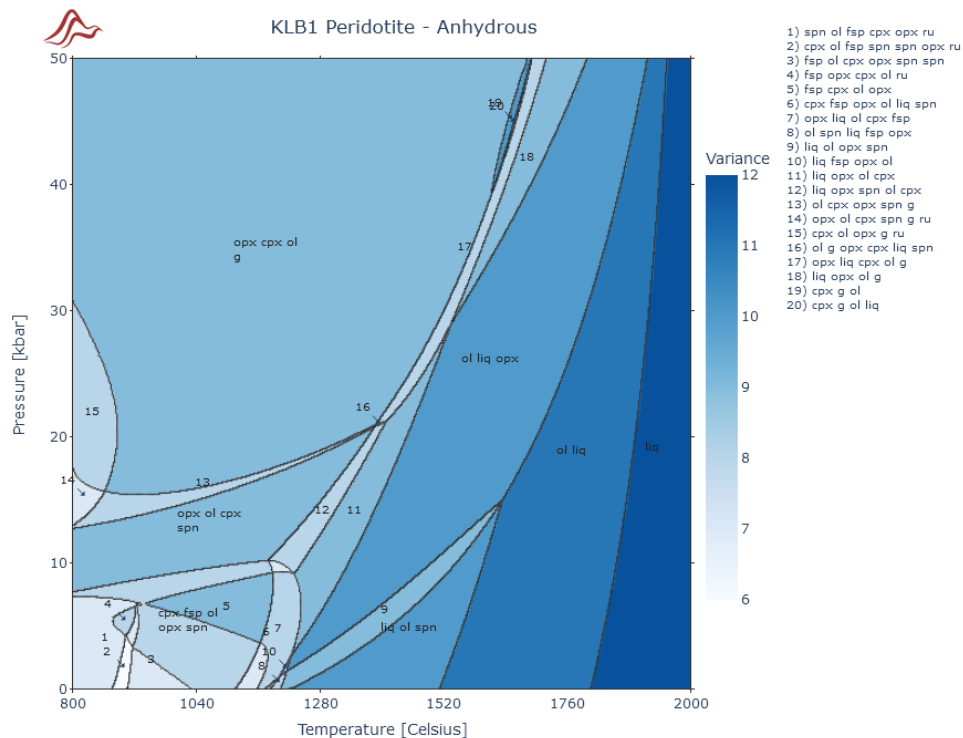


MAGEMinApp: introduction



MAGEMinApp contributors

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H. Ranocha,
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H. Dominguez
P. Lanari
J. Forshaw
T. Holland



MAGEMin github: ComputationalThermodynamics

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



<https://github.com/ComputationalThermodynamics/Resources>

The screenshot shows the GitHub repository page for 'Resources' by NicolasRiel. The repository is public and has 1 branch and 0 tags. The file tree shows a folder named 'GG2024' (added databases), a 'LICENSE' file (Initial commit), and a 'README.md' file (updated README). The 'Code' button is highlighted with a red box, and the 'Download ZIP' option in the dropdown menu is also highlighted with a red box. The right sidebar shows repository statistics (0 stars, 2 watching, 0 forks) and links to Readme, Activity, and Releases.

- 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)

```
seph42@DESKTOP-2V82075:~$ julia -t 6

Documentation: https://docs.julialang.org
Type "?" for help, "]" for Pkg help.

Version 1.10.0 (2023-12-25)
Official https://julialang.org/ release

julia> using MAGEMinApp
App()
Using libMAGEMin.dylib from MAGEMin_jll

julia> App()
[ Info: Listening on: 127.0.0.1:8050, thread id: 2
```

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

Favored way
(better performances on
Mac and Linux)

POWERSHELL

WINDOWS(NO WSL)

```
Windows PowerShell
Copyright (C) Microsoft Corporation. All rights reserved.

Try the new cross-platform PowerShell https://aka.ms/pscore6

PS C:\Users\Seph> $env:JULIA_NUM_THREADS=6
PS C:\Users\Seph> julia

Documentation: https://docs.julialang.org
Type "?" for help, "]" for Pkg help.

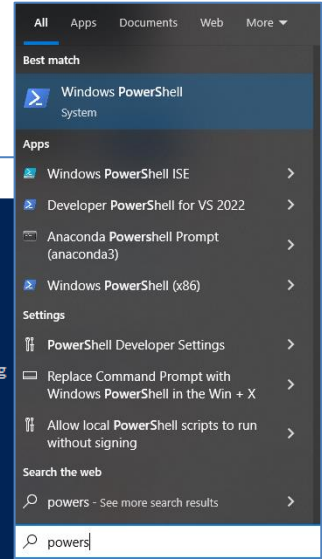
Version 1.9.3 (2023-08-24)
Official https://julialang.org/ release

julia> using MAGEMinApp
Using libMAGEMin.dylib from MAGEMin_jll

julia> App()
[ Info: Listening on: 127.0.0.1:8050, thread id: 1
```

