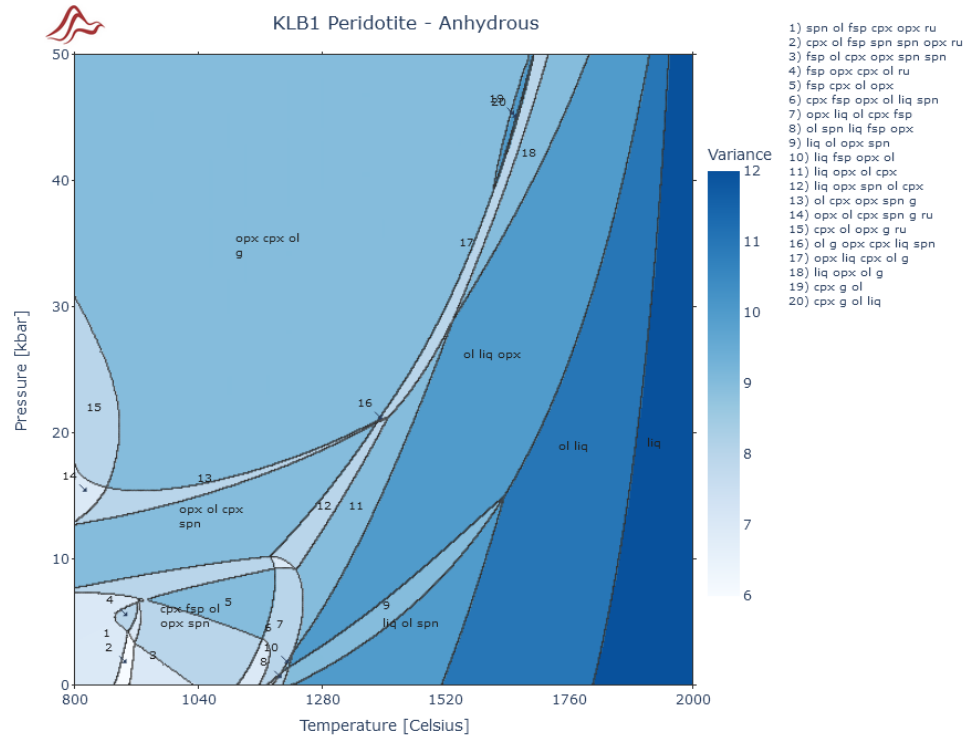


MAGeMinApp: phase diagrams tutorials



MAGEMinApp: phase diagrams interface

erc JGU JOHANNES GUTENBERG UNIVERSITÄT MAINZ

Reminder: Don't forget to properly cite the references used to create the diagrams by using the 'export references' buttons!

MAGEMin

File

Phase diagrams PTX path Isentropic path

Setup Diagram Trace-elements

Phase diagram parameters

Thermodynamic database Igneous (Holland et al., 2018)

Solution phase selection

Diagram type P-T diagram

H₂O-saturated at solidus false

☐ Limit Ca-opt 0.5

TE predictive model false

Pressure [kbar] 0.01 20.01

Temperature [°C] 800 1400

Initial grid subdivision 3

Refinement type Phases only

Refinement levels 2

Buffer no buffer

Solver Hybrid

Verbose none

Specific Cp 00

Bulk-rock composition

Drag and drop or select bulk-rock file

KLB1 Peridotite - Anhydrous

oxide	mol_fraction
SiO ₂	38.494
Al ₂ O ₃	1.776
CaO	2.304
MgO	50.566
FeO	5.886
K ₂ O	0.01
Na ₂ O	0.25
TiO ₂	0.1
O	0.096
Cr ₂ O ₃	0.189
H ₂ O	0

General parameters

Title KLB1 Peridotite - Anhydrous

Update Reset

filename Save state Load state

File

Phase diagrams PTX path Isentropic path

Setup Diagram Trace-elements

Phase diagram parameters

Thermodynamic database Igneous (Holland et al., 2018)

Solution phase selection

MAGEMinApp: first P-T phase diagram

- Select the following setup (nearly default)

Phase diagram parameters

Thermodynamic database: Igneous (Holland et al., 2018)

Solution phase selection: ☐

Diagram type: P-T diagram

☐ Limit Ca-opx: 0,5

TE predictive model: **true**

Kd's database: O. Laurent (2012)

Zr saturation: Crisp and Berry (2022)

Pressure [kbar]: min 0,01 max 20,01

Temperature [°C]: min 800 max 1400

Initial grid subdivision: 3

Refinement type: Phases only

Refinement levels: 2

Buffer: no buffer

Solver: Hybrid

Verbose: none

Specific Cp: G0

Bulk-rock composition

Drag and drop or select bulk-rock file

KLB1 Peridotite - Anhydrous

oxide	mol_fraction
SiO2	38.494
Al2O3	1.776
CaO	2.824
MgO	50.566
FeO	5.886
K2O	0.01
Na2O	0.25
TiO2	0.1
O	0.096
Cr2O3	0.109
H2O	0

Igneous (Holland et al., 2018)

Trace-element composition

Drag and drop or select trace-element file

Pyrolite (Primitive Mantle)

- Select Pyrolite for trace-element composition

General parameters

Title: KLB1 Peridotite - Anhydrous

Update Reset

filename Save state Load state

Compute phase diagram

State/CSV directory: /home/seph42/MAGEMinApp.jl_v04.0

- Click compute phase diagram

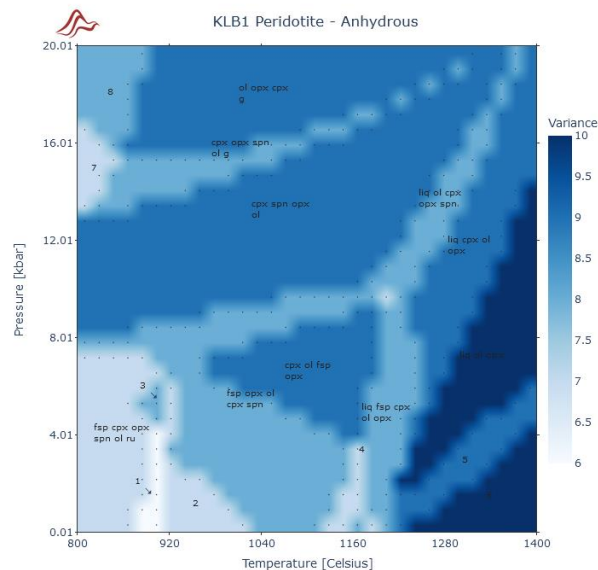
MAGEMinApp: first phase diagram

- 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):

Phase diagrams PTX path Isentropic path
Setup Diagram Trace-elements



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

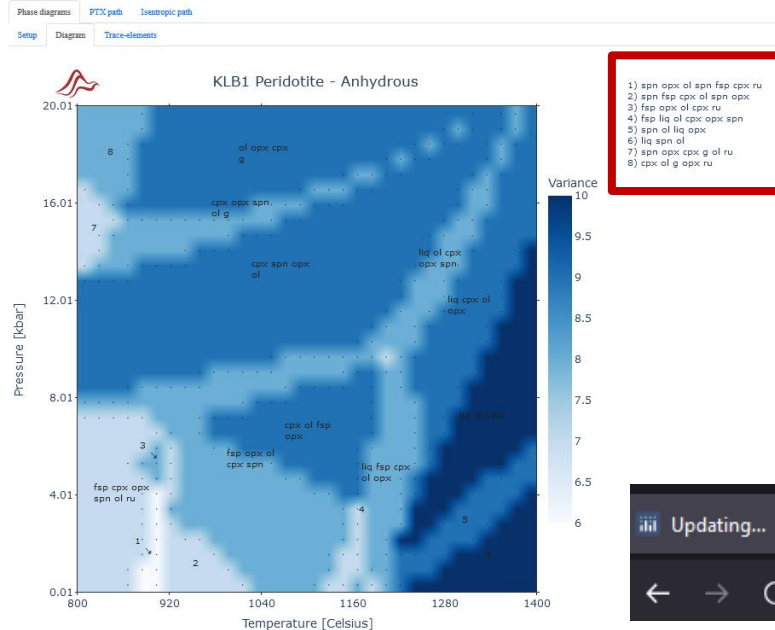
- List of stable phase mineral assemblage that cannot fit the size of the field

