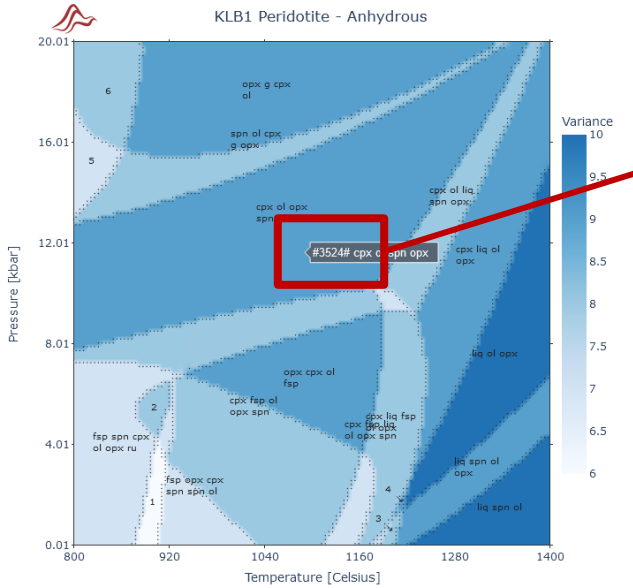
```
output path: /home/seph42/MAGEMinApp.jl_v04.0
Saving data to csv... 100%
```

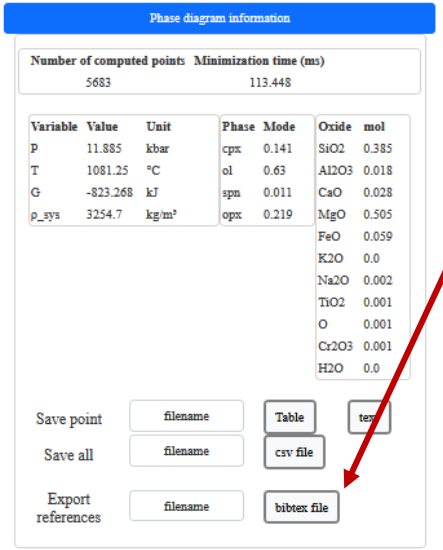
- The "csv" file is a complete save of all information of the phase diagram. When the number of points becomes larges (e.g., > 50k points) it can take a few minutes to save a file bigger than a few Go.

	A	B	C	D	E	F	G	H	I	J	
1	point[#]	X[0.0-1.0]	P[kbar]	T[°C]	phase	mode[mol	mode[wt%	log10(fO2	log10(dQF	aH2O	a
2	1	1	0.635	818.75	system	100	100	-11.6936	2.559878	0	(
3	1	1	0.635	818.75	fsp	6.959184	6.970663	-	-	-	-
4	1	1	0.635	818.75	spn	0.174666	0.248471	-	-	-	-
5	1	1	0.635	818.75	cpx	6.119897	6.341448	-	-	-	-
6	1	1	0.635	818.75	ol	69.78836	69.61555	-	-	-	-
7	1	1	0.635	818.75	opx	16.87659	16.72111	-	-	-	-
8	1	1	0.635	818.75	ru	0.081307	0.102756	-	-	-	-
9	2	1	0.3225	846.875	system	100	100	-11.1585	2.557661	0	(
10	2	1	0.3225	846.875	fsp	6.946325	6.956501	-	-	-	-
11	2	1	0.3225	846.875	ol	69.78973	69.61939	-	-	-	-
12	2	1	0.3225	846.875	opx	16.94176	16.79384	-	-	-	-
13	2	1	0.3225	846.875	cpx	6.082929	6.30309	-	-	-	-
14	2	1	0.3225	846.875	spn	0.159418	0.226294	-	-	-	-
15	2	1	0.3225	846.875	ru	0.079834	0.100888	-	-	-	-
16	3	1	0.16625	860.9375	system	100	100	-10.9044	2.55316	0	
17	3	1	0.16625	860.9375	ol	69.7901	69.62	-	-	-	-
18	3	1	0.16625	860.9375	fsp	6.938948	6.94901	-	-	-	-
19	3	1	0.16625	860.9375	opx	16.97846	16.83468	-	-	-	-
20	3	1	0.16625	860.9375	cpx	6.061894	6.281553	-	-	-	-

MAGEMinApp: saving data

- You can save point wise information or the whole diagram data using the right panel
- First, let's click on any grid point



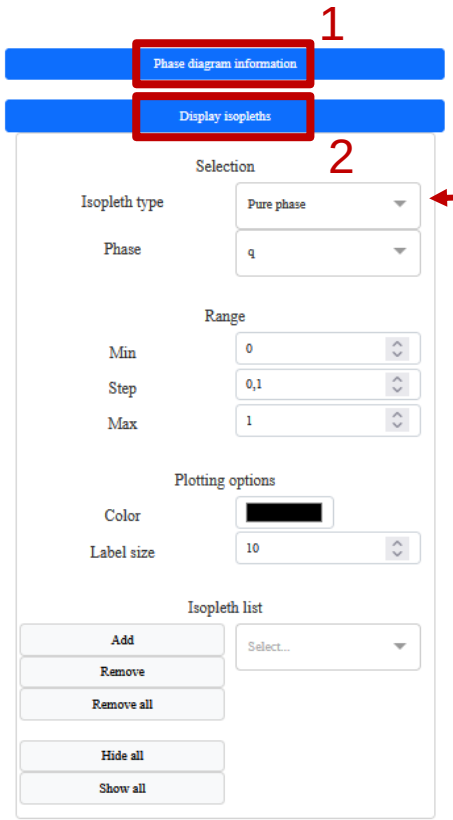


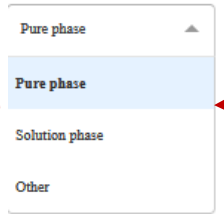
- **You can also save the references used to perform the calculation clicking on "bibtex file"!**

```
@article{holland2018melting,
 pages        = {881--900},
 info         = {ig},
 author       = {Holland, Tim JB and Green, Eleanor CR and Powell, Roger},
 journal      = {Journal of Petrology},
 title        = {Melting of peridotites through to granites: a simple thermodynamic model in the system KNCFMASHTOCr},
 publisher    = {Oxford University Press},
 number       = {5},
 doi          = {10.1093/petrology/egy048},
 year         = {2018},
 volume       = {59}
}

@article{riel2022magemin,
 pages        = {e2022GC010427},
 info         = {MAGEMin},
 author       = {Riel, Nicolas and Kaus, Boris JP and Green, ECR and Berlie, Nicolas},
 journal      = {Geochemistry, Geophysics, Geosystems},
 title        = {MAGEMin, an efficient Gibbs energy minimizer: application to igneous systems},
 publisher    = {Wiley Online Library},
 number       = {7},
 doi          = {https://doi.org/10.1029/2022GC010427},
 year         = {2022},
 volume       = {23}
}
```

