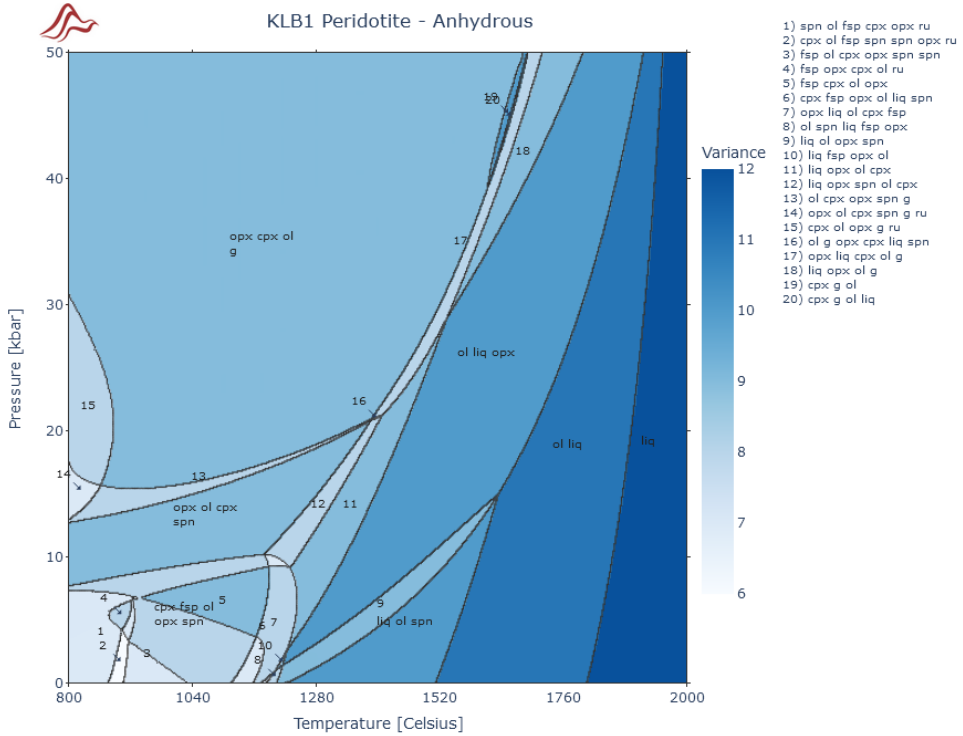
MAGEMinApp: introduction

Granulites & Granulites 2024

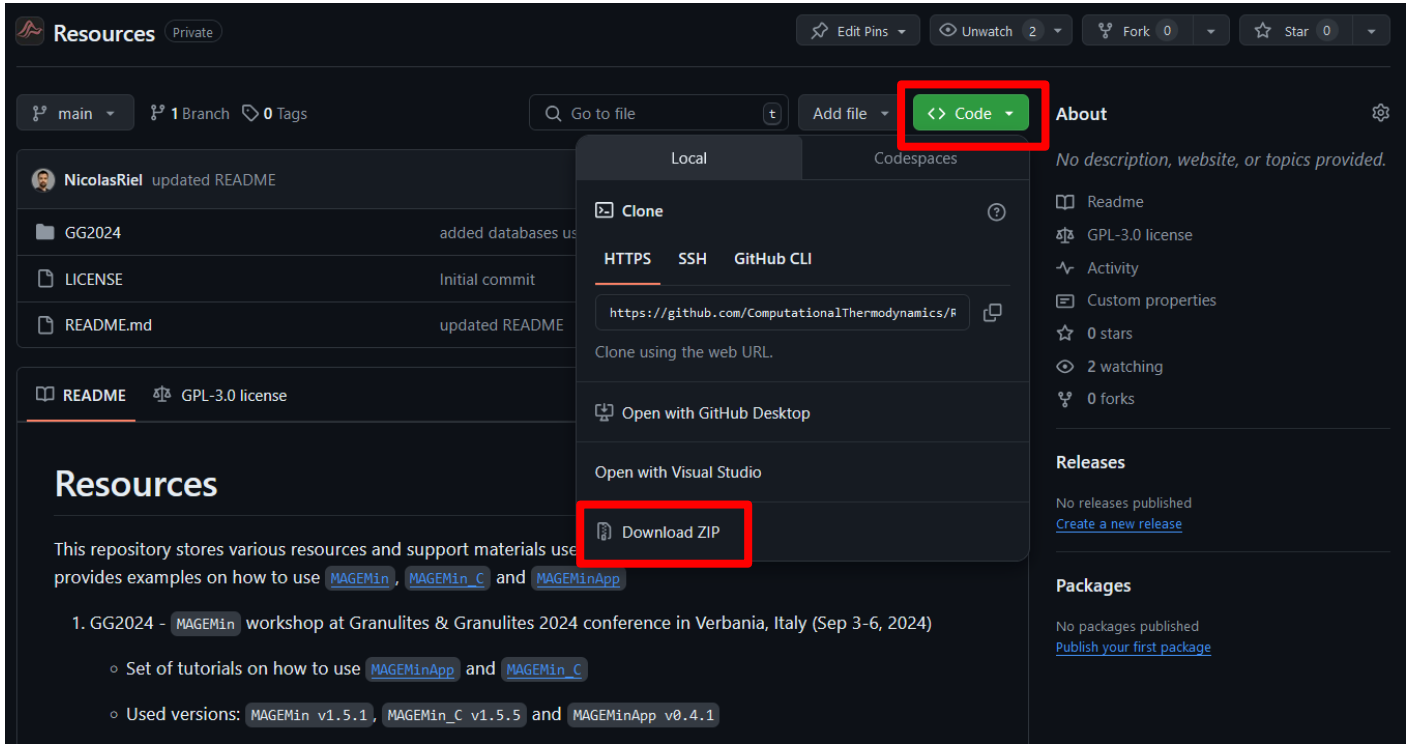
MAGEMin



MAGEMin github: ComputationalThermodynamics

- **First, download the resources for the shortcourse from Github:**

https://github.com/ComputationalThermodynamics/Resources

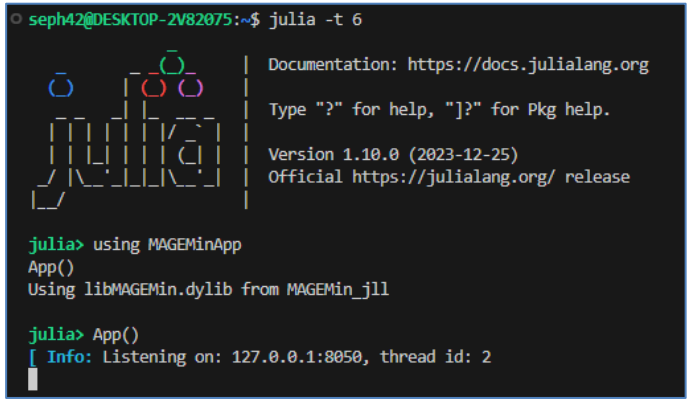


- **The GG2024 folder includes:**

- Bulk rock input file example
- Trace element input file
- Reference database used in MAGEMinApp
- The pdfs used in the short course
- MAGEMin_C Julia scripts used during the course

MAGEMinApp: launching the App in parallel

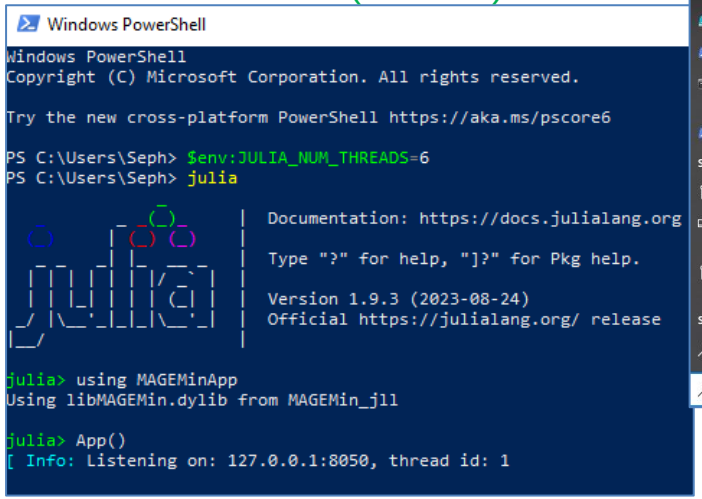
VISUAL STUDIO CODE
MAC, LINUX AND WINDOWS(USING WSL)

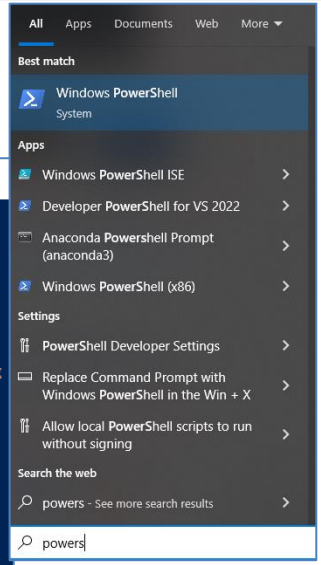



```
julia –t 6
using MAGEMinApp
App()
```