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

Around 2.5 times slower
than using WSL



MAGEMinApp: interface (Phase diagrams)

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

☐ Limit Ca-ox: 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 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

ig

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

MAGEMinApp: interface (Phase diagrams)

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

☐ Limit Ca-ox

0,5

TE predictive model

false

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
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K2O	0.01
Na2O	0.25
TiO2	0.1
O	0.096
Cr2O3	0.109
H2O	0

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

- Save/load state
- Compute diagram

Grid properties

Bulk rock
composition(s)

MAGEMinApp: Thermodynamic database

Phase diagram parameters

Thermodynamic database

Solution phase selection

Diagram type

TE predictive model

Pressure [kbar]

Temperature [°C]

Initial grid subdivision

Refinement type

Refinement levels

Buffer

Solver

Verbose

Specific Cp

Igneous (Holland et al., 2018)

Metapelite (White et al., 2014)

Metabasite (Green et al., 2016)

Igneous (Holland et al., 2018)

Ultramafic (Evans & Frost, 2021)

min max

0,01 20,01

min max

800 1400

3

Phases only

2

no buffer

Hybrid

none

G0

id=6a7eedc6-5f5b-4ca6-a39d-d968df521e13, MAGEMinApp GUI v=0.4.0

- **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

Phase diagram parameters

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

Solution phase selection

- ☒ spin
- ☒ bi
- ☒ cd
- ☒ cpx
- ☒ ep
- ☒ g
- ☒ hb
- ☒ ilm
- ☒ liq
- ☒ ol
- ☒ opx
- ☒ fsp
- ☒ fl
- ☒ mu
- ☒ fper

Diagram type: P-T diagram

☐ Limit Ca-opx: 0,5

TE predictive model: false

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

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

MAGEMinApp: diagram types

Phase diagram parameters

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

Solution phase selection: ☐

Diagram type

TE predictive model

Pressure [kbar]: 0,01 (min) to 20,01 (max)

Temperature [°C]: 800 to 1400

Initial grid subdivision: 3

Refinement type: Phases only

Refinement levels: 2

Buffer: no buffer

Solver: Hybrid

Verbose: none

Specific Cp: G0

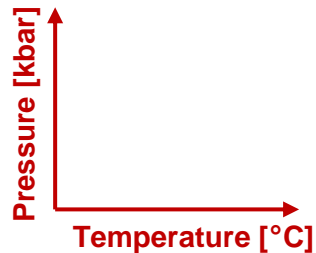
P-T diagram (selected)

P-X diagram

T-X diagram

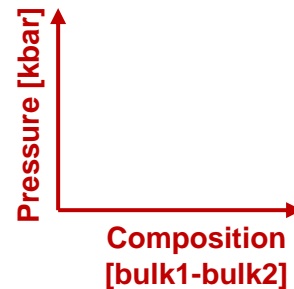
PT-X diagram

P-T



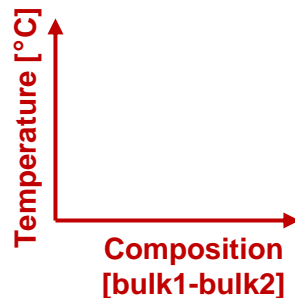
P-X

Fixed temperature

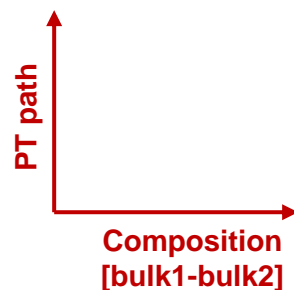


T-X

Fixed pressure



PT-X



MAGEMinApp: Trace element predictive model

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

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

- 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

Watson & Harrison (1983)

Boehnke et al. (2013)

Crisp and Berry (2022)