MAGEMinApp: fields isocontours and isopleths

- Clicking on the “phase diagram information” panel will fold it
- Then click on “Display isopleths” panel to unfold it

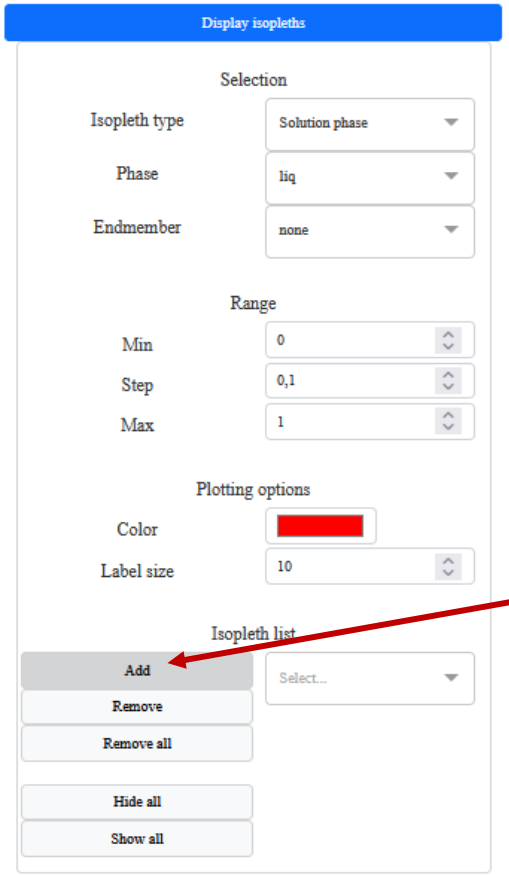




- **Here you can select what to contour: Pure phase, Solution phase or Other (fields)**
- **Here you can select min, step and max values**
- **Here you can select the color of the isocontour**
- **And here you can manage the isocontour list**

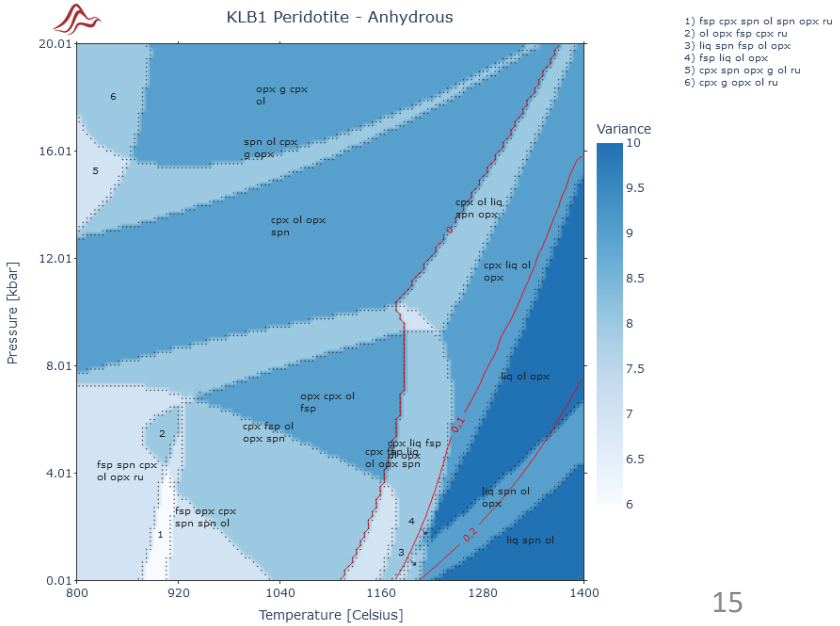
MAGEMinApp: fields isocontours and isopleths

- Let's contour melt fraction



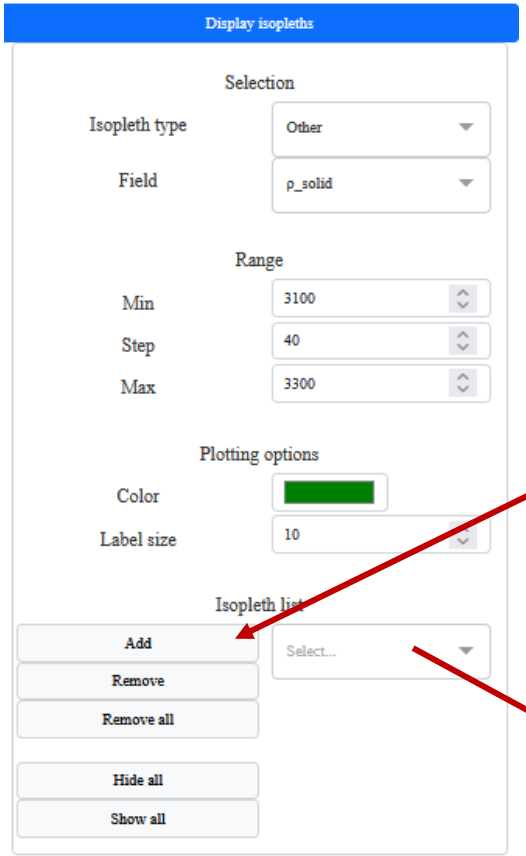
- **Select:**
  Isopleth type = "Solution phase"
  Phase = "liq"
  Endmember = "none"
  → This will display the mode in mol%