Favored way (better performances on Mac and Linux)

POWERSHELL
WINDOWS(NO WSL)

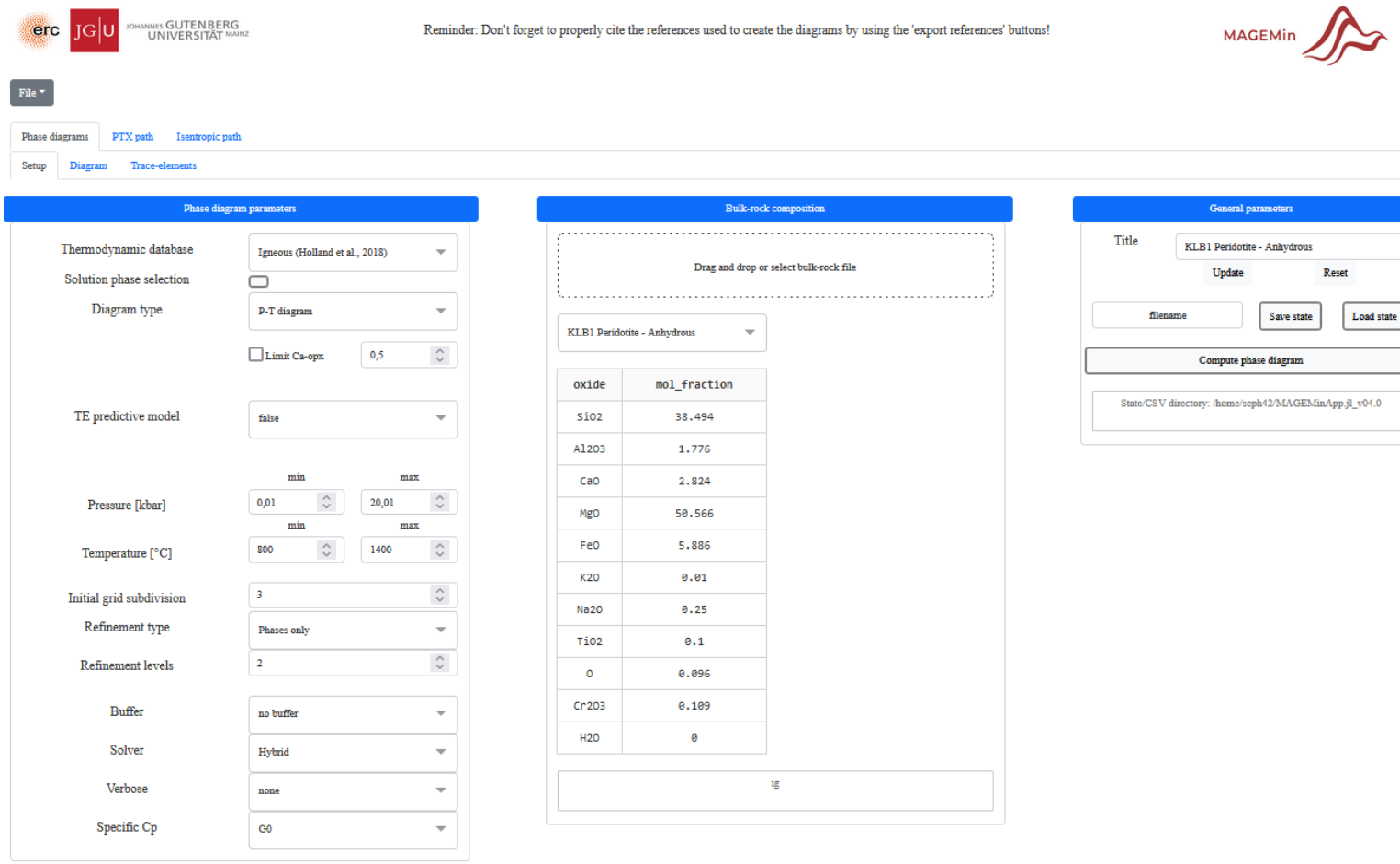




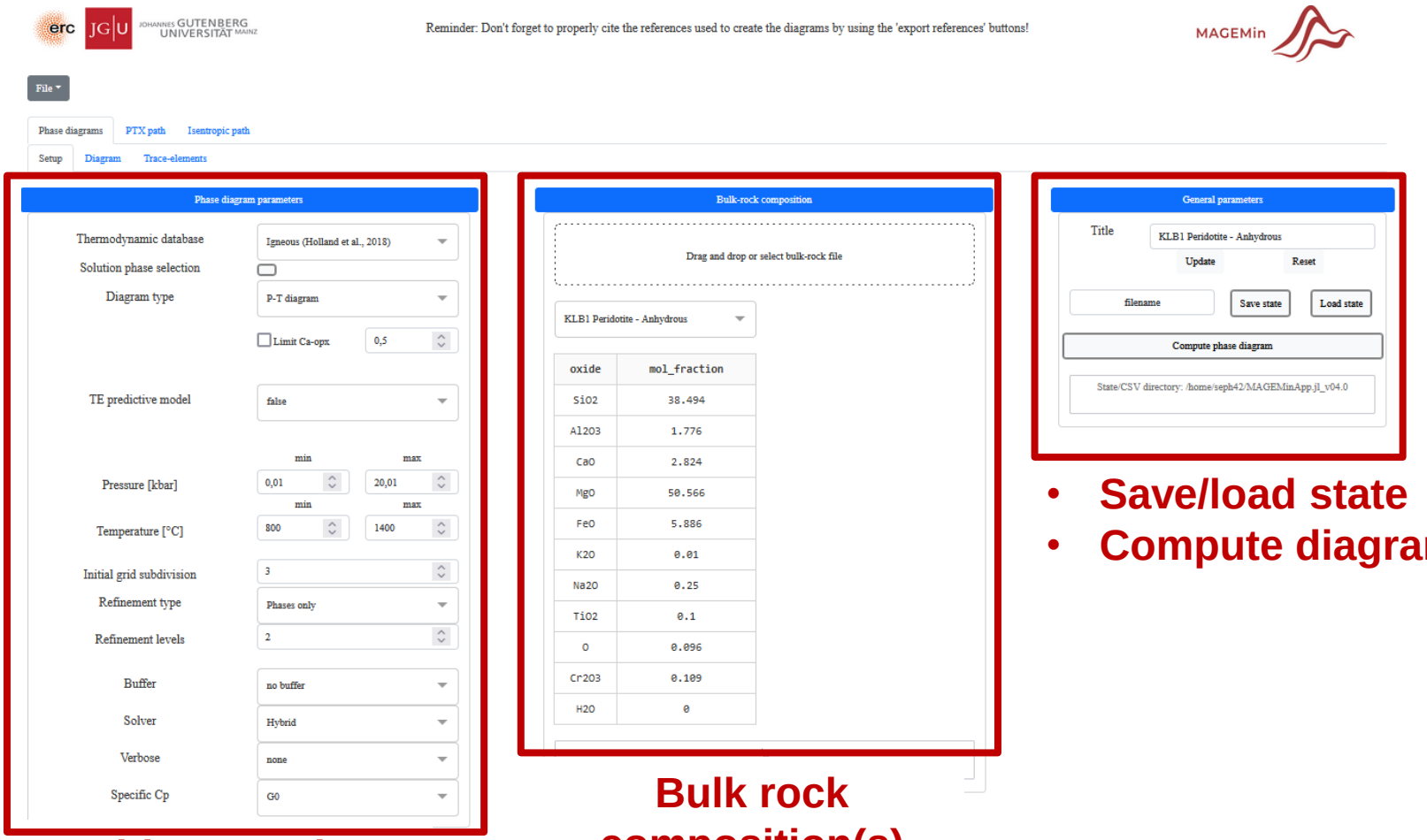

```
$env:JULIA_NUM_THREADS=6
julia
using MAGEMinApp
App()
```

Around 2.5 times slower than using WSL

MAGEMinApp: interface (Phase diagrams)



MAGEMinApp: interface (Phase diagrams)