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

Trace-element composition

Drag and drop or select trace-element file

Pyrolite (Primitive Mantle) ▾

elements	µg/g
Rb	0.6
Ba	6.6
Th	0.0795
U	0.0203
Nb	0.658
Ta	0.037
La	0.648
Ce	1.675
Pb	0.15
Pr	0.254
Sr	19.9
Nd	1.25

MAGEMinApp: grid subdivision and refinement

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: false

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

Temperature [°C]: min 800 max 1400

Initial grid subdivision: 3

Refinement type: Phases only

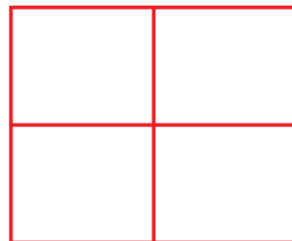
Refinement levels: 2

Buffer: no buffer

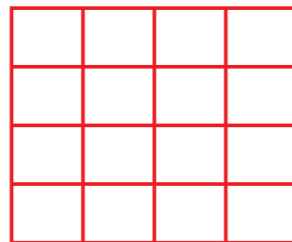
Solver: Hybrid

Verbose: none

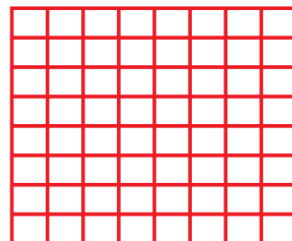
Specific Cp: G0



1 initial grid subdivisions



2 initial grid subdivisions



3 initial grid subdivisions

MAGeMinApp: grid subdivision and refinement

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: false

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