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):

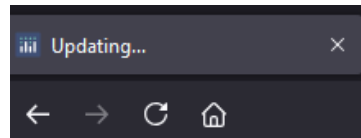


1) spn opx ol spn fsp cpx ru
2) spn fsp cpx ol spn opx
3) fsp opx ol cpx ru
4) fsp liq ol cpx opx spn
5) spn ol liq opx
6) liq spn ol
7) spn opx cpx g ol ru
8) cpx ol g opx ru

- 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"

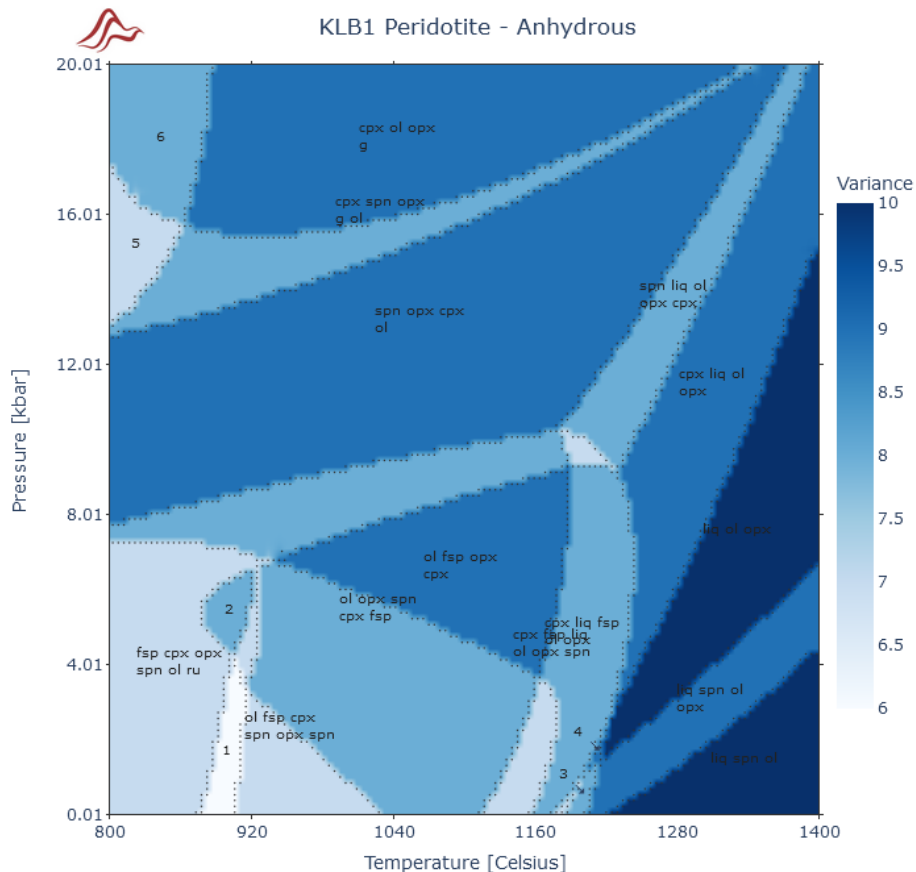


- Note that during any loading/calculation the title of your MAGEMinApp web-browser tab indicates "Updating..."
Wait until the message is gone before new actions!



MAGMinApp: 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

Phase diagram information	
Number of computed points	Minimization time (ms)
5680	109.18
Save point	filename
Save all	filename
Export references	filename
	Table
	csv file
	text
	bibtex file

- 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	Phase	Mode	Oxide	mol
P	8.604	kbar	fsp	0.021	SiO2	0.385
T	982.813	°C	cpx	0.127	Al2O3	0.018
G	-816.909	kJ	ol	0.616	CaO	0.028
p_sys	3245.7	kg/m²	opx	0.225	MgO	0.505
			spn	0.012	FeO	0.059
					K2O	0.0
					Na2O	0.002
					TiO2	0.001
					O	0.001
					Cr2O3	0.001
					H2O	0.0

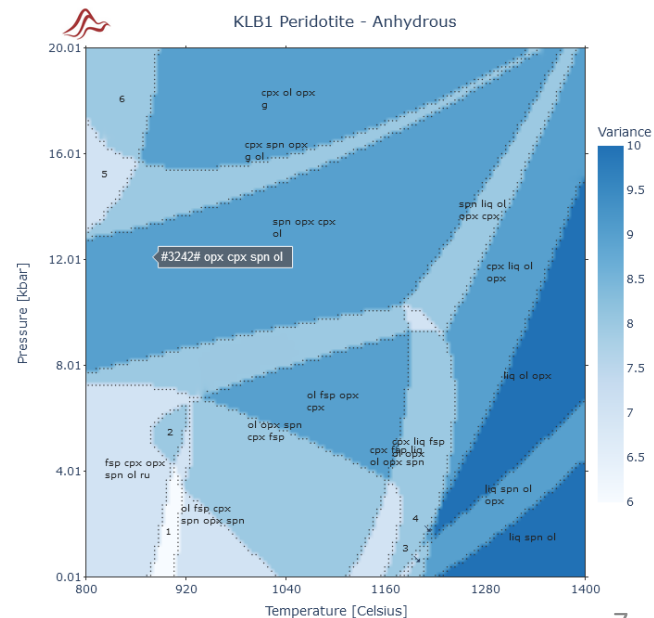
MAGEMinApp: colormap range

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

Display options

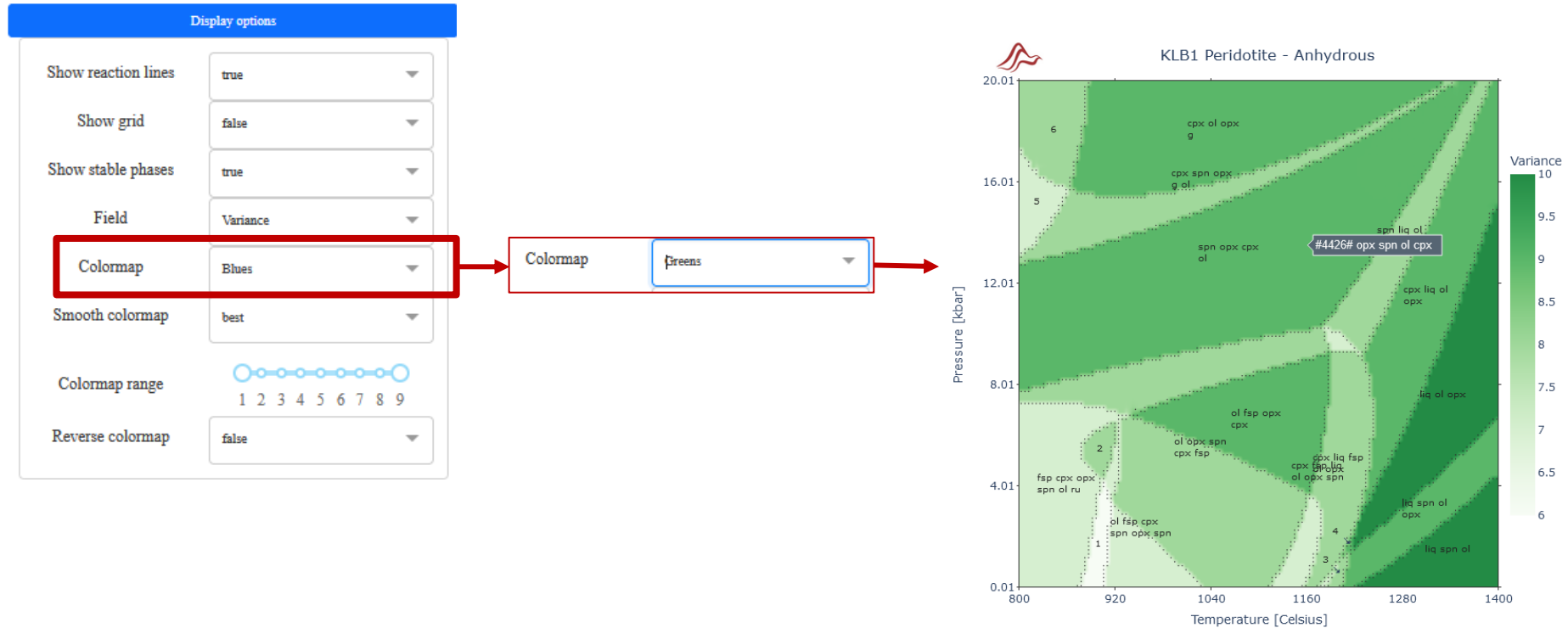
Show reaction lines	true
Show grid	false
Show stable phases	true
Field	Variance
Colormap	Blues
Smooth colormap	best
Colormap range	
Reverse colormap	false