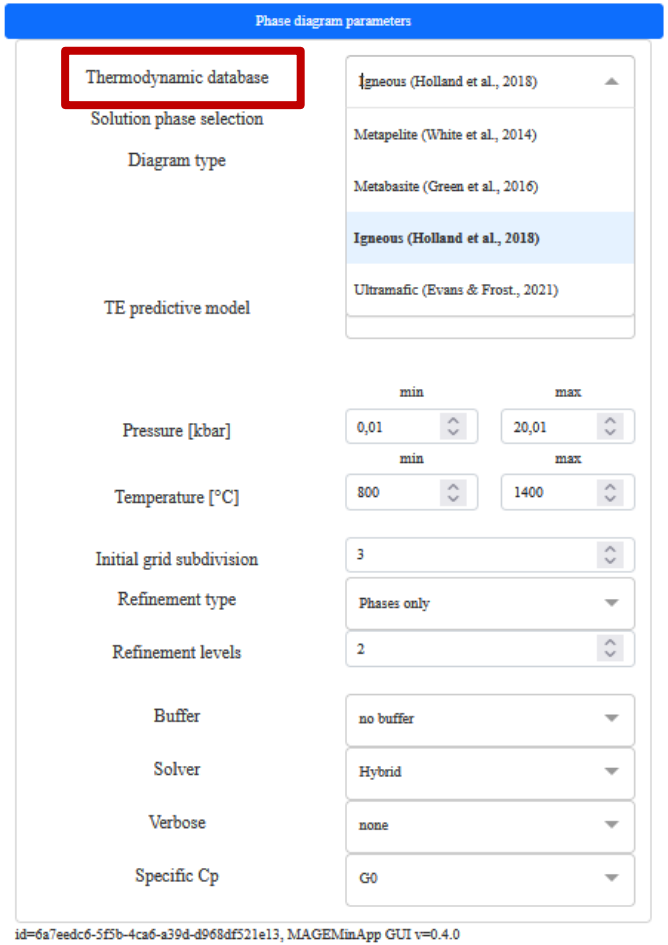


- **Save/load state**
- **Compute diagram**

Grid properties

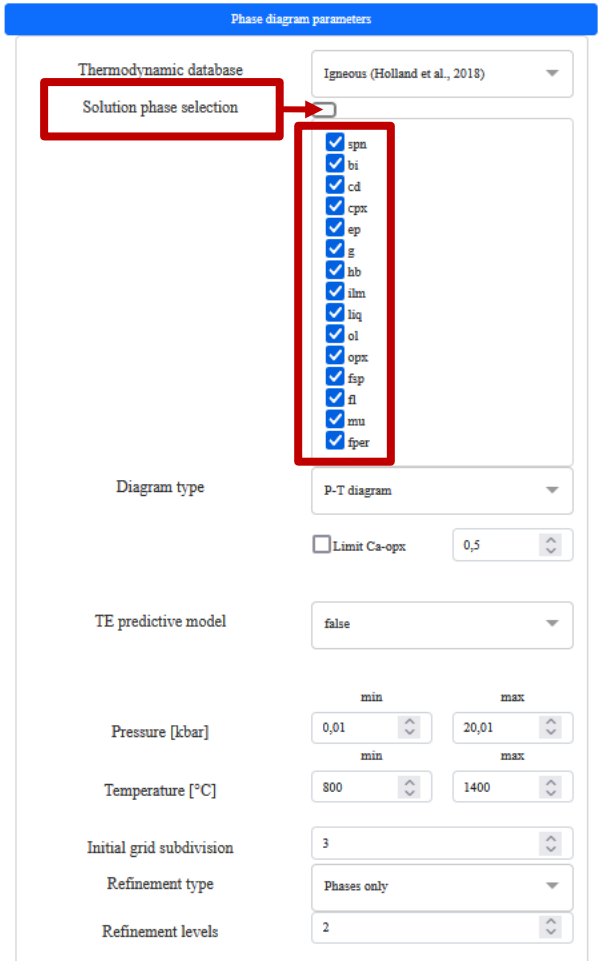
Bulk rock composition(s)

MAGEMinApp: Thermodynamic database



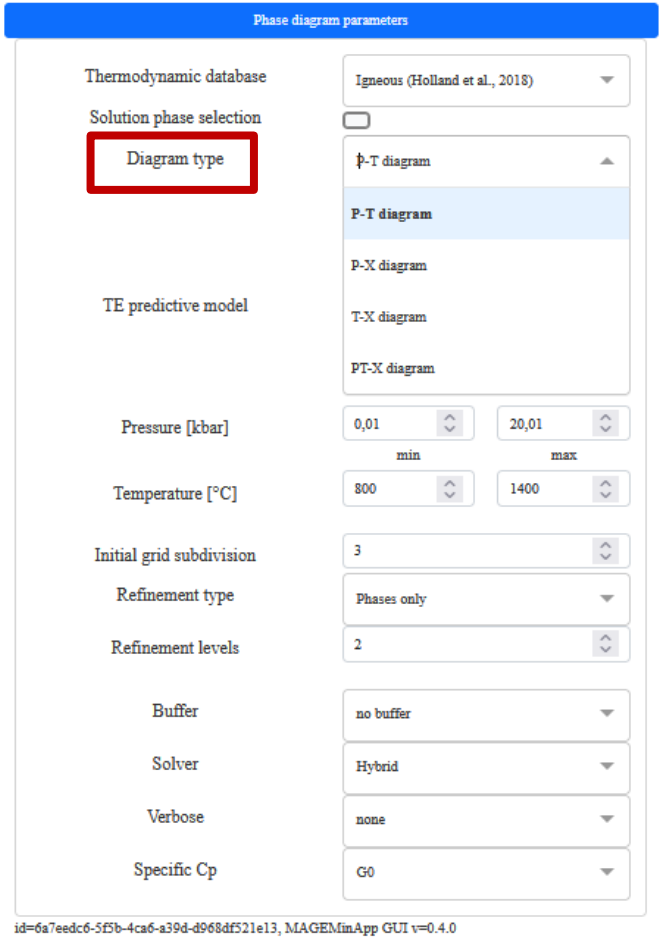
- **Metapelite (White et al., 2024)**
  MnNCKFMASHTO
- **Metabasite (Green et al., 2016)**
  NCKFMASHTO
- **Igneous (Holland et al., 2018)**
  NCKFMASHTOCr
- **Ultramafic (Evans & Frost, 2021)**
  FMASOSH
- **Dry igneous alkaline (Weller et al., in review)**
  NCKFMASHTOCr (upcoming)
- **Mantle (Stixrude and Lithgow-Bertelloni, 2011)**
  NCFMAS (upcoming)

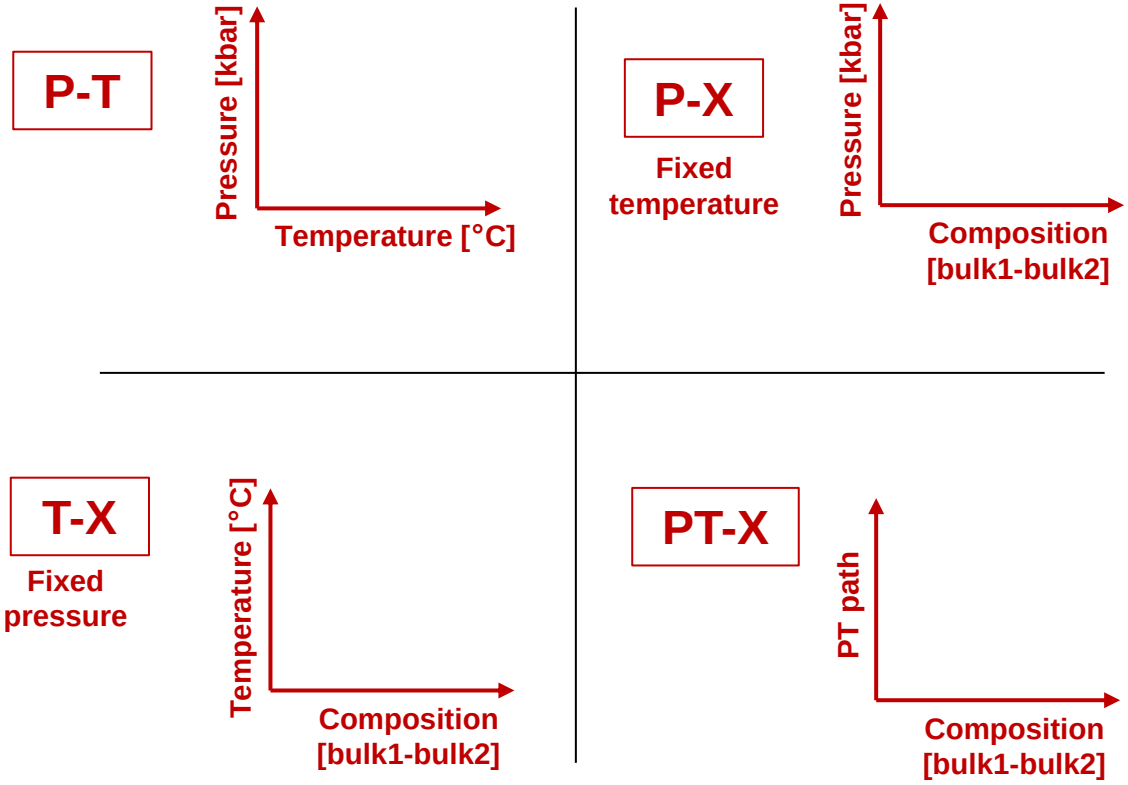
MAGEMinApp: solution phase selection



- **Allow to deactivate solution phase models**
- **Note that solution phase models from different dataset cannot be mixed (yet)**