- **Change the color to what you like then click add**



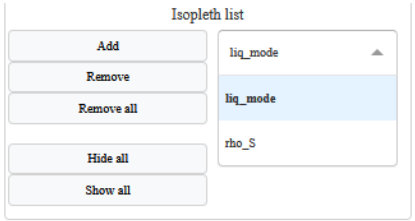
MAGEMinApp: fields isocontours and isopleths

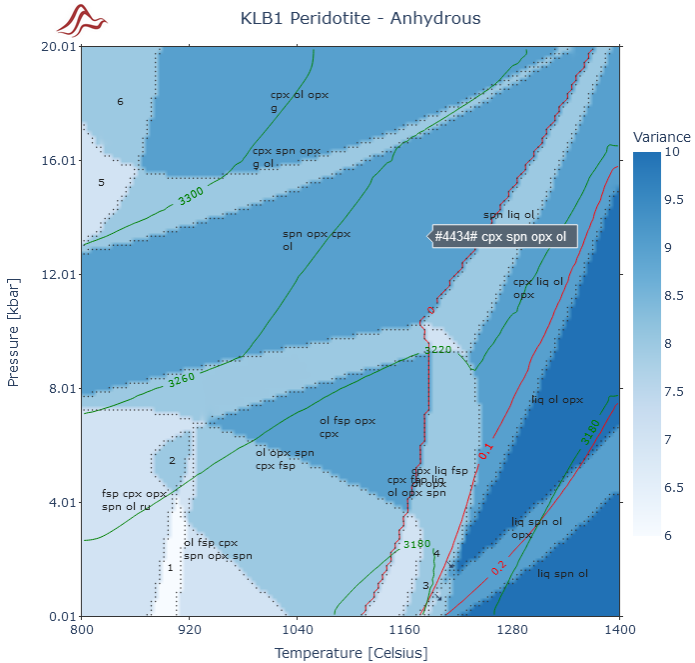
- Adding density contour



- **Select:**
  Isopleth type = “Other”
  Phase = “rho_solid”

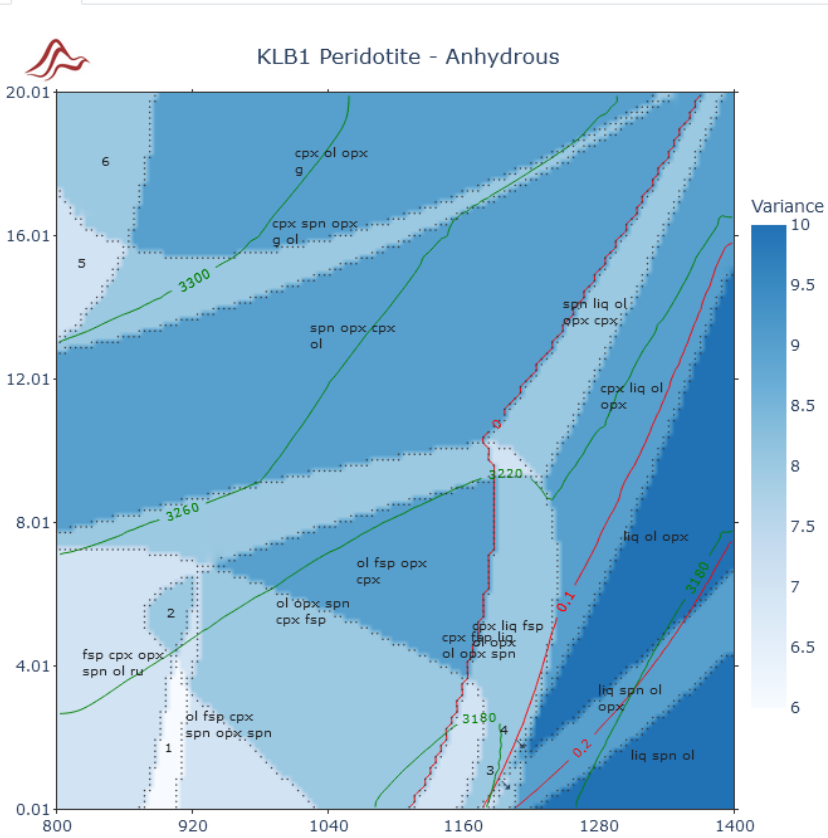
- **Change the color to what you like then click add**

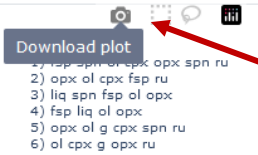




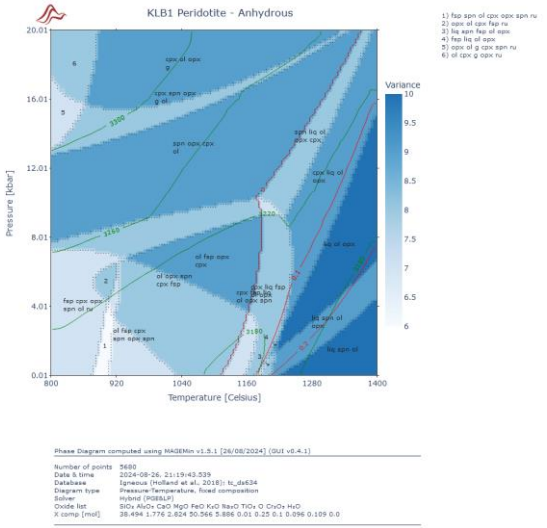
- **The isopleth list allow you to remove select isocontour**

MAGEMinApp: save figure(s)





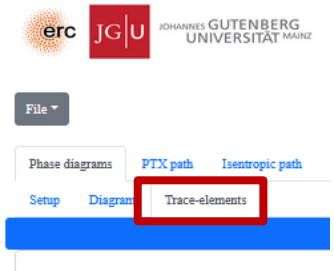
Click here to save the plot as an “svg” vector file that can be opened in Inksape



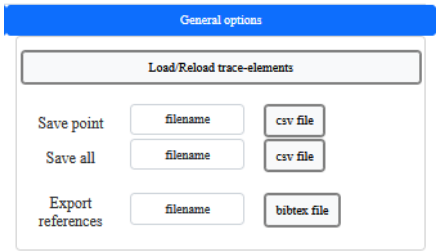
- **All plots and figures in the app can be saves in the same way**

