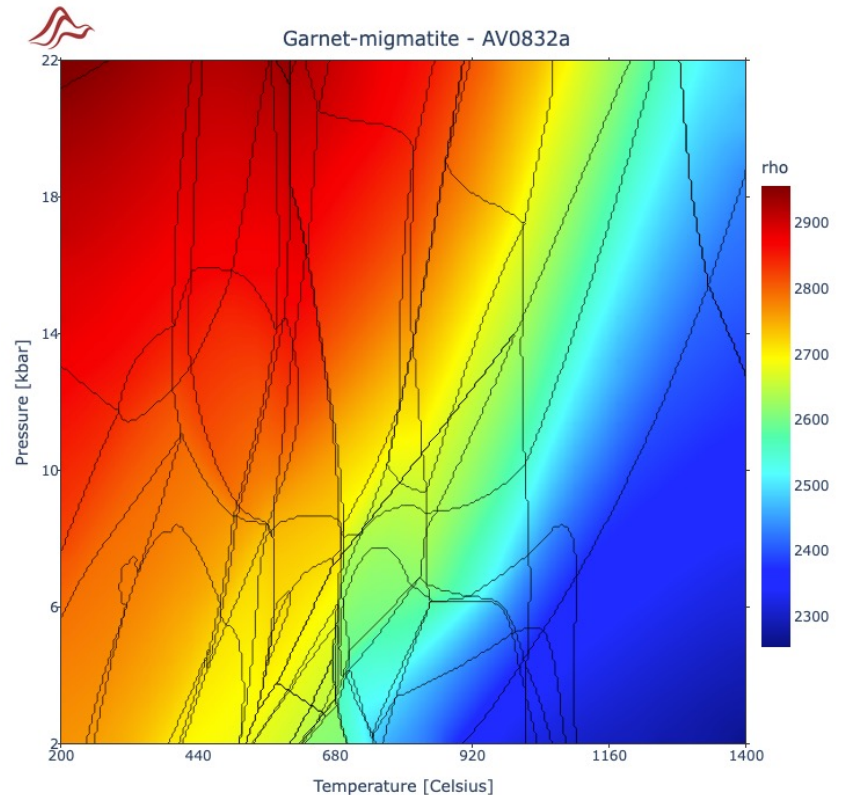
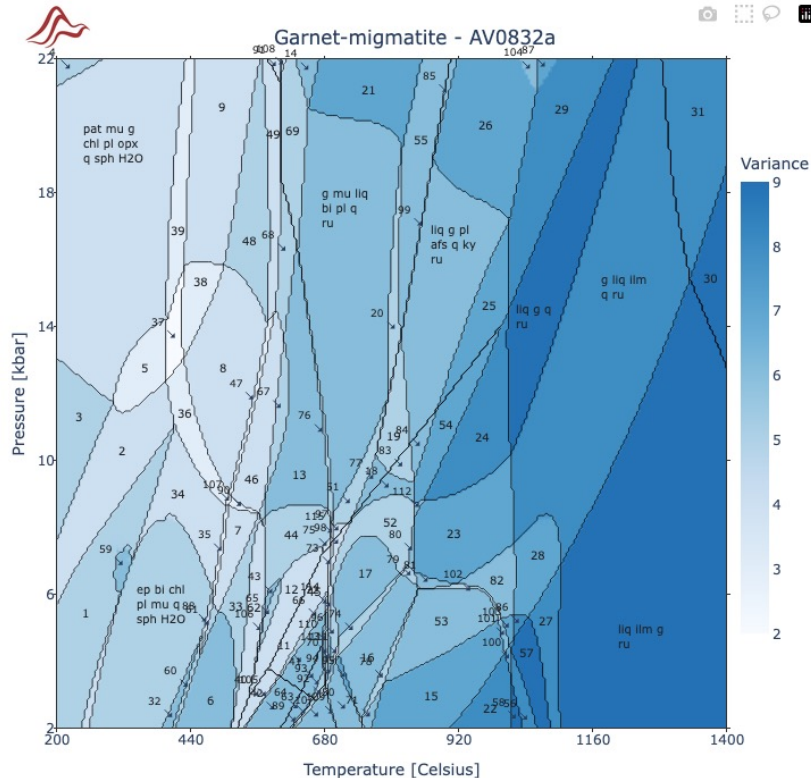