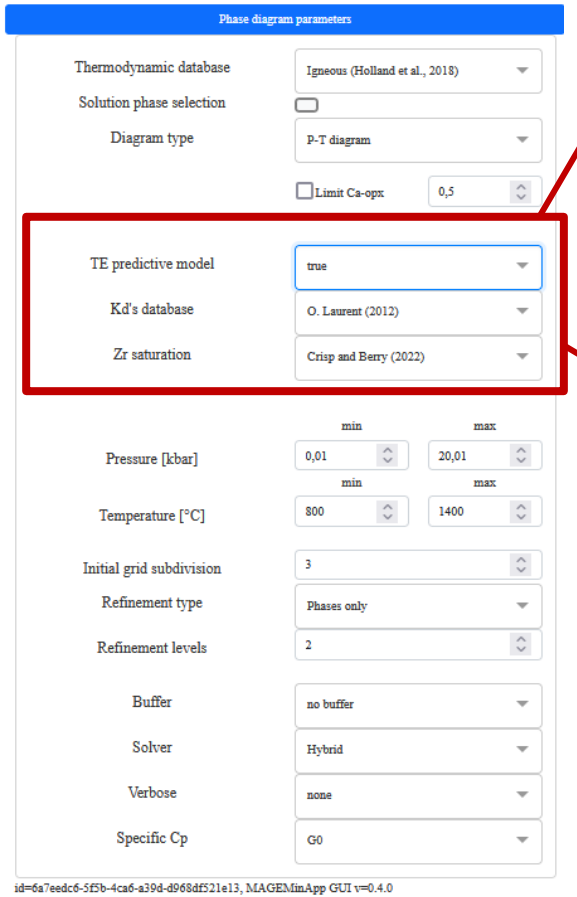
MAGEMinApp: diagram types



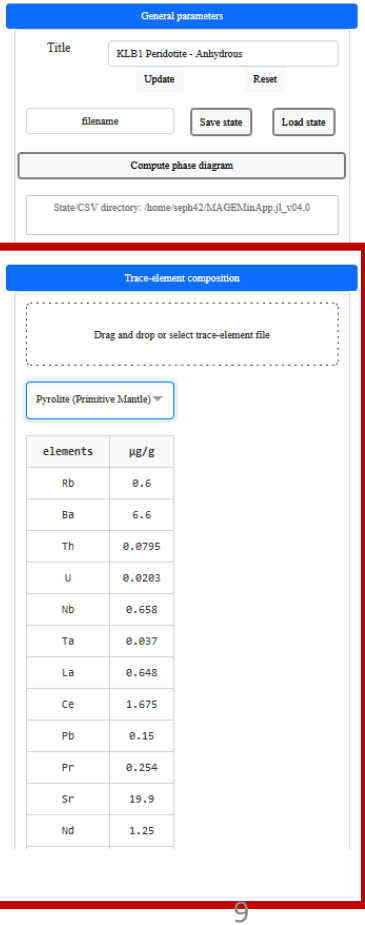


MAGEMinApp: Trace element predictive model

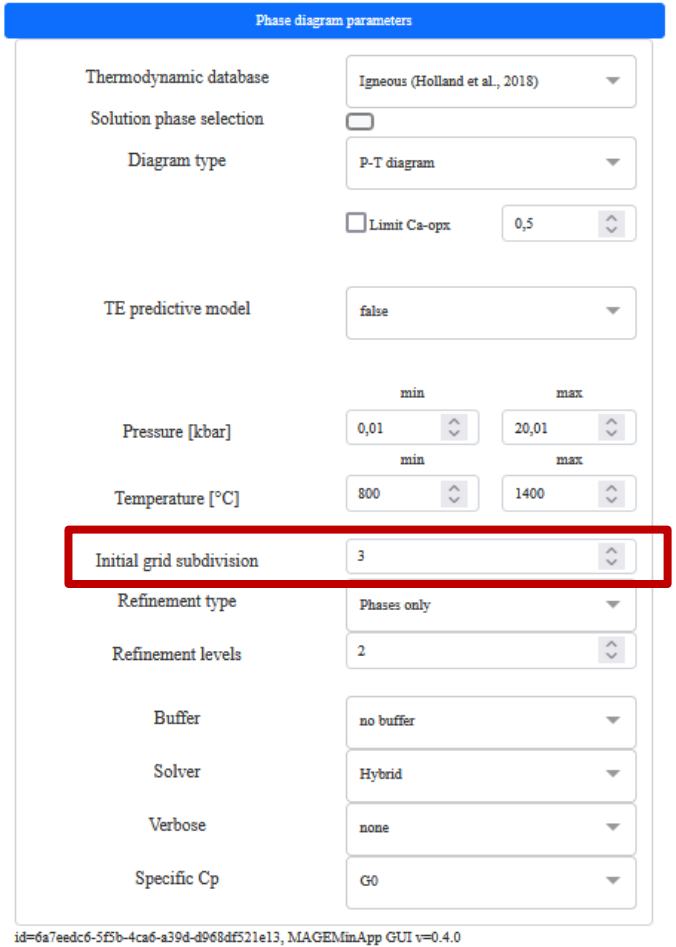
Implemented with the help of J-F Moyen (LMV) and H. Dominguez (Uni - Bern)



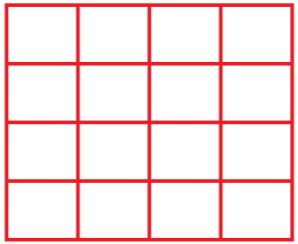
- **Activate trace-element partitioning at supra-solidus conditions**
- **Displays trace element bulk panel on the right**
- **Gives the option to select among 3 zirconium saturation models**