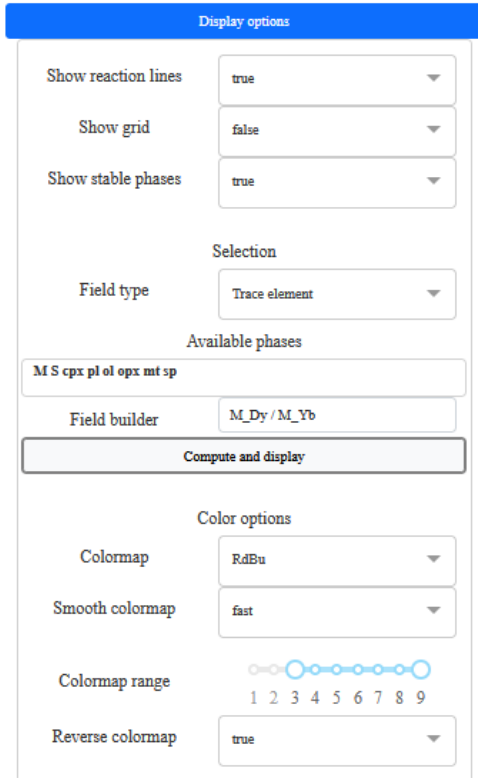
MAGEMinApp: trace elements

- Click on “Trace-elements” tab



- Then on the right panel,
  click “Load/Reload trace-elements”





- Then in display option,
  Field type → “Trace element”
  then
  click “Compute and display”

- Then click on anywhere in supra-solidus fields

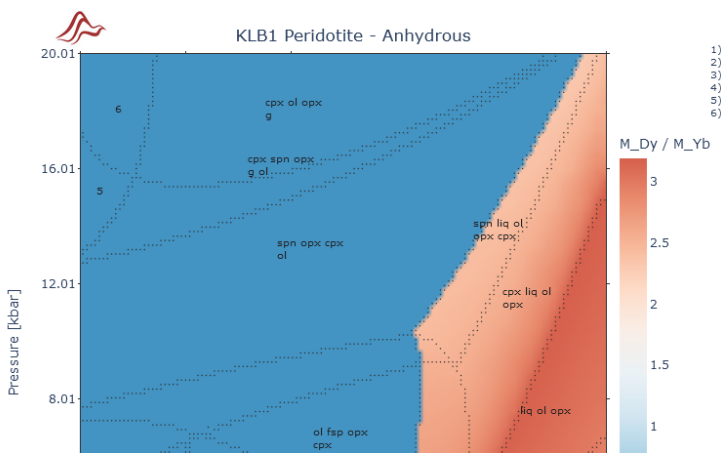
MAGEMinApp: trace elements

- Which yields:

This plot displays TE spectrum

Here you can choose to display REE or all TE

Here you can change the normalization



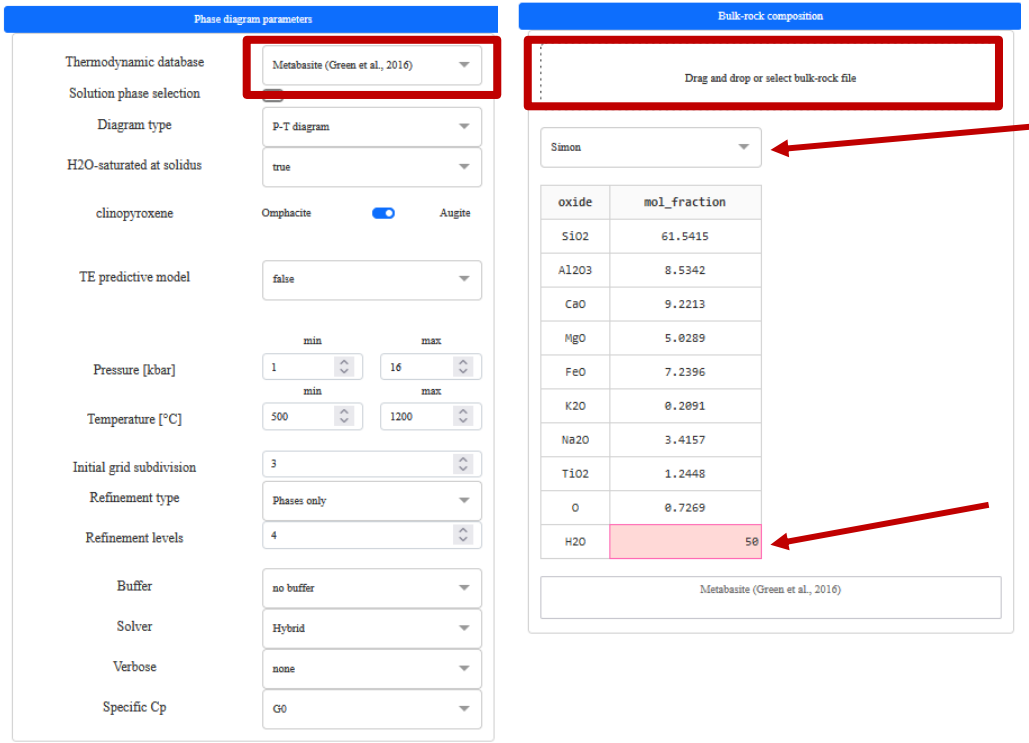
Here you can save point/all information

Here you can display custom made fields

Note that:
M → melt
S → solid
M_Dy → Dy in melt in ug/g
Operators should be separated by a space