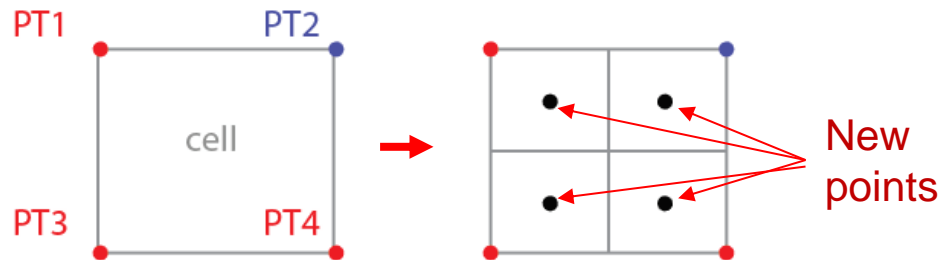
Buffer: no buffer

Solver: Hybrid

Verbose: none

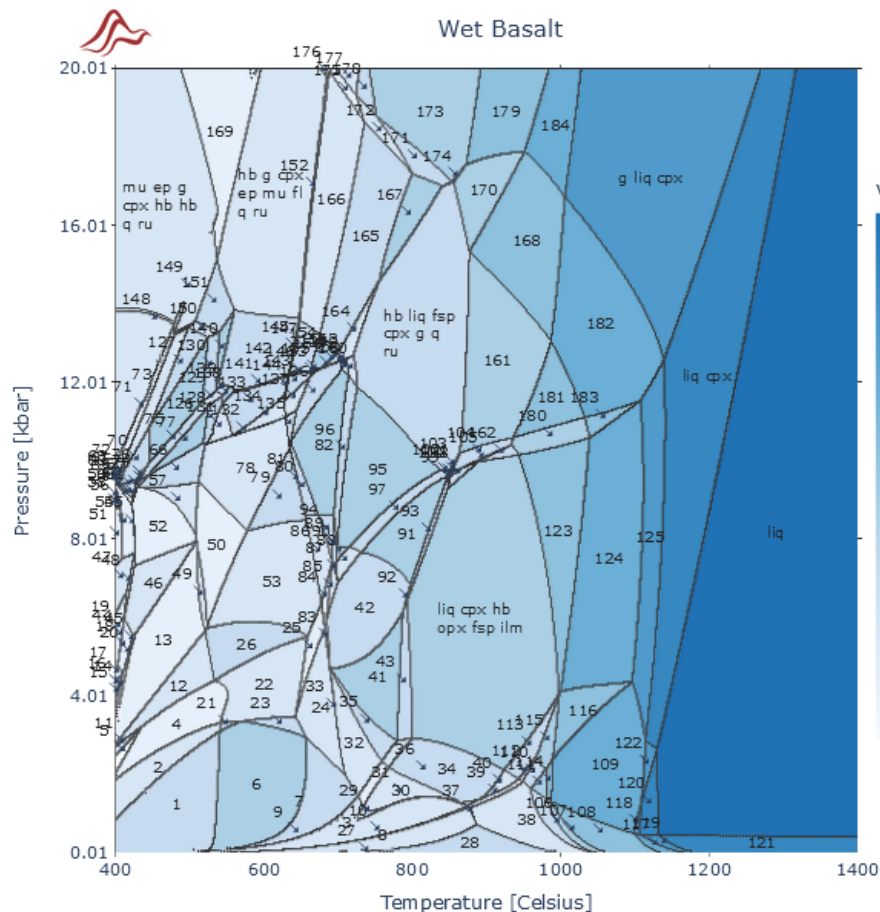
Specific Cp: G0

- **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 si
- 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	Phase	Mode	Oxide	mol
P	7.198	kbar	opx	0.06	SiO ₂	0.501
T	884.375	°C	liq	0.198	Al ₂ O ₃	0.087
G	-916.164	kJ	hb	0.274	CaO	0.117
p _{sys}	2936.0	kg/m ³	cpx	0.224	MgO	0.121
p _{solid}	3104.2	kg/m ³	fsp	0.238	FeO	0.078
p _{melt}	2241.8	kg/m ³	ilm	0.006	K ₂ O	0.002
					Na ₂ O	0.025
					TiO ₂	0.01
					O	0.005
					Cr ₂ O ₃	0.0
					H ₂ O	0.054

Save point

filename

Table

Table light

Save all

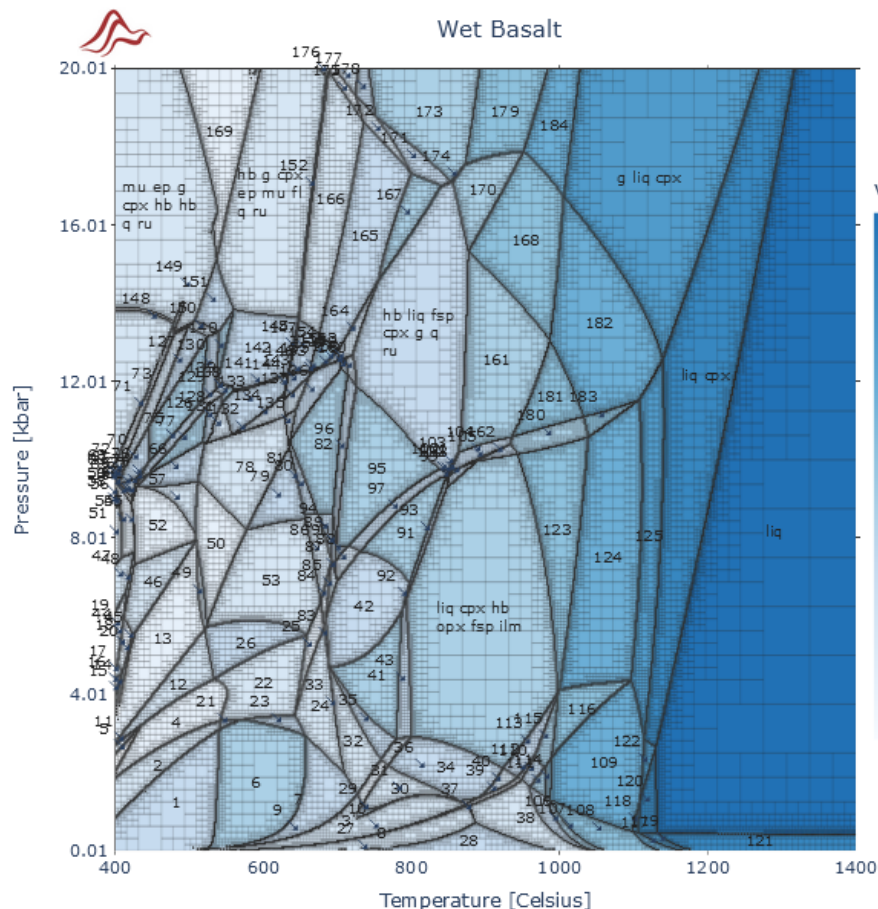
filename

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 opx 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	Phase	Mode	Oxide	mol
P	7.198	kbar	opx	0.06	SiO ₂	0.501
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					TiO ₂	0.01
					O	0.005
					Cr ₂ O ₃	0.0
					H ₂ O	0.054