MAGEMinApp: grid subdivision and refinement



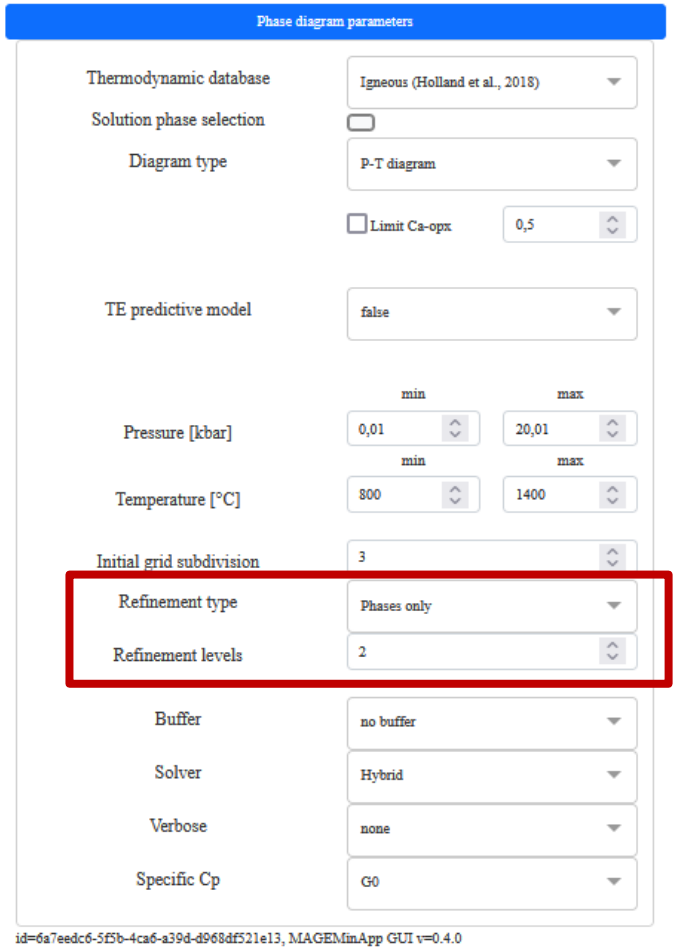
1 initial grid subdivision



2 initial grid subdivisions

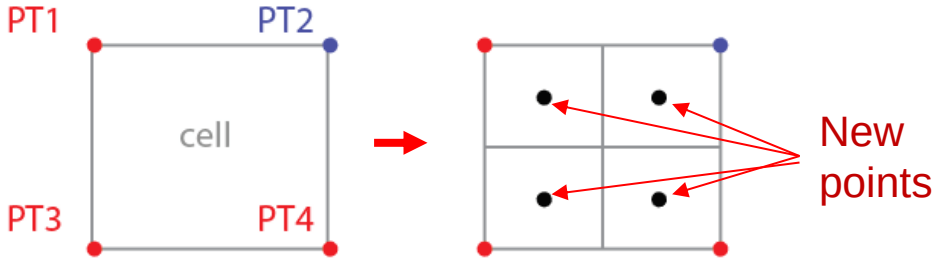
3 initial grid subdivisions

MAGEMinApp: grid subdivision and refinement



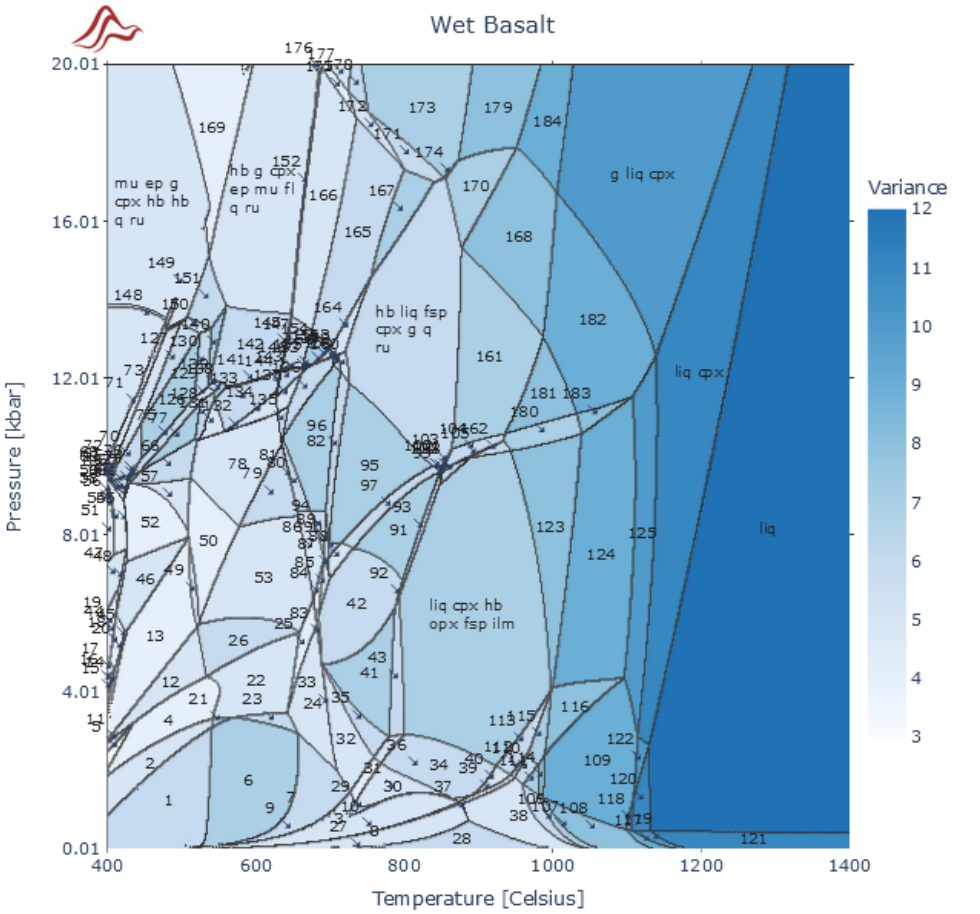
- **Phase only**
  refines (split) cells when a phase change is recorded in one of the four corners

- **Dominant end-member**
  refines (split) cells when the dominant end-member of any solution phase model changes in one of the four corners



- **Refinement levels**
  Number of successive grid refinements

MAGEMinApp: grid refinement



1) hb fl spn fsp hb ilm bi
2) fsp fl hb ilm spn bi hb sph
3) ilm hb fsp spn opx bi cpx fl
4) ilm fl hb hb bi fsp spn q sph
5) hb fl bi hb spn ilm fsp q ru s
6) spn hb ilm fsp bi fl
7) spn hb ilm bi cpx fsp fl
8) ol bi fl spn opx cpx fsp ilm
9) bi spn fsp hb cpx spn opx fl
10) cpx opx ol ilm hb fl fsp spn
11) bi hb spn fl hb fsp q ru sph
12) bi spn hb hb fl fsp q sph
13) hb spn fsp hb ep fl bi q sph
14) ep fl hb hb fsp spn bi q ru s
15) bi fsp hb fl ep spn hb q ru
16) mu hb hb bi ep spn fsp q n
17) fsp bi ep hb hb spn q ru
18) ep hb hb spn fsp bi q ru sp
19) ep hb bi fsp ilm spn hb q n
20) spn fsp hb mu ep hb bi q n
21) hb bi ilm fl fsp spn sph
22) hb fsp ilm fl bi spn q sph
23) fsp fl hb spn bi ilm q
24) fsp hb bi fl spn cpx ilm q
25) bi spn hb fsp fl cpx ilm q sp
26) hb fl fsp spn bi q sph
27) ilm ol cpx fsp fsp spn opx f
28) spn ol fl opx cpx fsp ilm
29) fsp cpx opx fl bi hb ilm
30) hb fsp fl spn opx cpx ilm bi
31) hb opx bi fl liq ilm fsp cpx
32) ilm hb fsp fl cpx liq spn bi
33) fl spn fsp cpx hb liq bi ilm c
34) hb ilm cpx opx fl fsp liq
35) fsp cpx hb liq fl ilm spn
36) liq cpx hb fsp fl opx spn ilm
37) fsp opx ol cpx ilm liq bi spn
38) cpx spn opx ilm fl liq fsp ol
39) liq ol spn fl fsp ilm cpx opx
40) fl ol cpx hb opx liq fsp ilm
41) liq spn cpx fsp ilm hb
42) hb fsp ilm liq spn cpx q
43) opx fsp hb cpx ilm liq spn
44) hb fsp bi ep hb spn ilm q n
45) hb ep hb fsp bi spn mu q s
46) hb ep spn fsp hb bi q sph
47) bi hb ep hb ilm spn fsp q
48) ilm hb ep fsp spn bi hb q sp
49) fl spn hb fsp bi ep q sph
50) fl hb bi cpx spn ep fsp q sp

Grid refinement

Refine phase boundaries

Phase diagram information

Number of computed points	Minimization time (ms)
55699	195.413

Variable	Value	Unit
P	7.198	kbar
T	884.375	°C
G	-916.164	kJ
ρ_sys	2936.0	kg/m³
ρ_solid	3104.2	kg/m³
ρ_melt	2241.8	kg/m³

Phase	Mode
opx	0.06
liq	0.198
hb	0.274
cpx	0.224
fsp	0.238
ilm	0.006

Oxide	mol
SiO2	0.501
Al2O3	0.087
CaO	0.117
MgO	0.121
FeO	0.078
K2O	0.002
Na2O	0.025
TiO2	0.01
O	0.005
Cr2O3	0.0
H2O	0.054

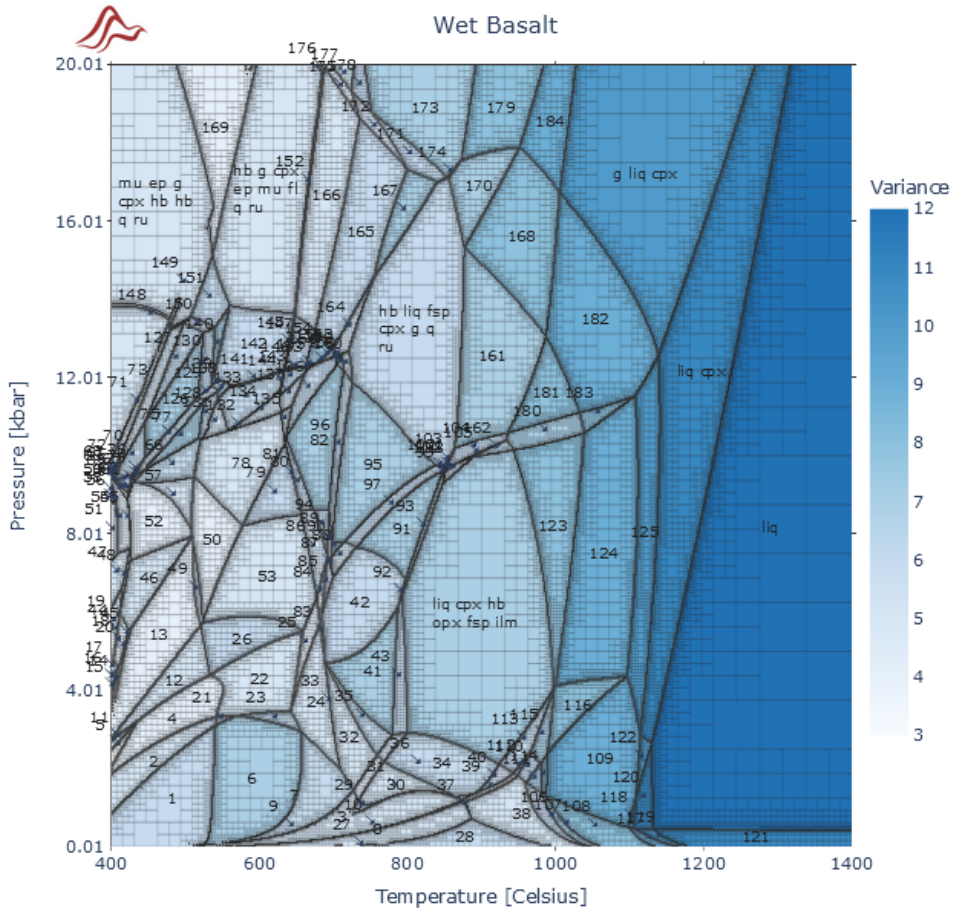
Save point | filename | Table | Table light