MAGEMinApp: custom bulk rock composition

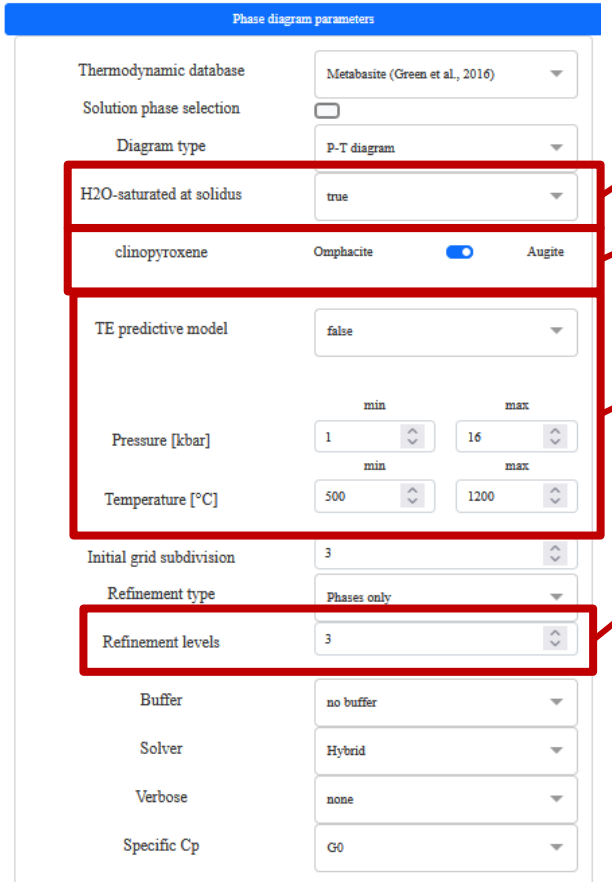
- In Tab “Phase diagrams”, “Setup” select “Metabasite”
  then drag and drop \Resources\GG2024\bulkrock_composition_input_files\bulk-rock_ref.dat in the middle panel “Bulk-rock composition”



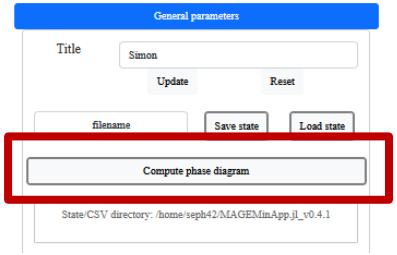
- In the bulk-rock dropdown menu, select “Simon” bulk

- Change the water content to 50 to oversaturate

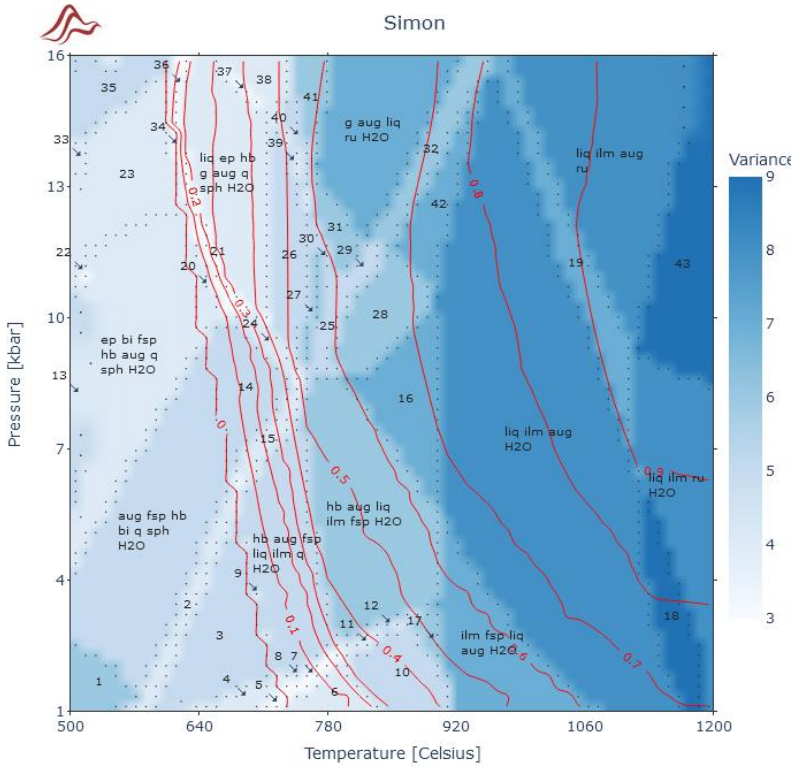
MAGEMinApp: diagram with saturated water at solidus



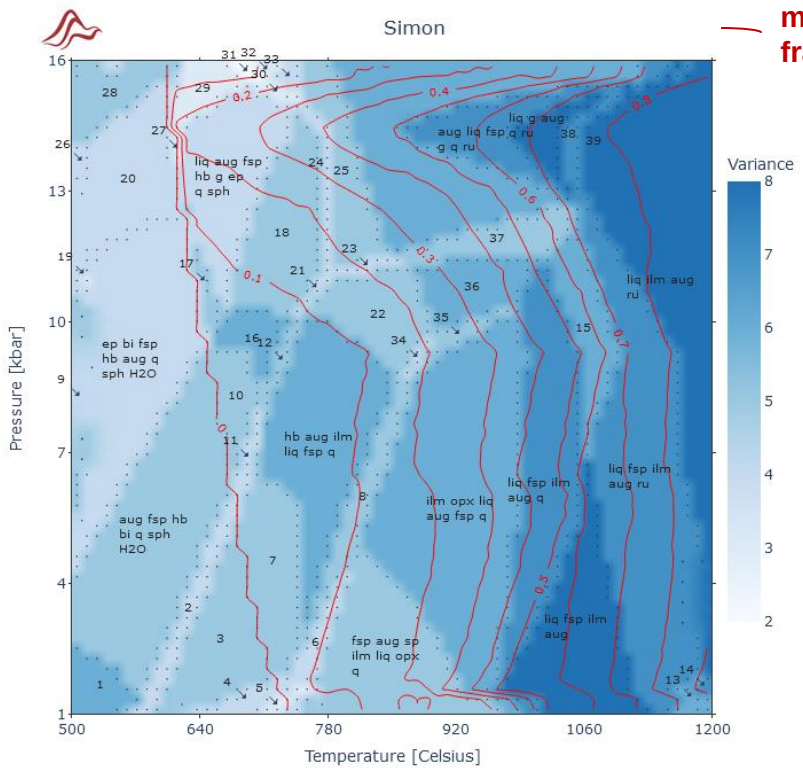
- **Select "H2O-saturated at solidus" = true**
  This activates automatic saturation of water at solidus
- **Select Augite for the suprasolidus conditions**
- **Choose to activate or not TE modeling**
- **Choose the range of PT conditions you want**
- **Select a level of refinement according to your computer performances**
- **Then compute the diagram…**