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



MAGEMinApp: colormap

- You can of course change the colormap



MAGEMinApp: grid display

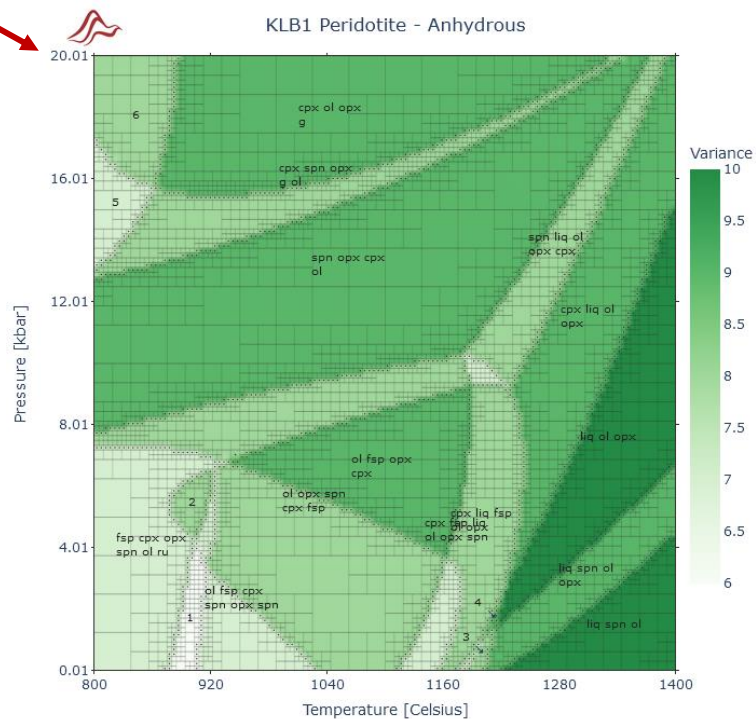
- display the grid...

Display options

Show reaction lines	true
Show grid	false
Show stable phases	true
Field	Variance
Colormap	Blues
Smooth colormap	best
Colormap range	<input type="radio"/> 1 <input type="radio"/> 2 <input type="radio"/> 3 <input type="radio"/> 4 <input type="radio"/> 5 <input type="radio"/> 6 <input type="radio"/> 7 <input type="radio"/> 8 <input type="radio"/> 9
Reverse colormap	false


Show grid

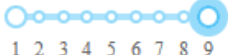
true



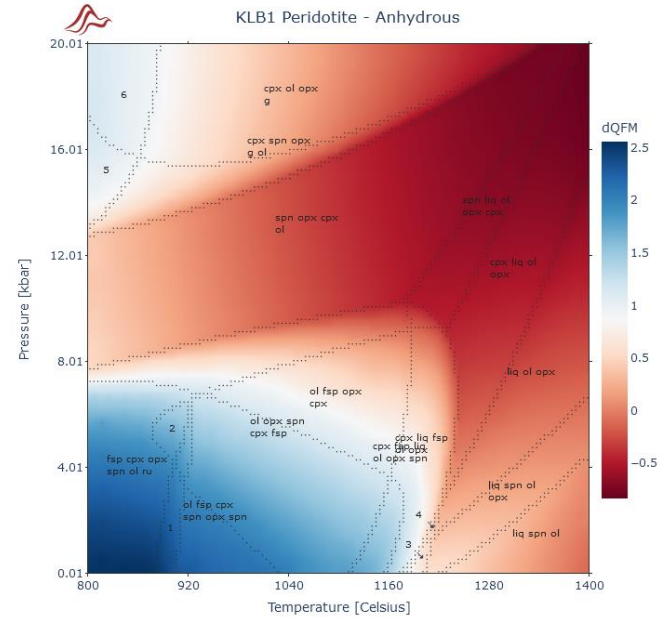
MAGEMinApp: field

- change the field to be displayed

Display options	
Show reaction lines	true
Show grid	false
Show stable phases	true
Field	Variance
Colormap	Blues
Smooth colormap	best
Colormap range	
Reverse colormap	false

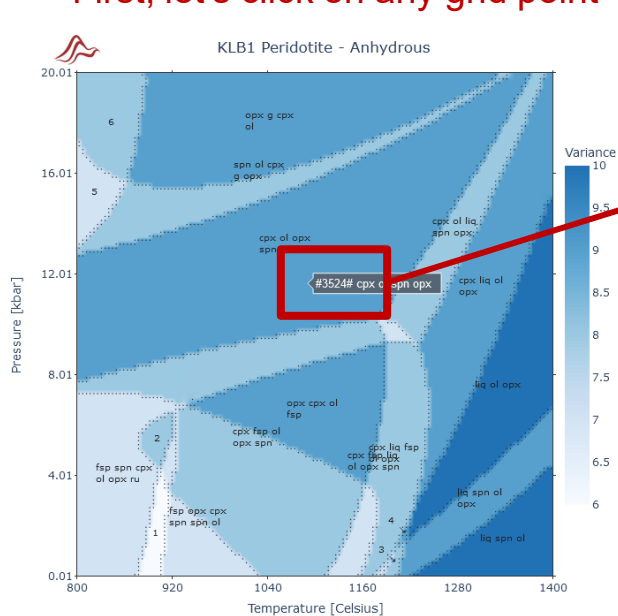
Display options	
Show reaction lines	true
Show grid	false
Show stable phases	true
Field	log10(dQFM)
Colormap	RdBu
Smooth colormap	best
Colormap range	
Reverse colormap	false

- 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



Phase diagram information

Number of computed points: 5683 Minimization time (ms): 113.448

Variable	Value	Unit	Phase	Mode	Oxide	mol
P	11.885	kbar	cpx	0.141	SiO ₂	0.385
T	1081.25	°C	ol	0.63	Al ₂ O ₃	0.018
G	-823.268	kJ	spn	0.011	CaO	0.028
p_sys	3254.7	kg/m ²	opx	0.219	MgO	0.505
					FeO	0.059
					K ₂ O	0.0
					Na ₂ O	0.002
					TiO ₂	0.001
					O	0.001
					Cr ₂ O ₃	0.001
					H ₂ O	0.0