Save all | filename | Table

Display isopleths

Display options

MAGEMinApp: grid refinement



1) hb fl spn fsp hb ilm bi
2) fsp fl hb ilm spn bi hb sph
3) ilm hb fsp spn opx bi cpx fl
4) ilm fl hb hb bi fsp spn q sph
5) hb fl bi hb spn ilm fsp q ru s
6) spn hb ilm fsp bi fl
7) spn hb ilm bi cpx fsp fl
8) ol bi fl spn opx cpx fsp ilm
9) bi spn fsp hb cpx spn opx fl
10) cpx opx ol ilm hb fl fsp spn
11) bi hb spn fl hb fsp q ru sph
12) bi spn hb hb fl fsp q sph
13) hb spn fsp hb ep fl bi q sph
14) ep fl hb hb fsp spn bi q ru s
15) bi fsp hb fl ep spn hb q ru
16) mu hb hb bi ep spn fsp q n
17) fsp bi ep hb hb spn q ru
18) ep hb hb spn fsp bi q ru sp
19) ep hb bi fsp ilm spn hb q n
20) spn fsp hb mu ep hb bi q n
21) hb bi ilm fl fsp spn sph
22) hb fsp ilm fl bi spn q sph
23) fsp fl hb spn bi ilm q
24) fsp hb bi fl spn cpx ilm q
25) bi spn hb fsp fl cpx ilm q sp
26) hb fl fsp spn bi q sph
27) ilm ol cpx fsp fsp spn opx f
28) spn ol fl opx cpx fsp ilm
29) fsp cpx opx fl bi hb ilm
30) hb fsp fl spn opx cpx ilm bi
31) hb opx bi fl liq ilm fsp cpx
32) ilm hb fsp fl cpx liq spn bi
33) fl spn fsp cpx hb liq bi ilm c
34) hb ilm cpx opx fl fsp liq
35) fsp cpx hb liq fl ilm spn
36) liq cpx hb fsp fl opx spn ilm
37) fsp opx ol cpx ilm liq bi spn
38) cpx spn opx ilm fl liq fsp ol
39) liq ol spn fl fsp ilm cpx opx
40) fl ol cpx hb opx liq fsp ilm
41) liq spn cpx fsp ilm hb
42) hb fsp ilm liq spn cpx q
43) opx fsp hb cpx ilm liq spn
44) hb fsp bi ep hb spn ilm q n
45) hb ep hb fsp bi spn mu q s
46) hb ep spn fsp hb bi q sph
47) bi hb ep hb ilm spn fsp q
48) ilm hb ep fsp spn bi hb q s
49) fl spn hb fsp bi ep q sph
50) fl hb bi cpx spn ep fsp q sp

Grid refinement

Refine phase boundaries

Phase diagram information

Number of computed points	Minimization time (ms)
55699	195.413

Variable	Value	Unit
P	7.198	kbar
T	884.375	°C
G	-916.164	kJ
ρ_sys	2936.0	kg/m³
ρ_solid	3104.2	kg/m³
ρ_melt	2241.8	kg/m³

Phase	Mode
opx	0.06
liq	0.198
hb	0.274
cpx	0.224
fsp	0.238
ilm	0.006

Oxide	mol
SiO2	0.501
Al2O3	0.087
CaO	0.117
MgO	0.121
FeO	0.078
K2O	0.002
Na2O	0.025
TiO2	0.01
O	0.005
Cr2O3	0.0
H2O	0.054

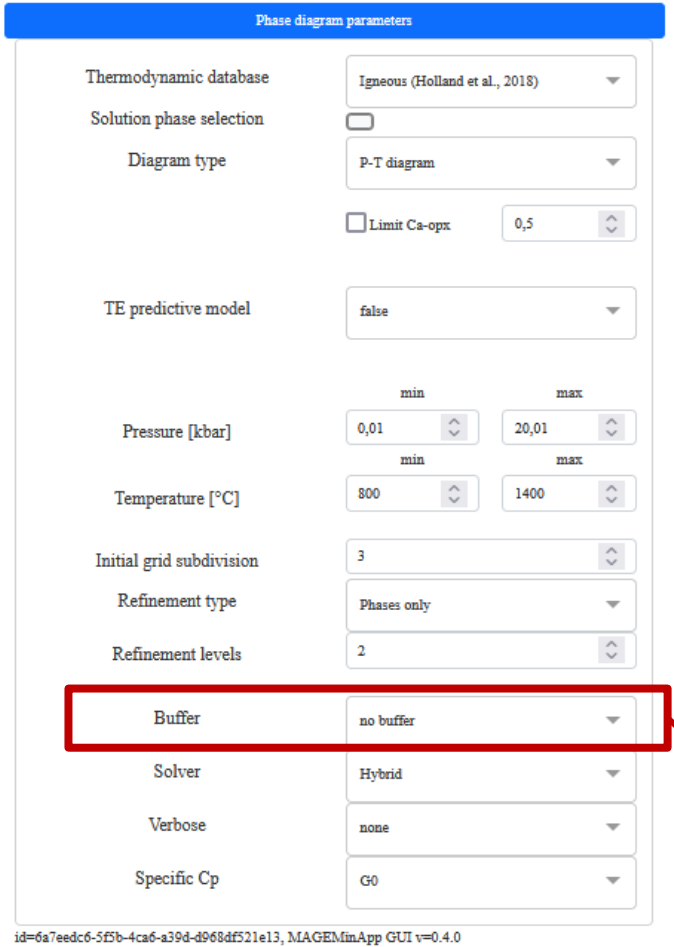
Save point | filename | Table | Table light

Save all | filename | Table

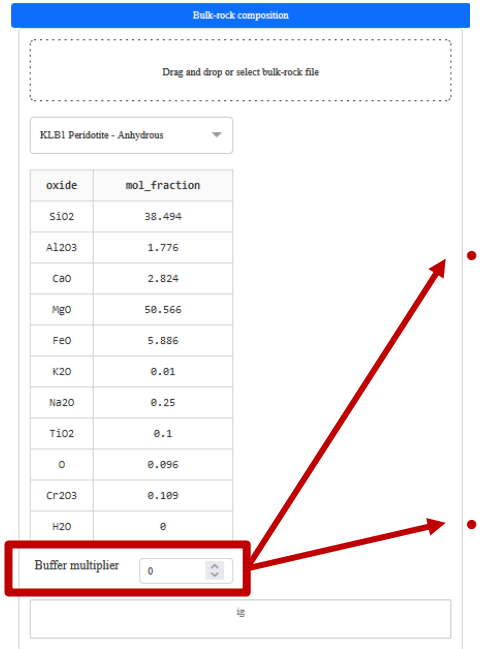
Display isopleths

Display options

MAGEMinApp: buffers

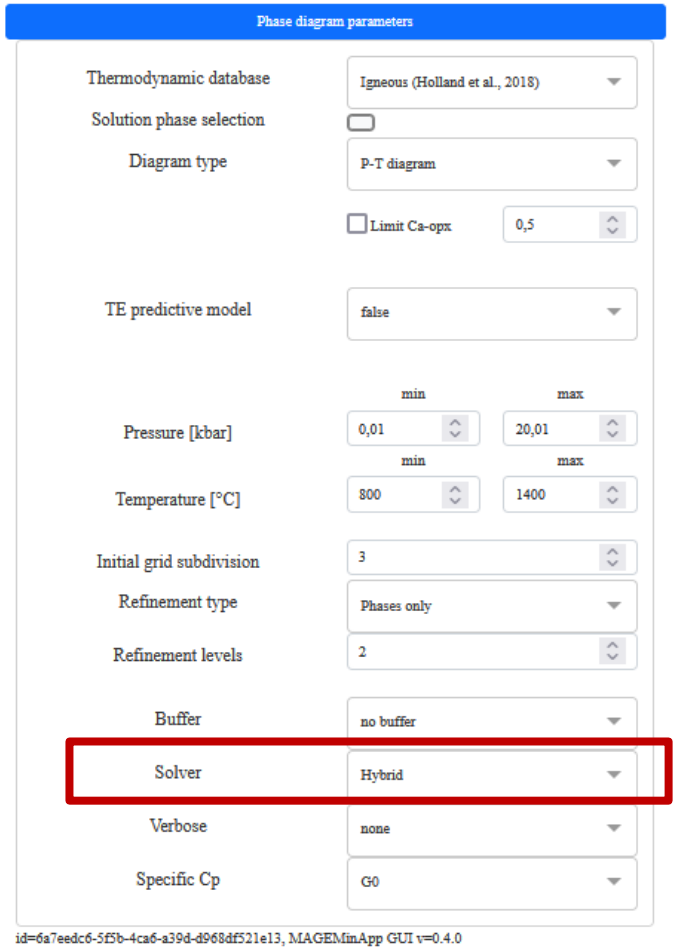


- **Oxygen buffers**
  QFM, MW, QIF, CCO, HM, NNO
- **Fix activity**
  H2O, O2, SiO2, FeO, MgO, Al2O3, TiO2