LaMEM short course

17-21 02 2025 Heidelberg

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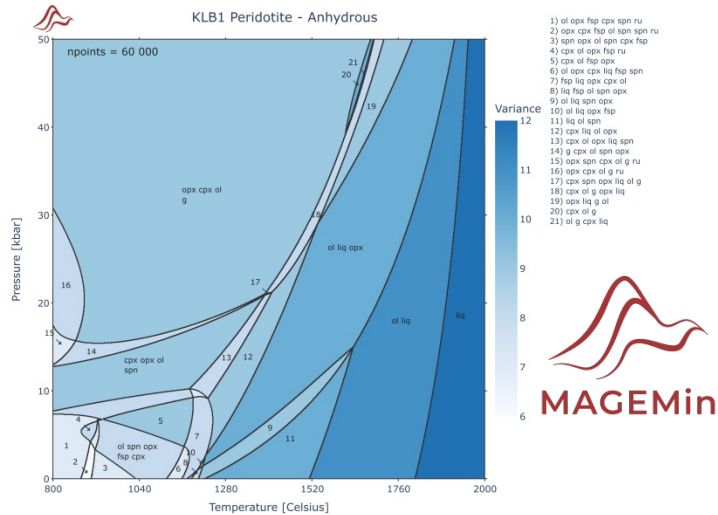
How to compute density diagram for LaMEM using MAGEMin?



MAGEMinApp.jl

using MAGEMinApp

(<https://github.com/ComputationalThermodynamics>)



Julia -t 5 #threaded
Julia>] add MAGEMinApp
Julia> using MAGEMinApp
Julia> App()

<http://127.0.0.1:8050/>

web browser

erc JGU UNIVERSITÄT ERLANGEN-NÜRNBERG

File

Simulation Phase Diagram P-T path TE modeling

Phase diagram parameters

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

Diagram type: P-T diagram

clinopyroxene: Omphacite ☒ Augite

Pressure [kbar]: min 0.01 max 20.01

Temperature [°C]: min 400 max 1400

Initial grid subdivision: 3

Refinement type: Phases only

Refinement levels: 4

Buffer: no buffer

Solver: Hybrid

Verbose: none

Bulk-rock composition

Drag and drop or select bulk-rock file

Natural amphibolites and low-temperature

oxide	mol_fraction
SiO2	51.08
Al2O3	9.68
CaO	13.26
MgO	11.21
FeO	11.66
K2O	0.16
Na2O	0.79
TiO2	1.37
O	0.8
H2O	28

Menzies (Green et al., 2016)

General parameters

Title: Natural amphibolites and low-temperature granulites

Update Reset

Filename: --

Load Save

Compute phase diagram

id=62d49318-3749-4151-ba1b-07a534753d62, MAGEMinApp OUT v=0.1.1

MAGEMin – phase diagrams

Phase diagrams | PTX path | Isentropic path | General information

Setup | Diagram | Trace-elements

Phase diagram parameters

Thermodynamic database: **Metabasite (Green et al., 2016)** 1

Phase selection: ☐ Solution phase ☐ Pure phase

Diagram type: P-T diagram

Solidus H₂O-saturated: false

clinopyroxene: ☐ Omphacite: ☒ Augite: ☐

TE predictive model: false

Pressure [kbar]: min 2 max 22

Temperature [°C]: min 200 max 1400 2

Initial grid subdivision: 3 8 × 8 grid

Refinement type: Phases only

Refinement levels: 4 3

Buffer: no buffer

Solver: Hybrid

Verbose: none

Specific Cp: G0

Bulk-rock composition

mol% ▼

Drag and drop or select bulk-rock file

SM89 oxidised average MORB composition 4

oxide	fraction
SiO ₂	52.47
Al ₂ O ₃	9.1
CaO	12.21
MgO	12.71
FeO	8.15
K ₂ O	0.23
Na ₂ O	2.61
TiO ₂	1.05
O	1.47
H ₂ O	20