Save point

filename

Table Table light

Save all

filename

Table

Display isopleths

Display options

MAGEMinApp: buffers

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: false

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

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

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

Buffer multiplier: 0

- **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

Phase diagram parameters

Thermodynamic database	Igneous (Holland et al., 2018)
Solution phase selection	<input type="checkbox"/>
Diagram type	P-T diagram
<input type="checkbox"/> Limit Ca-opx	0,5
TE predictive model	false
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

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

MAGEMinApp: solvers

Phase diagram parameters

Thermodynamic database	Igneous (Holland et al., 2018)
Solution phase selection	<input type="checkbox"/>
Diagram type	P-T diagram
<input type="checkbox"/> Limit Ca-opx	0,5
TE predictive model	false
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

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

MAGEMinApp: Specific heat capacity

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: false

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

- Method to compute specific heat capacity

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

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

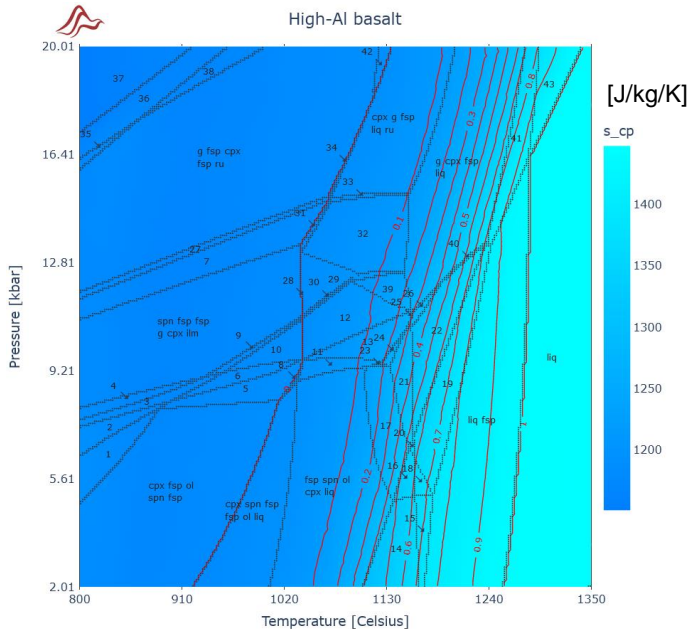
- Can be computed using

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

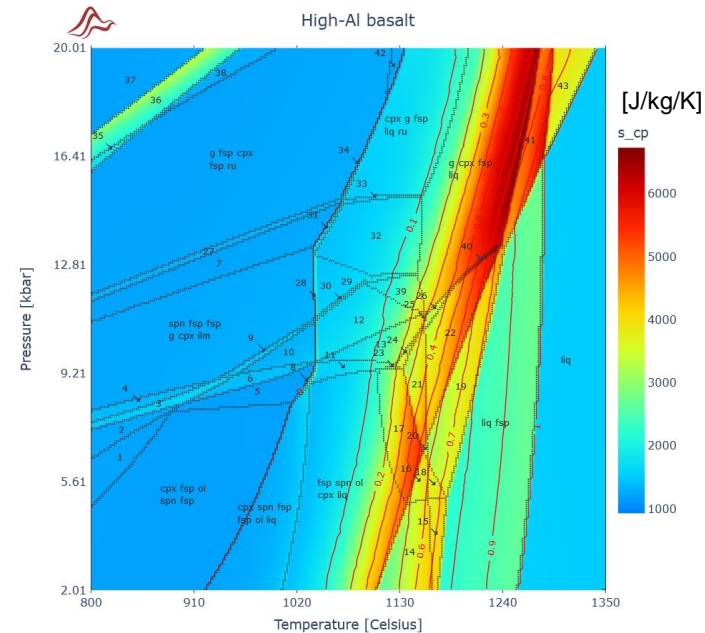
Specific heat capacity: what difference does it make?