Save point filename Table **text**

Save all filename csv file

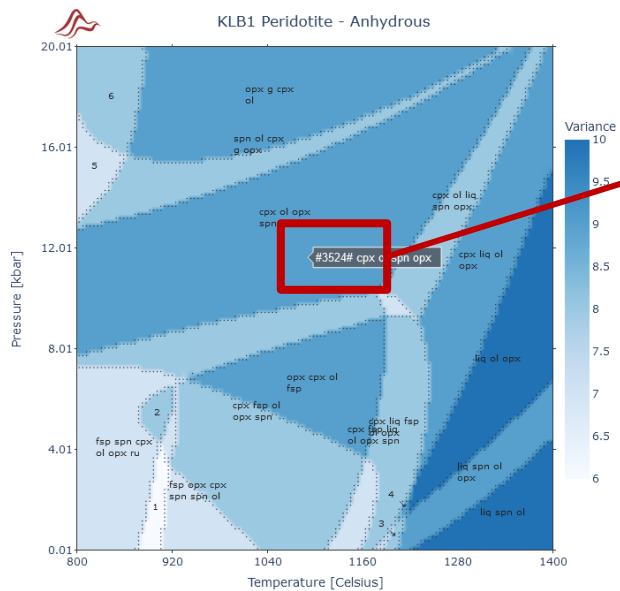
Export references filename bibtext file

- 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

```
1 =====
2 ...cpx...ol...spn...opx...{11.8850;1081.2500}...kbar/°C
3
4 End-members-fractions[wt-fr]:
5 ...di...cfs...cats...crdi...cess...chuf
6 ...0.596337...0.066411...0.012233...0.017320...0.022295...0.032958
7 ...mont...fa...fo...cfm
8 ...0.003522...0.177025...0.819402...0.000051
9 ...nsp...isp...nhc...ihc...nmt...imt
10 ...0.553107...0.231982...0.141464...0.021306...-0.013429...0.02323
11 ...en...fs...fm...odi...mgts...crer
12 ...0.639219...0.053216...0.082200...0.045373...0.118856...0.023216
13
14 Oxide-compositions-[wt-fr]:
15 ...SiO2...Al2O3...CaO...MgO...FeO...
16 ...SYS...0.448600...0.035124...0.030719...0.395275...0.082032
17 ...cpx...0.531572...0.054166...0.175962...0.168373...0.038435
18 ...ol...0.408187...0.000000...0.000952...0.490787...0.100073
19 ...spn...0.000000...0.636768...0.000000...0.230242...0.083187
20 ...opx...0.527534...0.074349...0.012709...0.309750...0.064255
21
22 Stable-mineral-assemblage:
23 ...phase...fraction[wt]...G[kJ]...V_molar[cm3/mol]...
24 ...cpx...+0.14461...-3457.26908...+66.64026...
25 ...ol...+0.62836...-2339.30393...+45.23134...
26 ...spn...+0.01071...-2446.84718...+41.03734...
27 ...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



Phase diagram information

Number of computed points: 5683 Minimization time (ms): 113.448

Variable	Value	Unit	Phase	Mode	Oxide	mol
P	11.885	kbar	cpx	0.141	SiO ₂	0.385
T	1081.25	°C	ol	0.63	Al ₂ O ₃	0.018
G	-823.268	kJ	spn	0.011	CaO	0.028
p_sys	3254.7	kg/m ²	opx	0.219	MgO	0.505
					FeO	0.059
					K ₂ O	0.0
					Na ₂ O	0.002
					TiO ₂	0.001
					O	0.001
					Cr ₂ O ₃	0.01
					H ₂ O	0.0

Save point filename Table text

Save all filename csv file

Export references filename bibtex file

- 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!

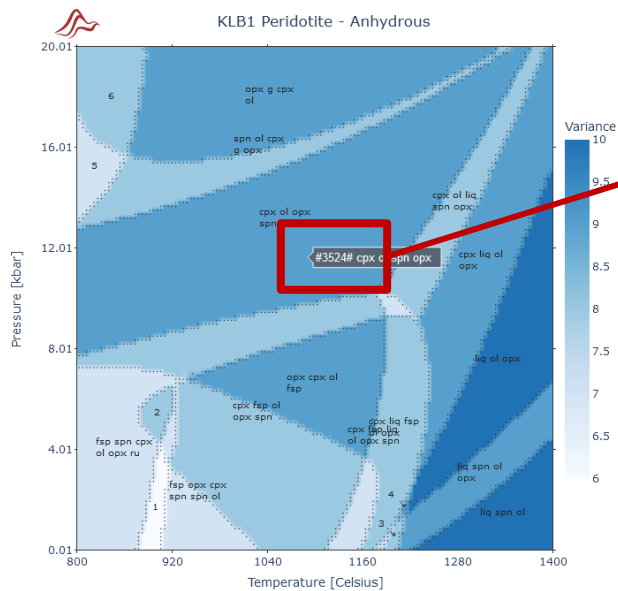
```
output path: /home/seph42/MAGEMinApp.jl_v04.0
Saving data to csv... 100%
```

- 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(fO ₂)	log10(dQ/aH ₂ O)		a
2	1	1	1	0.635	818.75 system	100	100	-11.6936	2.559878	0	(
3	1	1	1	0.635	818.75 fsp	6.959184	6.970663	-	-	-	-
4	1	1	1	0.635	818.75 spn	0.174666	0.248471	-	-	-	-
5	1	1	1	0.635	818.75 cpx	6.119897	6.341448	-	-	-	-
6	1	1	1	0.635	818.75 ol	69.78836	69.61555	-	-	-	-
7	1	1	1	0.635	818.75 opx	16.87659	16.72111	-	-	-	-
8	1	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



Phase diagram information

Number of computed points: 5683 Minimization time (ms): 113.448

Variable	Value	Unit	Phase	Mode	Oxide	mol
P	11.885	kbar	cpx	0.141	SiO ₂	0.385
T	1081.25	°C	ol	0.63	Al ₂ O ₃	0.018
G	-823.268	kJ	spn	0.011	CaO	0.028
p_sys	3254.7	kg/m ³	opx	0.219	MgO	0.505
					FeO	0.059
					K ₂ O	0.0
					Na ₂ O	0.002
					TiO ₂	0.001
					O	0.001
					Cr ₂ O ₃	0.001
					H ₂ O	0.0

Save point filename Table test

Save all filename csv file

Export references filename bibtex file

You can also save the references used to perform the calculation clicking on “bibtex file”!