MAGEMinApp: diagram with saturated water at solidus

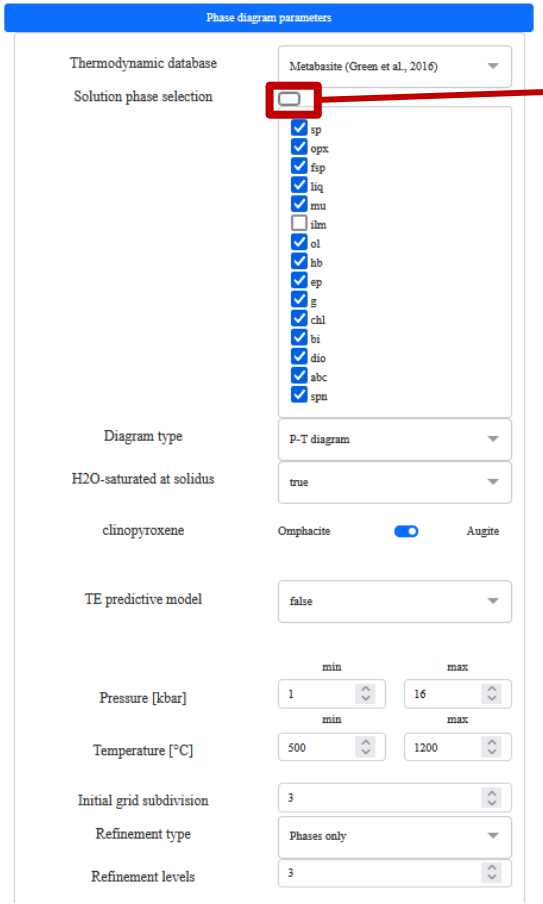


“H2O-saturated at solidus” = false



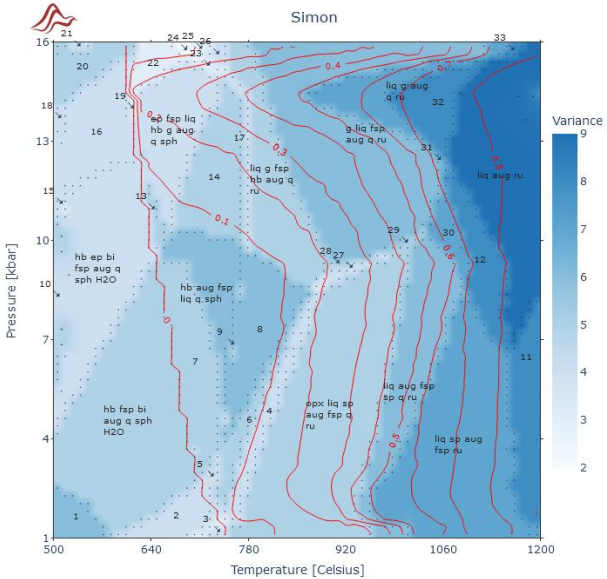
“H2O-saturated at solidus” = true

MAGEMinApp: deactivating a solution phase model



- **Go back to setup then click on "Solution phase selection" to unfold the list of solution phase model belonging to the "Metabasite" database**

- **Unselect "ilm" and re-compute the diagram**



"H2O-saturated at solidus" = true

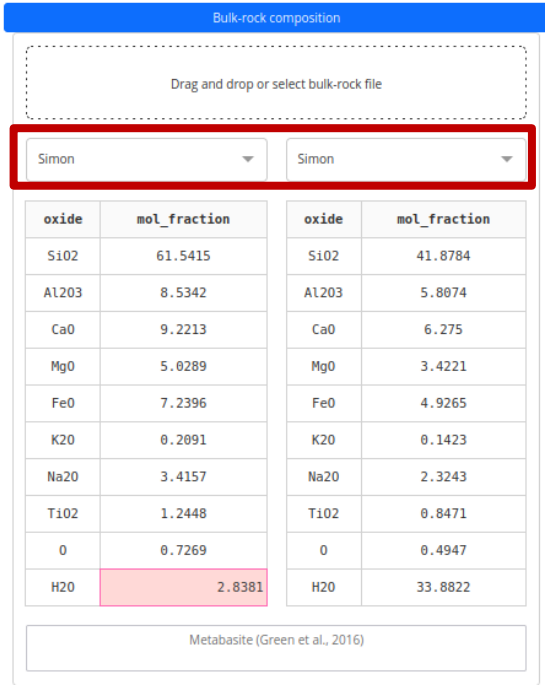
MAGEMinApp: T-X phase diagrams

- Open \Resources\GG2024\bulkrock_composition_input_files\bulk-rock_ref.dat in a text editor
- Copy the “Simon” composition and change the water content to 50.0 (do not add “;” at the end)
  this provides the second bulk rock composition that will be used in the T-X diagram

```
# HEADER
title; comments; db; sysUnit; oxide; frac; frac2
# BULK-ROCK COMPOSITION
Test 2;Moo et al., 2000;ig;mol;[SiO2, Al2O3, CaO, MgO, FeO, K2O, Na2O, TiO2, O, Cr2O3, H2O];
[48.97, 11.76, 13.87, 4.21, 8.97, 1.66, 10.66, 1.36, 1.66, 0.01, 5.0];
K167;Moo et al., 2000;ig;mol;[SiO2, Al2O3, CaO, MgO, FeO, K2O, Na2O, TiO2, O, Cr2O3, H2O];
[50.3162, 8.0778, 11.6616, 11.3262, 9.1893, 0.4312, 2.4051, 2.271, 4.312, 0.0096, 0.0];
Test 3;Coin & Kwak, 1984;mb;wt;[SiO2, Al2O3, CaO, MgO, Fe2O3, K2O,Na2O, TiO2, FeO, H2O];
[55.12, 12.76, 4.32, 5.21, 2.45, 1.66, 10.66, 1.36, 1.66, 2.0];
Simon;Shorn Simon, 2023;mb;mol;[SiO2, Al2O3, CaO, MgO, FeO, K2O, Na2O, TiO2, O, H2O];
[61.8,8.57,9.26,5.05,7.27,0.21,3.43,1.25,0.73,2.85];
[61.8,8.57,9.26,5.05,7.27,0.21,3.43,1.25,0.73,50]
```