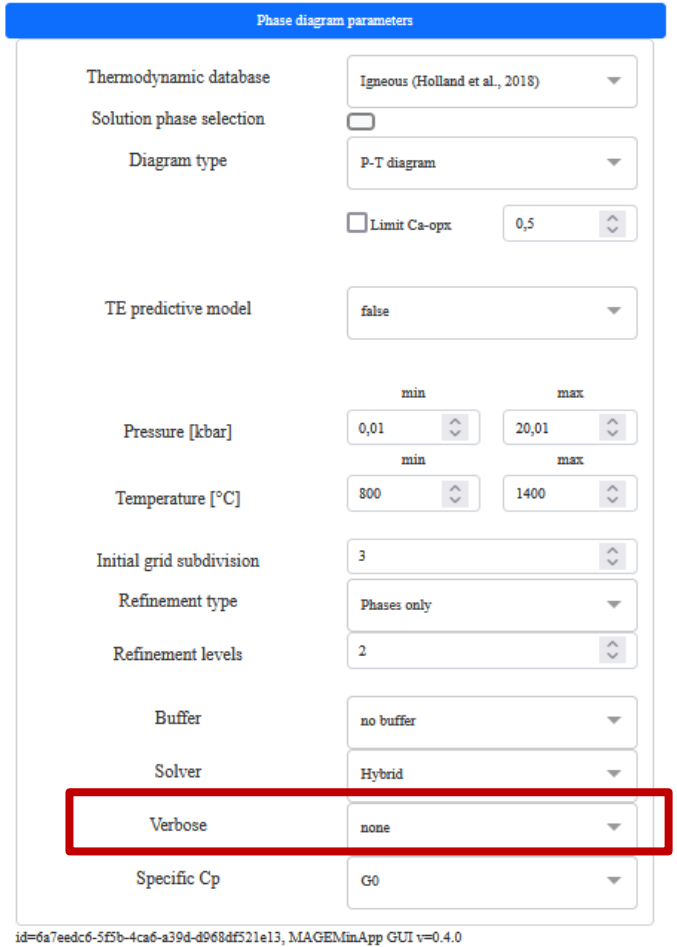
- **Selecting a buffer displays the option to apply a shift in the RTlog scale**
  e.g., +2 QFM
- **Allow to provide the activity value in case activity is selected**

MAGEMinApp: solvers



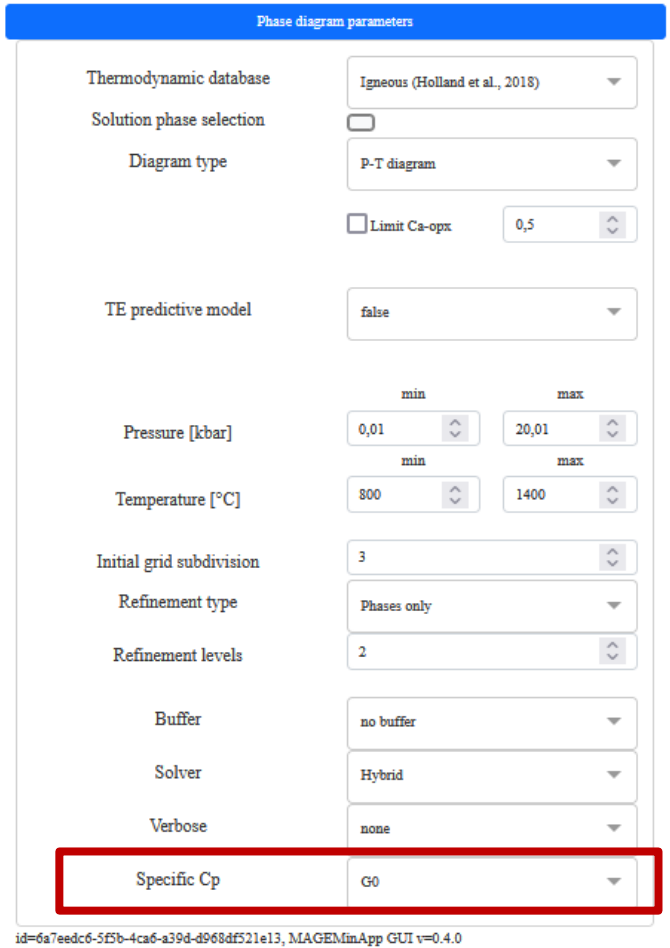
- **Default MAGEMin solver to perform stable phase equilibria calculation**
  No need to be changed in normal use

MAGEMinApp: solvers



- **Displays details of the calculation(s) in the Julia terminal**
  mostly used for debugging

MAGEMinApp: Specific heat capacity



- **Method to compute specific heat capacity**

$$Cp = -T\,\frac{\Delta^2 G}{\Delta T^2} = -T\,\frac{G^{(T+\delta T)} + G^{(T-\delta T)} - 2G^{(T)}}{\delta T^2}$$

where Cp is the specific heat capacity, T is the temperature

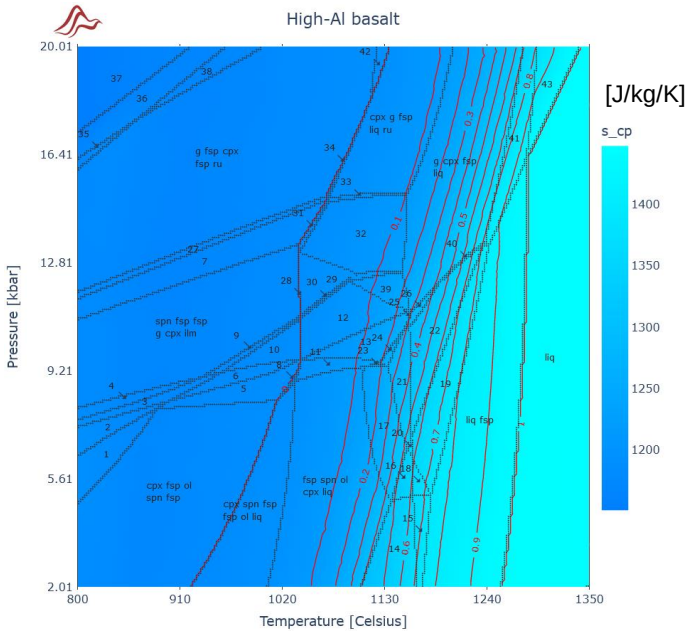
- **Can be computed using**

1. phase aggregate (G_0) ***Without reactions***
2. phase assemblage (G_{system}) ***With reactions***

- **Note that when G_system is selected, solver must be set to legacy**
  higher accuracy at suprasolidus conditions is needed to compute Gibbs second derivative

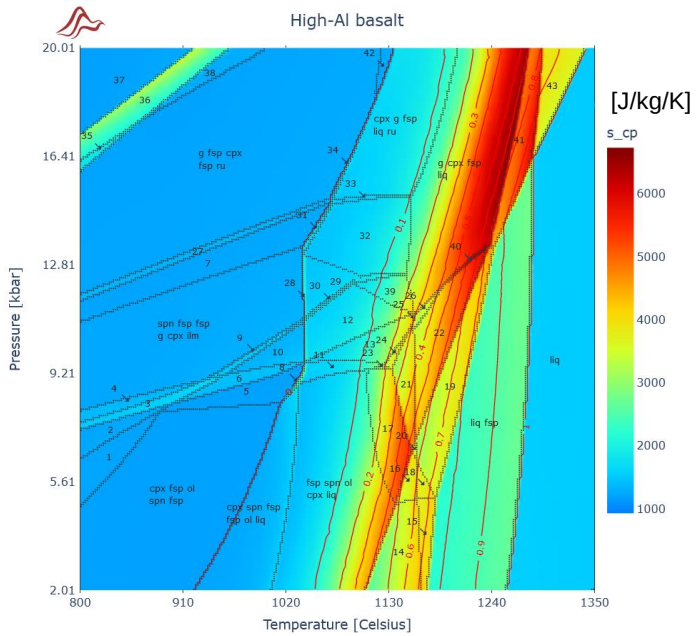
Specific heat capacity: what difference does it make?