```
1 @article{holland2018melting,
2   pages = {881--900},
3   info = {doi = {10.1016/j.jpet.2018.08.001}},
4   author = {Holland, Tim JB and Green, Eleanor CR and Powell, Roger},
5   journal = {Journal of Petrology},
6   title = {Melting of peridotites through to granites: a simple thermodynamic model in the system KNCFMASH+H2O},
7   publisher = {Oxford University Press},
8   number = {5},
9   doi = {10.1093/petrology/egy048},
10  year = {2018},
11  volume = {59}
12 }
13
14 @article{riel2022magemin,
15   pages = {e2022gc010427},
16   info = {doi = {10.1029/2022gc010427}},
17   author = {Riel, Nicolas and Kaus, Boris JP and Green, ECR and Berlie, Nicolas},
18   journal = {Geochemistry, Geophysics, Geosystems},
19   title = {MAGEMin, an efficient Gibbs energy minimizer: application to igneous systems},
20   publisher = {Wiley Online Library},
21   number = {7},
22   doi = {https://doi.org/10.1029/2022gc010427},
23   year = {2022},
24   volume = {23}
25 }
```

MAGEMinApp: fields isocontours and isopleths

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

1

Phase diagram information

Display isopleths

2

Selection

Isopleth type: Pure phase

Phase: q

Range

Min: 0

Step: 0,1

Max: 1

Plotting options

Color: [Black color swatch]

Label size: 10

Isopleth list

Add

Remove

Remove all

Hide all

Show all

Select...

Pure phase

Pure phase

Solution phase

Other

- 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

MAGMinApp: fields isocontours and isopleths

- Let's contour melt fraction

Display isopleths

Selection

Isopleth type
Solution phase

Phase
liq

Endmember
none

Range

Min
0

Step
0,1

Max
1

Plotting options

Color

Label size
10

Isopleth list

Add

Remove

Remove all

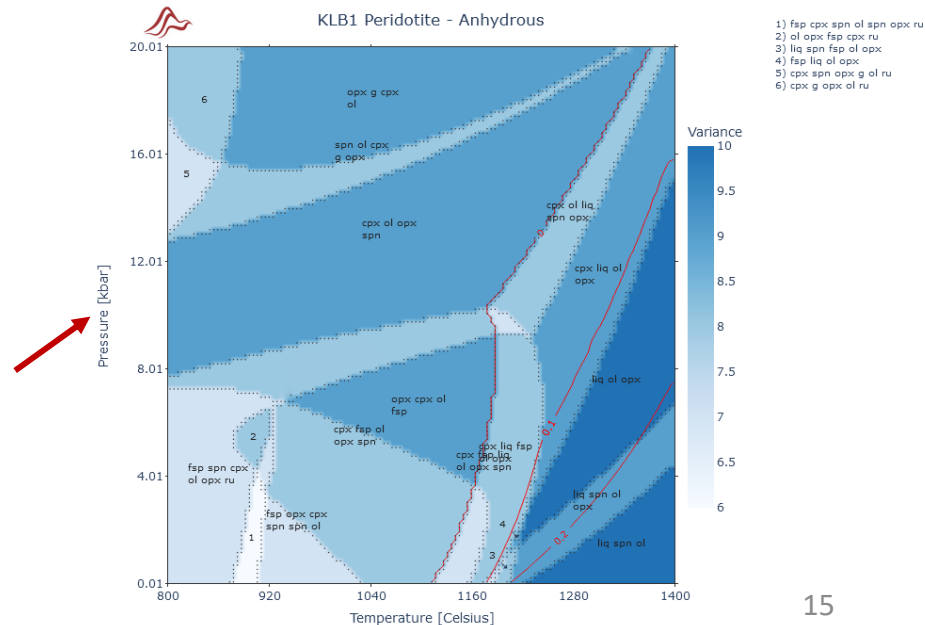
Hide all

Show all

Select...

- 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

Display isopleths

Selection

Isopleth type: Other

Field: ρ_{solid}


Range

Min: 3100

Step: 40

Max: 3300

Plotting options

Color: 

Label size: 10

Isopleth list

Add

Remove

Remove all

Hide all

Show all

Select...

- Select:
Isopleth type = "Other"
Phase = "rho_solid"

- Change the color to what you like then click add

Isopleth list

Add

Remove

Remove all

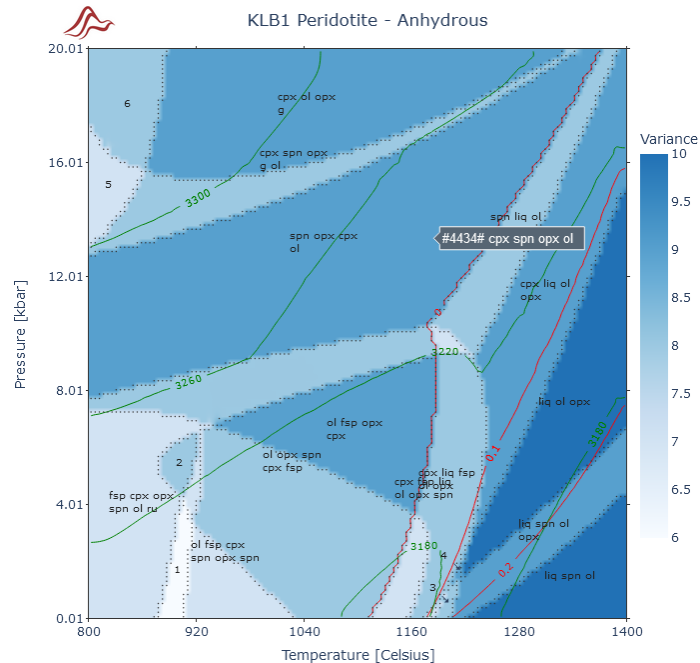
Hide all

Show all

liq_mode

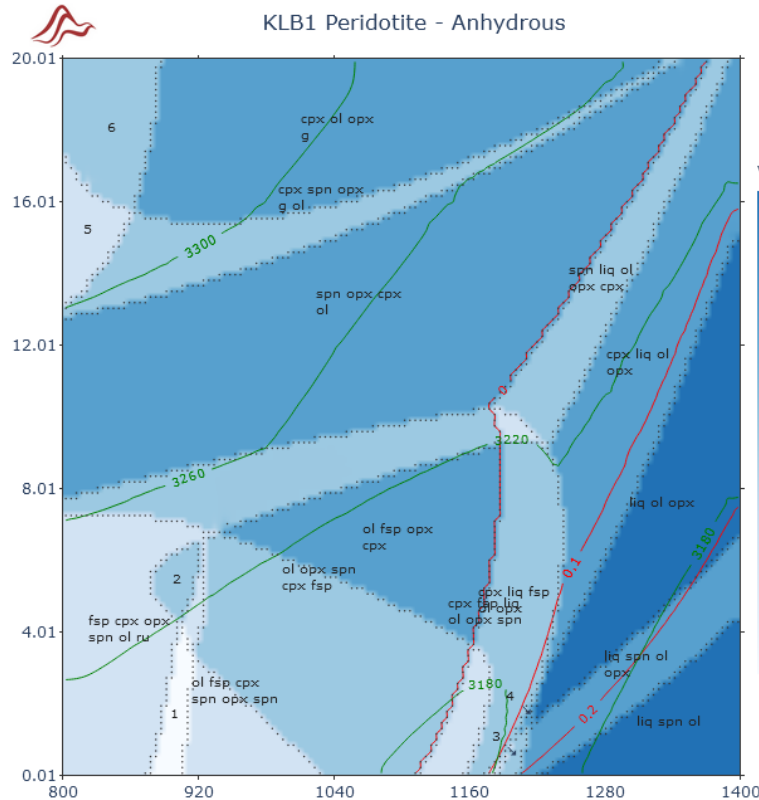
liq_mode

rho_S

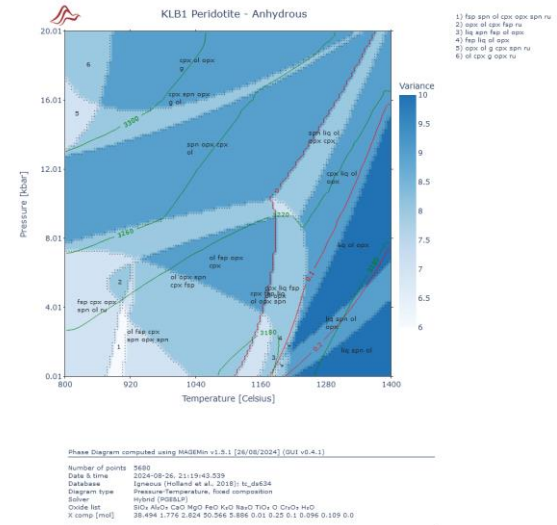


- The isopleth list allow you to remove select isocontour

MAGMinApp: save figure(s)



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



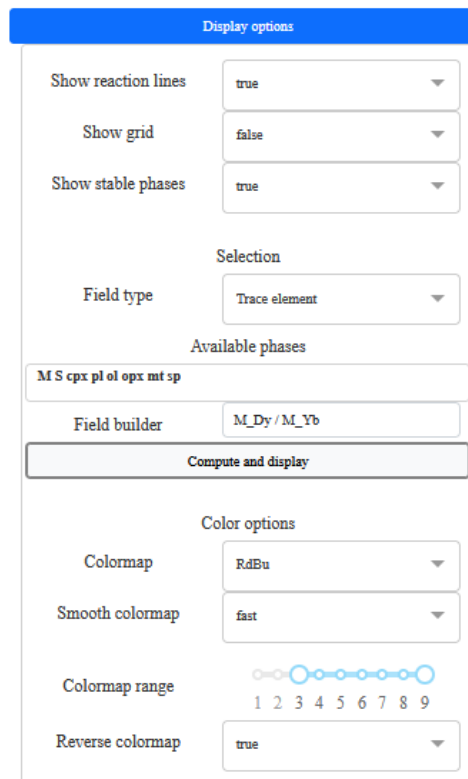
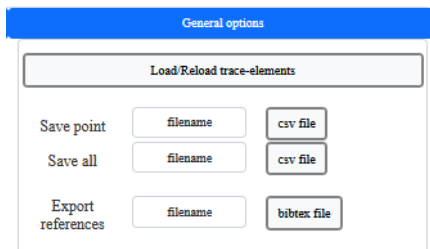
- All plots and figures in the app can be saves in the same way

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

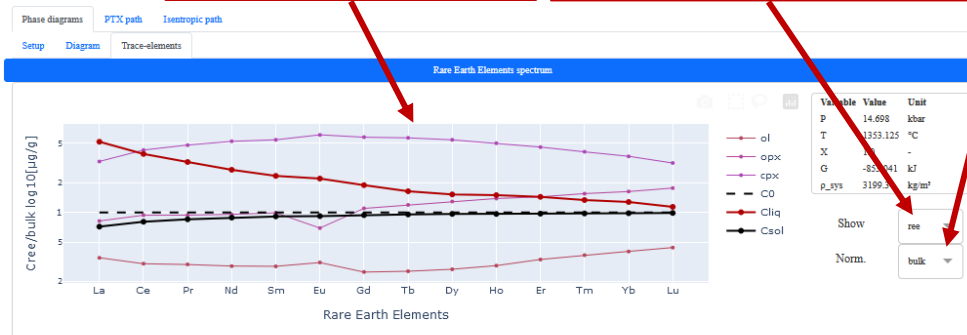
MAGEMinApp: trace elements

- Which yields:

This plot displays TE spectrum

Here you can choose to display REE or all TE

Here you can change the normalization



General options

Load/Reload trace-elements

Save point:

Save all:

Export references:

Here you can save point/all information

Display options

Show reaction lines: ☒

Show grid: ☐

Show stable phases: ☒

Selection:

Field type:

Available phases:

Field builder:

Compute and display

Color options

Colormap:

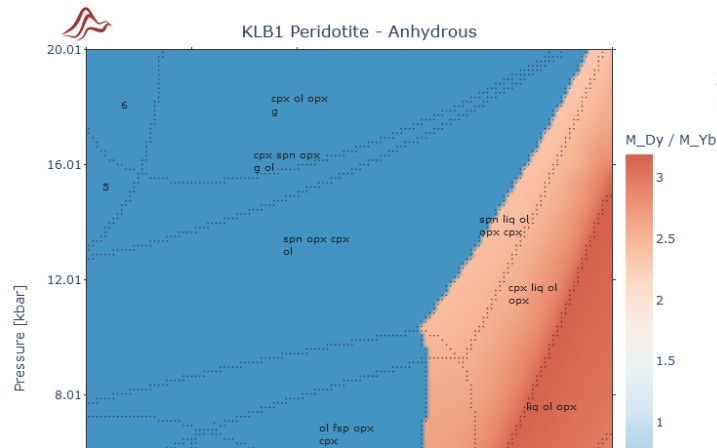
Smooth colormap:

Colormap range:

Reverse colormap: ☒

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



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

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”

Phase diagram parameters

Thermodynamic database