- In “Setup” tab load the modified bulk-rock_ref.dat
- Change “Diagram type” to “T-X diagram”
  This displays a new table in the central “Bulk-rock composition” panel

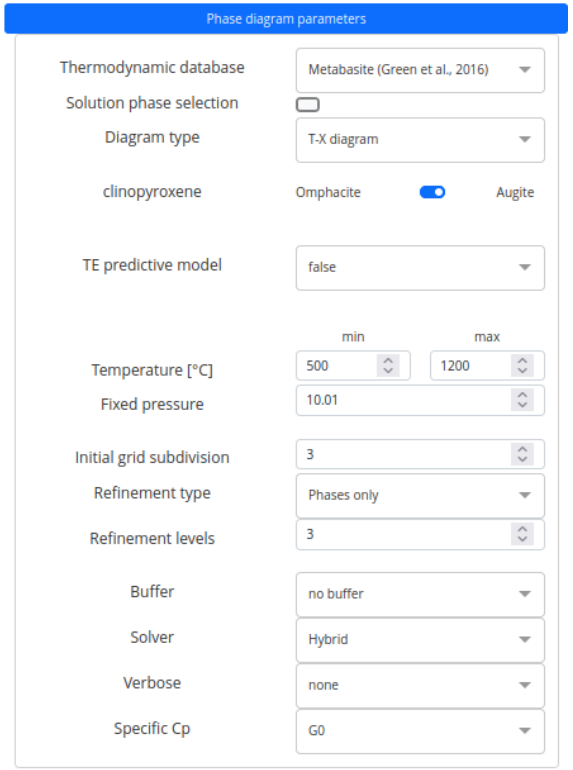
- Select Simon for both →
  Notice that the right table automatically loads the second “Simon” bulk-rock composition



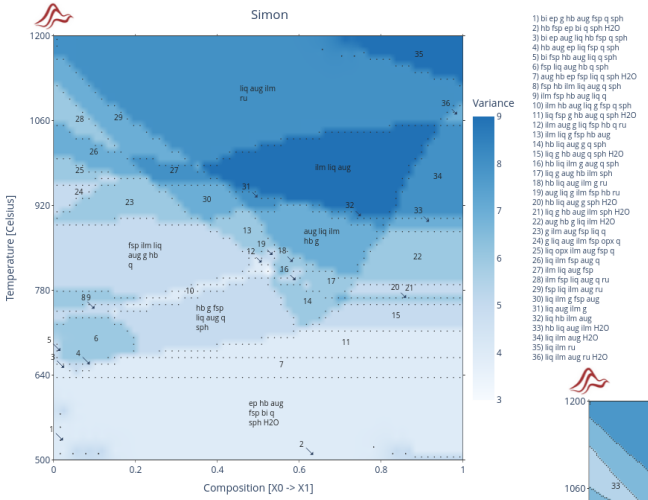
oxide	mol_fraction	oxide	mol_fraction
SiO2	61.5415	SiO2	41.8784
Al2O3	8.5342	Al2O3	5.8074
CaO	9.2213	CaO	6.275
MgO	5.0289	MgO	3.4221
FeO	7.2396	FeO	4.9265
K2O	0.2091	K2O	0.1423
Na2O	3.4157	Na2O	2.3243
TiO2	1.2448	TiO2	0.8471
O	0.7269	O	0.4947
H2O	2.8381	H2O	33.8822

MAGEMinApp: T-X phase diagrams

- Change the Phase-Diagram setup according to what you want
- Then compute the phase diagram

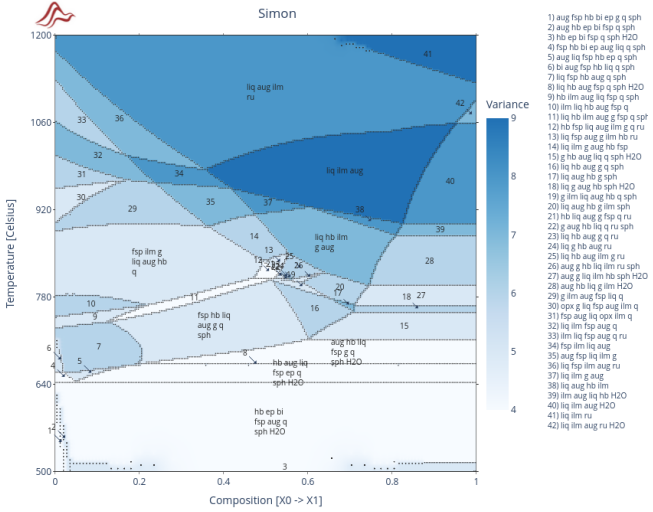


Set of parameters example



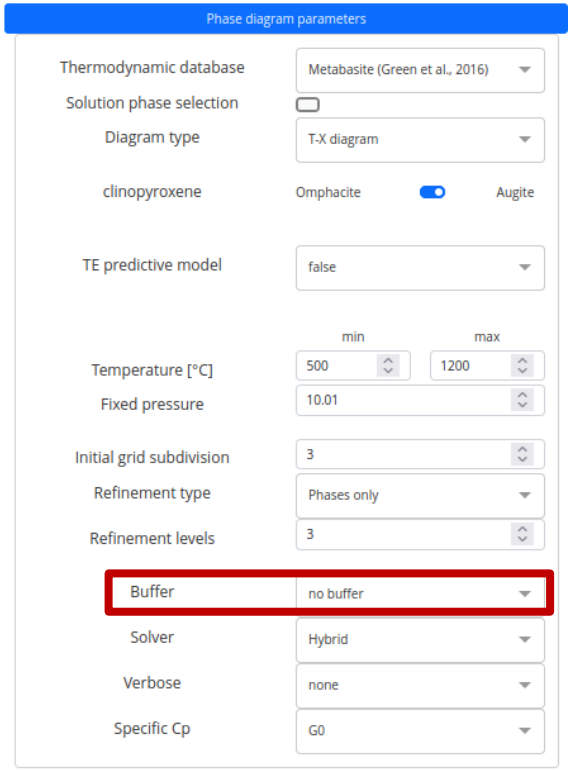
Example of phase diagram result using 3 refinements levels

And after 2 supplementary refinements...