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

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	2.824
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	0.109
H ₂ O	0

Buffer multiplier 0

ig

- 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

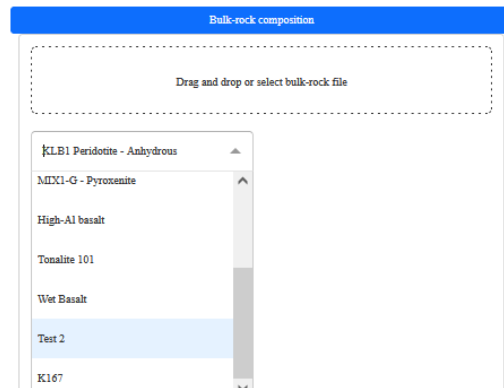
MAGEMinApp: bulk rock input file format

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 be provided for the database accounting for O**

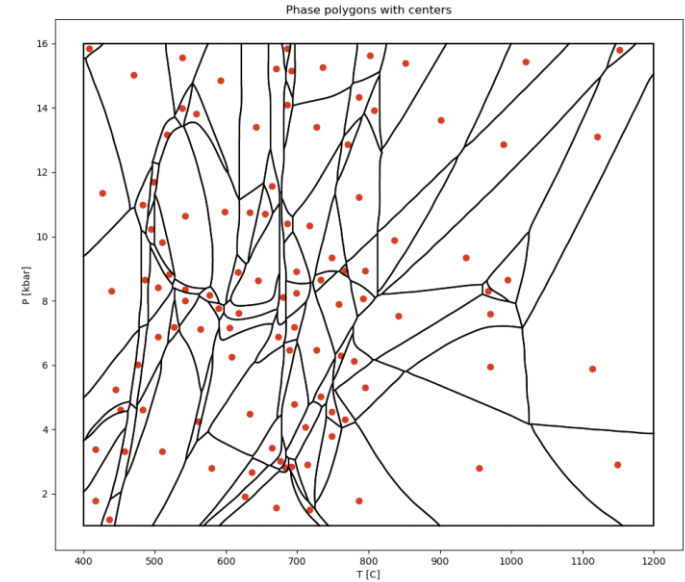
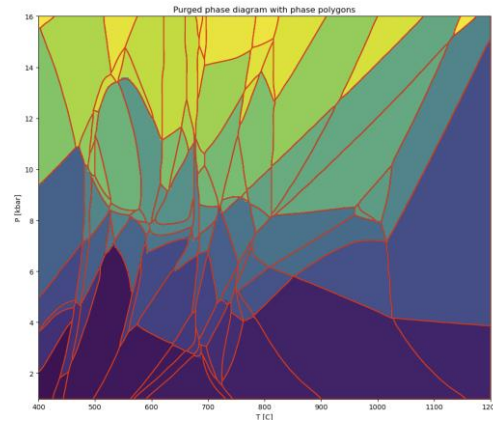
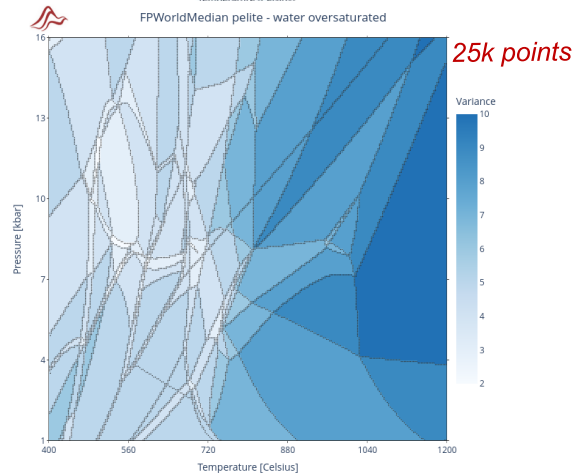
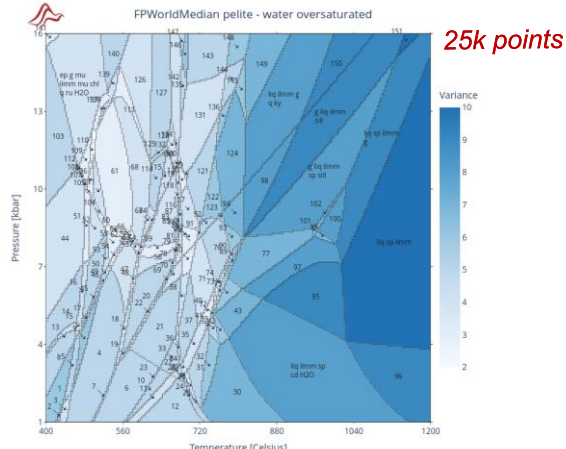


- **Once loaded, the bulk-rock composition appear in the dropdown menu**
Note that the bulk are attached to a database, this is why only Test 2 and K167 appear in the dropdown menu

MAGEMinApp: upcoming

- Improved reaction line extraction and field center finder

With Anton Popov (JGU Mainz)



→ 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   : -7.68888396800797
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    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
time_ms
```