Metabasite (Green et al., 2016)

Solution phase selection

Diagram type

P-T diagram

H2O-saturated at solidus

true

clinopyroxene

Omphacite

☒

Augite

TE predictive model

false

Pressure [kbar]

min

1

max

16

Temperature [°C]

min

500

max

1200

Initial grid subdivision

3

Refinement type

Phases only

Refinement levels

4

Buffer

no buffer

Solver

Hybrid

Verbose

none

Specific Cp

G0

Bulk-rock composition

Drag and drop or select bulk-rock file

Simon

oxide	mol_fraction
SiO2	61.5415
Al2O3	8.5342
CaO	9.2213
MgO	5.0289
FeO	7.2396
K2O	0.2091
Na2O	3.4157
TiO2	1.2448
O	0.7269
H2O	50

Metabasite (Green et al., 2016)

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

- Change the water content to 50 to oversaturate

MAGEMinApp: diagram with saturated water at solidus

Phase diagram parameters

Thermodynamic database: Metabasite (Green et al., 2016)

Solution phase selection: ☐

Diagram type: P-T diagram

H2O-saturated at solidus: true

clinopyroxene: Omphacite ☒ Augite

TE predictive model: false

Pressure [kbar]: min 1 max 16

Temperature [°C]: min 500 max 1200

Initial grid subdivision: 3

Refinement type: Phases only

Refinement levels: 3

Buffer: no buffer

Solver: Hybrid

Verbose: none

Specific Cp: G0

- 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...

General parameters

Title: Simon

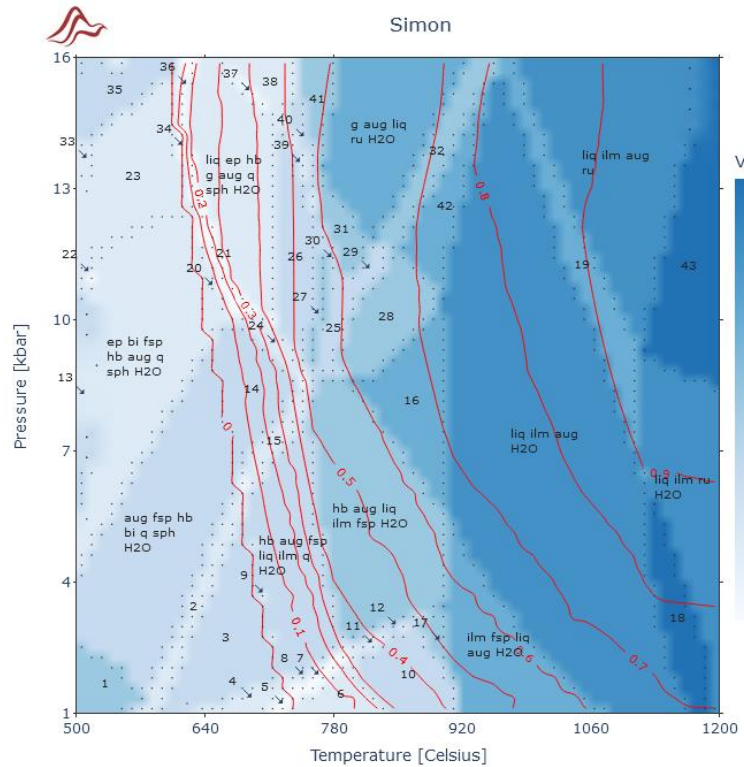
Update Reset

filename Save state Load state

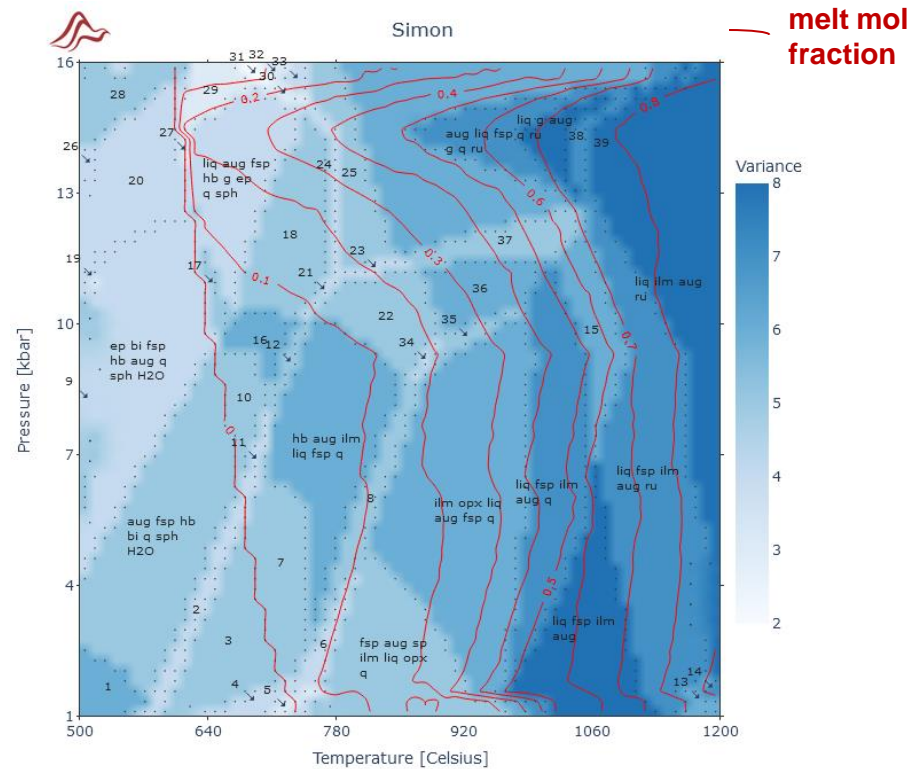
Compute phase diagram

State-CSV directory: /home/sepb42/MAGEMinApp_jl_v0.4.1

MAGEMinApp: diagram with saturated water at solidus



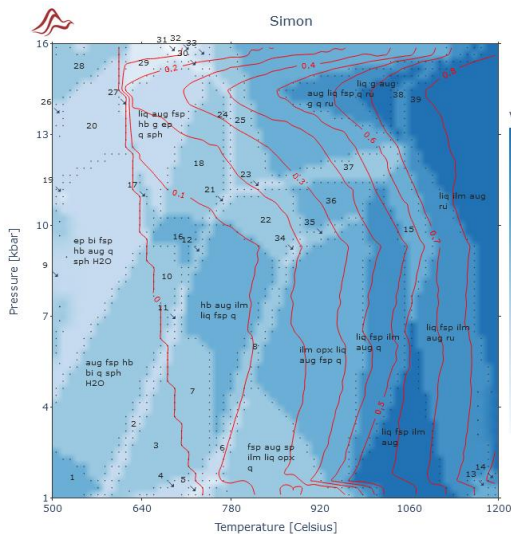
“H2O-saturated at solidus” = false



“H2O-saturated at solidus” = true

MAGEMinApp: diagram with saturated water at solidus

- You can check the water-saturation at solidus by plotting system H₂O-activity (a_{H_2O})

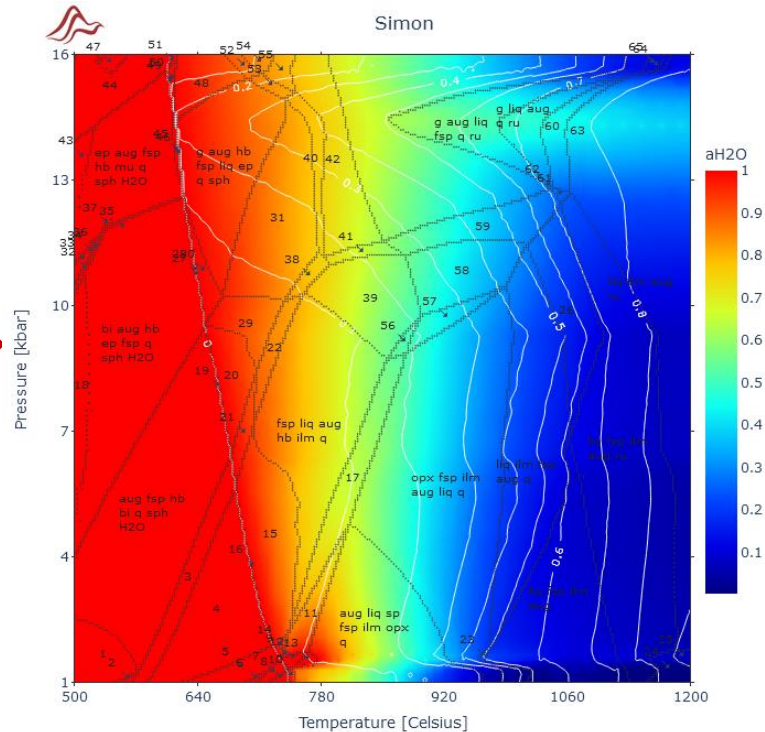


melt mol
fraction

Display options

Show reaction lines	<input checked="" type="checkbox"/>
Show grid	<input type="checkbox"/>
Show stable phases	<input checked="" type="checkbox"/>
Field	H ₂ O activity
Colormap	jet
Smooth colormap	best
Colormap range	<input type="checkbox"/> 1 <input type="checkbox"/> 2 <input type="checkbox"/> 3 <input type="checkbox"/> 4 <input type="checkbox"/> 5 <input type="checkbox"/> 6 <input type="checkbox"/> 7 <input type="checkbox"/> 8 <input type="checkbox"/> 9 <input type="checkbox"/>
Reverse colormap	<input type="checkbox"/>

"H₂O-saturated at solidus" = true



"H₂O-saturated at solidus" = true
+ few more refinement levels

MAGEMinApp: deactivating a solution phase model

Phase diagram parameters

Thermodynamic database: Metabasite (Green et al., 2016)

Solution phase selection: ☐

- ☒ sp
- ☒ opx
- ☒ fsp
- ☒ liq
- ☒ mu
- ☐ ilm
- ☒ ol
- ☒ hb
- ☒ ep
- ☒ g
- ☒ chl
- ☒ bi
- ☒ dio
- ☒ abc
- ☒ spn

Diagram type: P-T diagram

H₂O-saturated at solidus: true

clinopyroxene: Omphacite ☒ Augite

TE predictive model: false

Pressure [kbar]: min 1 max 16

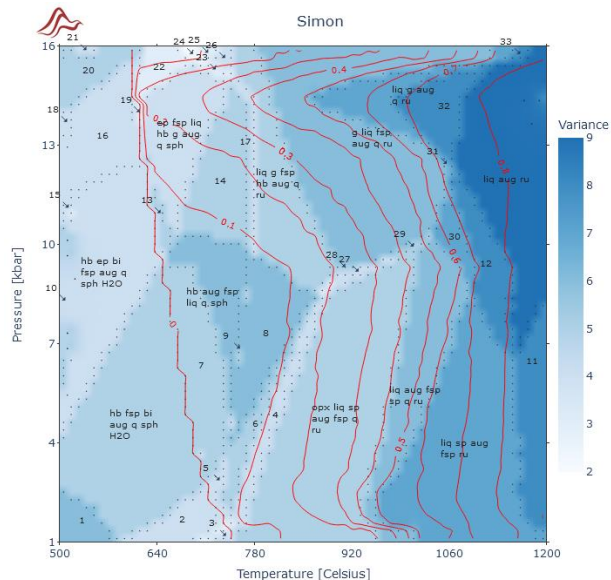
Temperature [°C]: min 500 max 1200

Initial grid subdivision: 3

Refinement type: Phases only

Refinement levels: 3

- 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

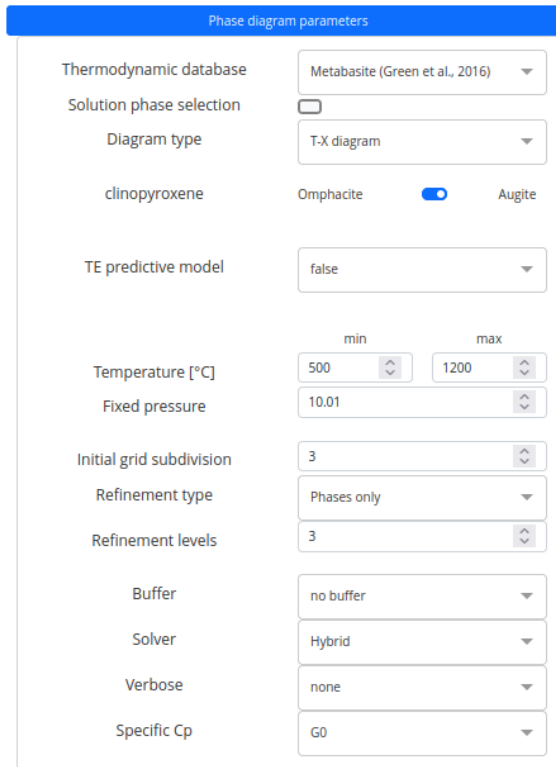
```
# HEADER
title; comments; db; sysUnit; oxide; frac; frac2
# BULK-ROCK COMPOSITION
Test 2;Moo et al., 2000;ig;mol:[SiO2, Al2O3, CaO, MgO, FeO, K2O, Na2O, TiO2, O, Cr2O3, H2O];
[48.97, 11.76, 13.87, 4.21, 8.97, 1.66, 10.66, 1.36, 1.66, 0.01, 5.0];
K167;Moo et al., 2000;ig;mol:[SiO2, Al2O3, CaO, MgO, 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