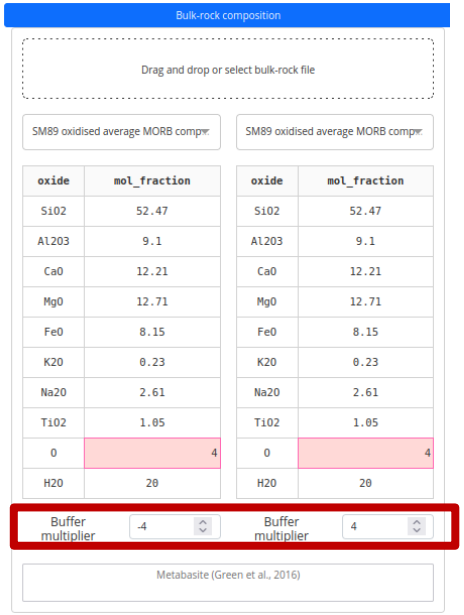
MAGEMinApp: T-X phase diagrams with buffer

- You can also change the buffer value in the RT log scale
- For instance, select QFM buffer

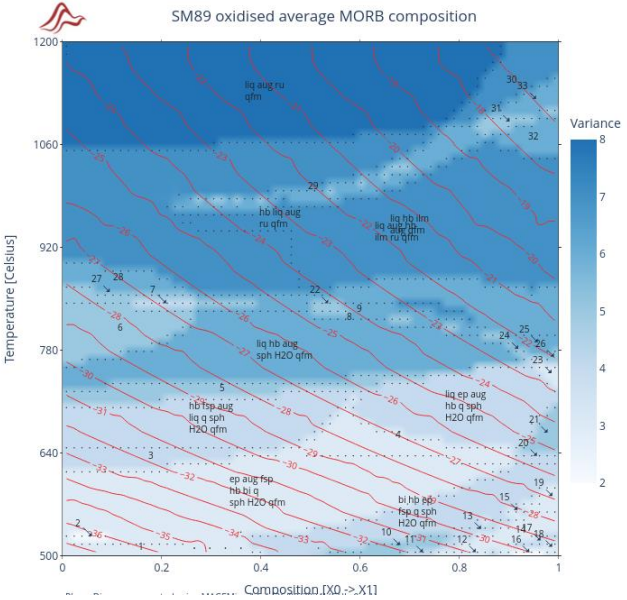


Set of parameters example

- Then select SM89 bulk-rock for both tables
- Oversaturate in oxygen (O)
- change the buffer multiplier values



- Compute and contour the field log10(fO2) (Oxygen fugacity)



MAGEMinApp: PT-X phase diagrams

- PT-X diagrams allow you to define a PT paths on the vertical axis and vary the composition in the horizontal axis

- Let's compute a Barrovian PT path phase diagram for metapelite while vayring the water content
- First select the "Metapelite" database, then change Diagram type to "PT-X diagram"

Phase diagram parameters

Thermodynamic database: Metapelite (White et al., 2014)

Solution phase selection: ☐

Diagram type: PT-X diagram

TE predictive model: false

Pressure-Temperature path (using pChip interpolation)

	P [kbar]	T [°C]
×	3	200
×	6	400
×	8	600
×	9	800
×	8	850
×	6	700
×	3	400

Add new point

Initial grid subdivision: 3

Refinement type: Phases only

Refinement levels: 3

Buffer: no buffer

Solver: Hybrid

Verbose: none

Specific Cp: G0

id=949306a2-415b-4eb8-b275-0bb3f1c162ed, MAGEMinApp GUI v=0.4.1

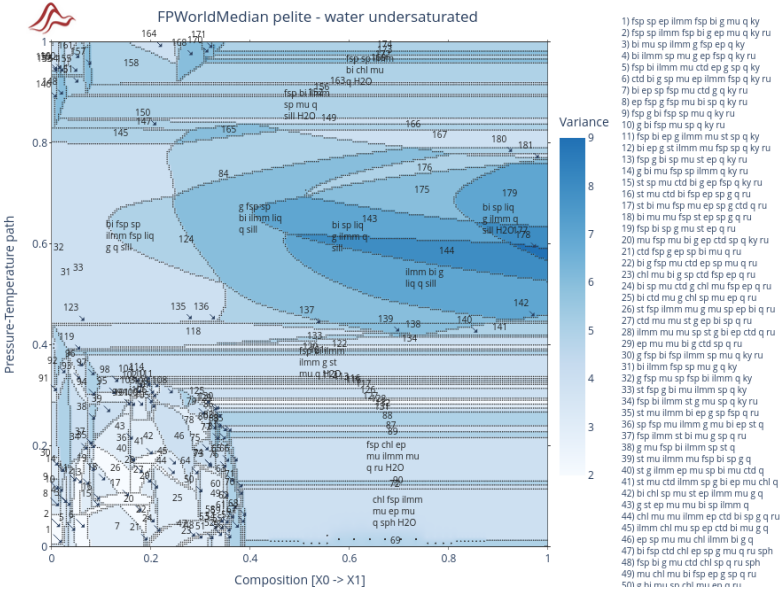
Bulk-rock composition

Drag and drop or select bulk-rock file

FPWorldMedian pelite - water under | FPWorldMedian pelite - water overs

oxide	mol_fraction	oxide	mol_fraction
SiO2	70.999	SiO2	70.999
Al2O3	12.805	Al2O3	12.805
CaO	0.771	CaO	0.771
MgO	3.978	MgO	3.978
FeO	6.342	FeO	6.342
K2O	2.7895	K2O	2.7895
Na2O	1.481	Na2O	1.481
TiO2	0.758	TiO2	0.758
O	0.72933	O	0.72933
MnO	0.075	MnO	0.075
H2O	5	H2O	30

Metapelite (White et al., 2014)



Note that if the field's list is cropped in the app, you can access the complete list of stable mineral assemblage in the "svg" when exporting the figure