G_0 differentiation (Cp without reaction)



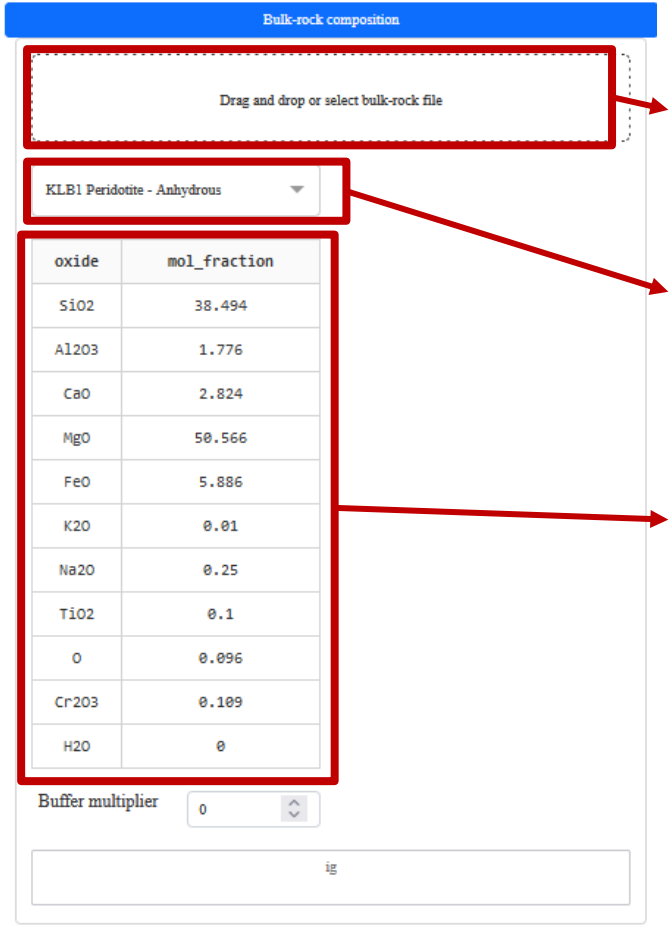
- Cheap to compute
- Ignores latent heat

G_{system} differentiation (Cp with reaction)



- More expensive to compute
- Correct heat budget
- To be chosen for geodynamic coupling

MAGEMinApp: bulk rock composition



- **Load custom bulk rock composition(s)**
- **Select predefined bulk rock composition for testing**
- **Bulk rock composition displayed in mol%**
  note that only the oxides taken into account in the database are displayed

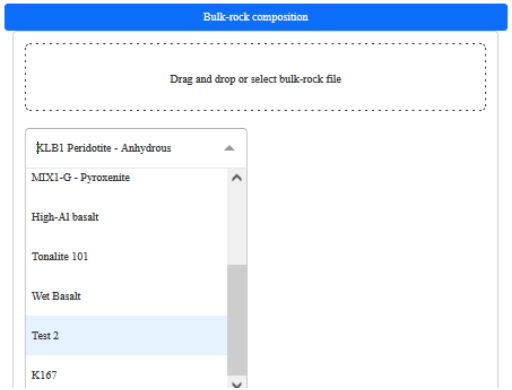
MAGEMinApp: bulk rock input file format

Example of input file provided in:

https://github.com/ComputationalThermodynamics/Resources/GG2024/bulkrock_composition_input_files/

```
# 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];
```

- **Note that either [..., Fe2O3, FeO,...] or [..., FeO, O, ...] must me provided for the database accounting for O**

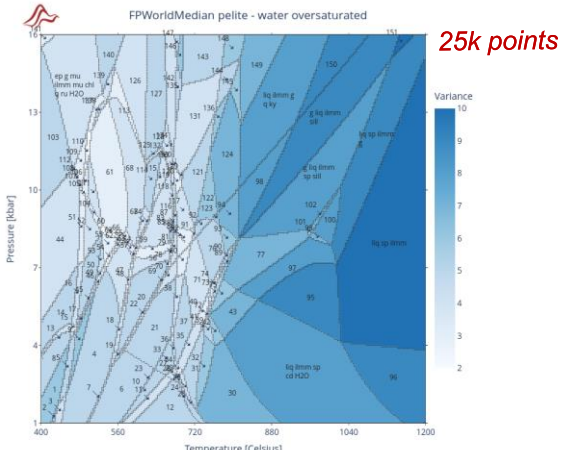


- **Once loaded, the bulk-rock composition appear in the dropdown menu**
  Note that the bulk are attached to a database, this is why only Test 2 and K167 appear in the dropdown menu

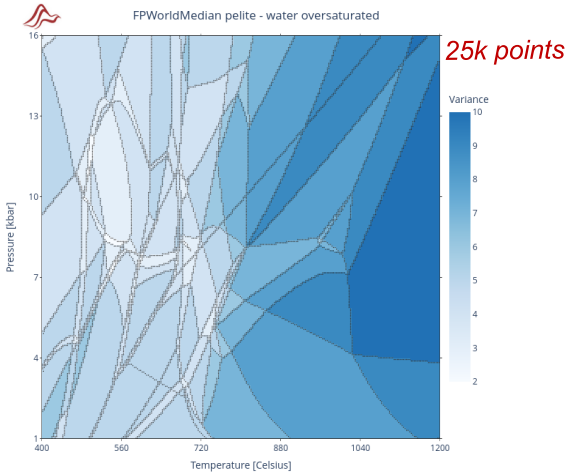
MAGEMinApp: upcoming

- Improved reaction line extraction and field center finder

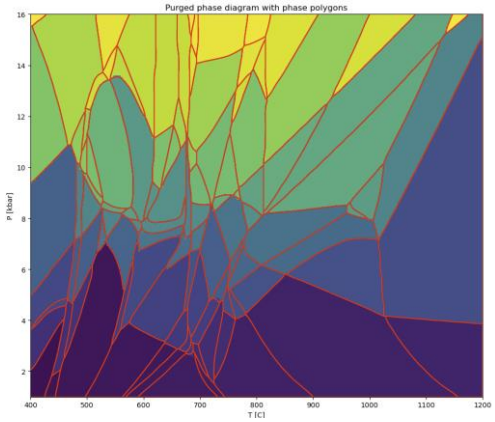
With Anton Popov (JGU Mainz)

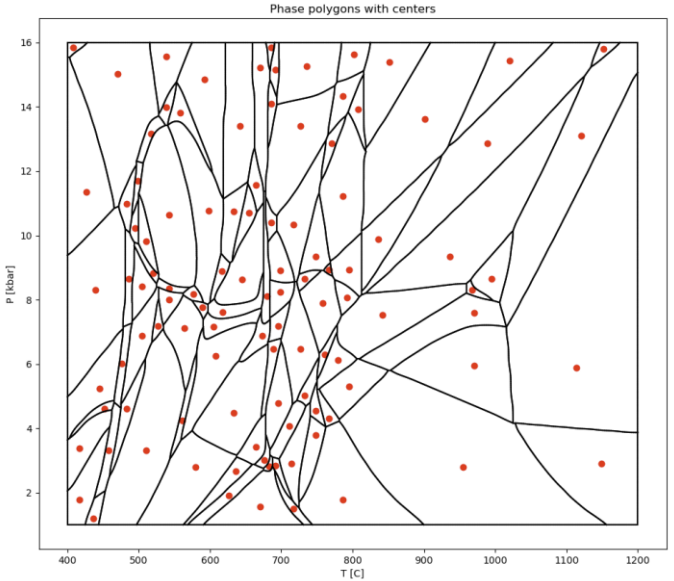


25k points



25k points





→ vectorized reaction lines and accurate labelling of non convex fields!

Julia interface: MAGEMin_C

https://github.com/ComputationalThermodynamics/MAGEMin_C

Install MAGEMin_C

```
julia> ]                    # opens the package manager
pkg> add MAGEMin_C          # MAGEMin_C
```

```
julia> using MAGEMin_C
julia> data     = Initialize_MAGEMin("ig", verbose=false);
julia> P,T      = 10.0, 1100.0
julia> Xoxides = ["SiO2"; "Al2O3"; "CaO"; "MgO"; "FeO"; "Fe2O3"; "K2O"; "Na2O"; "TiO2"; "Cr2O3"; "H2O"]
julia> X        = [48.43; 15.19; 11.57; 10.13; 6.65; 1.64; 0.59; 1.87; 0.68; 0.0; 3.0];
julia> sys_in   = "wt"
julia> out      = single_point_minimization(P, T, data, X=X, Xoxides=Xoxides, sys_in=sys_in)
```

```
julia> out     = single_point_minimization(P, T, data, X=X, Xoxides=Xoxides, sys_in=sys_in)
Pressure          : 10.0     [kbar]
Temperature       : 1100.0   [Celsius]
    Stable phase | Fraction (mol fraction)
             liq   0.75136
             cpx   0.20987
             opx   0.03877
    Stable phase | Fraction (wt fraction)
             liq   0.73007
             cpx   0.22897
             opx   0.04097
    Stable phase | Fraction (vol fraction)
             liq   0.77373
             cpx   0.19218
             opx   0.03409
Gibbs free energy : -916.874646  (45 iterations; 81.05 ms)
Oxygen fugacity          : -7.68808396800797
Delta QFM                : 1.2159893622277753
```

`out. `+ tab``

```
julia> out.
G_system        Gamma           MAGEMin_ver     M_sys           PP_vec          P_kbar          SS_vec          T_C             V               Vp              Vp_S            Vs              Vs_S
X               aAl2O3          aFeO            aH2O            aMgO            aSiO2           aTiO2           alpha           bulk            bulkMod         bulkModulus_M   bulkModulus_S   bulk_F
bulk_F_wt       bulk_M          bulk_M_wt       bulk_S          bulk_S_wt       bulk_res_norm   bulk_wt         cp              dQFM            dataset         enthalpy        entropy         fO2
frac_F          frac_F_wt       frac_M          frac_M_wt       frac_S          frac_S_wt       iter            mSS_vec         n_PP            n_SS            n_mSS           oxides          ph
ph_frac         ph_frac_vol     ph_frac_wt      ph_id           ph_type         rho             rho_F           rho_M           rho_S           s_cp            shearMod        shearModulus_S  status
time_ms
```