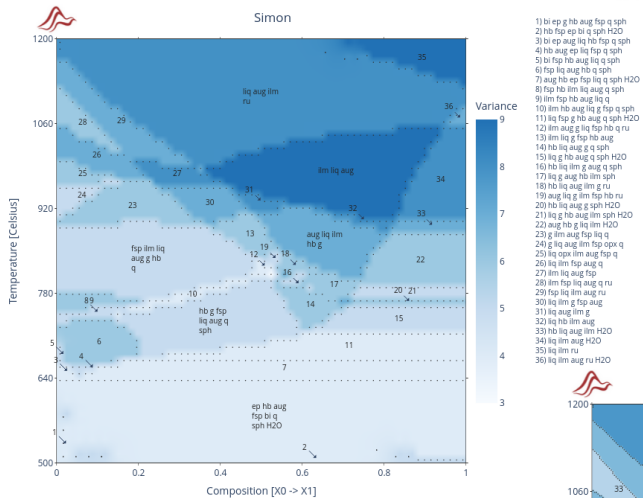
Bulk-rock composition			
Drag and drop or select bulk-rock file			
Simon		Simon	
oxide	mol_fraction	oxide	mol_fraction
SiO2	61.5415	SiO2	41.8784
Al2O3	8.5342	Al2O3	5.8074
CaO	9.2213	CaO	6.275
MgO	5.0289	MgO	3.4221
FeO	7.2396	FeO	4.9265
K2O	0.2091	K2O	0.1423
Na2O	3.4157	Na2O	2.3243
TiO2	1.2448	TiO2	0.8471
O	0.7269	O	0.4947
H2O	2.8381	H2O	33.8822
Metabasite (Green et al., 2016)			

MAGEMinApp: T-X phase diagrams

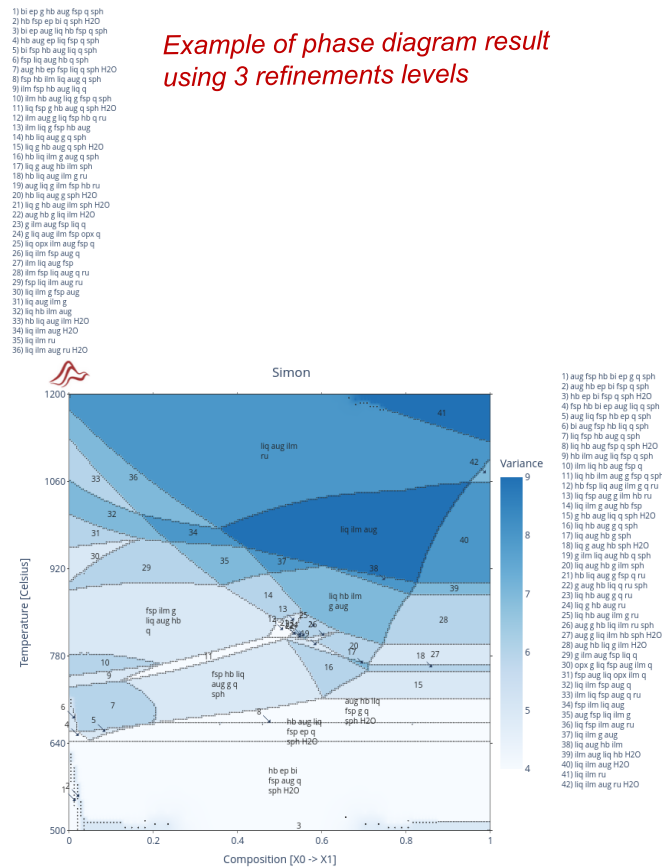
- Change the Phase-Diagram setup according to what you want
- Then compute the phase diagram



Set of parameters example



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

Phase diagram parameters

Thermodynamic database: Metabasis (Green et al., 2016)

Solution phase selection: ☐

Diagram type: T-X diagram

clinopyroxene: Omphacite ☒ Augite

TE predictive model: false

Temperature [°C]: min 500 max 1200
Fixed pressure: 10.01

Initial grid subdivision: 3

Refinement type: Phases only

Refinement levels: 3

Buffer: no buffer

Solver: Hybrid

Verbose: none

Specific Cp: G0

Set of parameters example

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

Bulk-rock composition

Drag and drop or select bulk-rock file

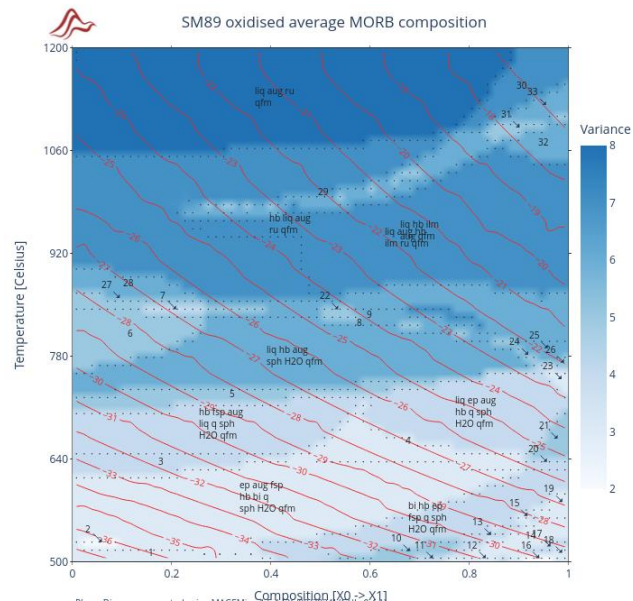
SM89 oxidised average MORB comp: SM89 oxidised average MORB comp:

oxide	mol_fraction	oxide	mol_fraction
SiO2	52.47	SiO2	52.47
Al2O3	9.1	Al2O3	9.1
CaO	12.21	CaO	12.21
MgO	12.71	MgO	12.71
FeO	8.15	FeO	8.15
K2O	0.23	K2O	0.23
Na2O	2.61	Na2O	2.61
TiO2	1.05	TiO2	1.05
O	4	O	4
H2O	20	H2O	20

Buffer multiplier: -4 Buffer multiplier: 4

Metabasis (Green et al., 2016)

- Compute and contour the field $\log_{10}(fO_2)$ (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 varying 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

Bulk-rock composition

Drag and drop or select bulk-rock file

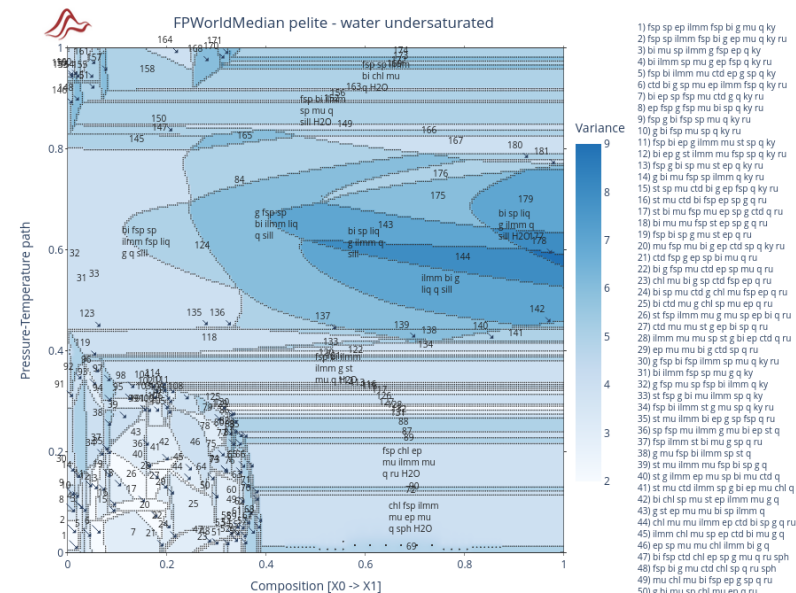
FPWorldMedian pelite - water underw

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

FPWorldMedian pelite - water oversw

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