Metabasite (Green et al., 2016)

id=3f380aa6-3537-40b4-a6c6-7c610b2c5117; MAGEMinApp GUI v=0.7.3; using 12/12 threads

1. Select database,
2. select P-T range → 200 to 1200° C 2 to 24 kbar,
3. select levels of refinement = 4,
4. choose MORB composition

MAGEMin – phase diagrams

General parameters

Title: SM89 oxidised average MORB composition

Update Reset

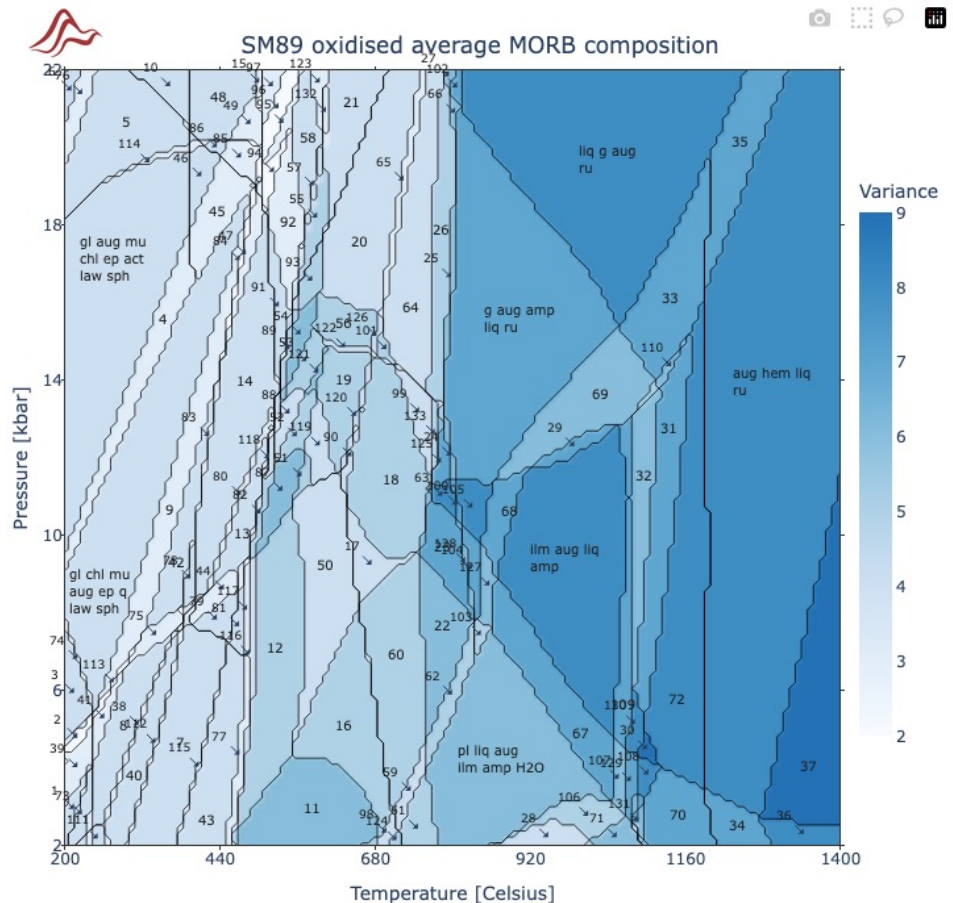
Compute phase diagram

Save/Load Diagram

filename Save state Load state

State/CSV directory: /Users/nicolasriehl/seph/MAGEMinApp.jl_v0.7.3

1. Compute diagram (wait a few minutes)



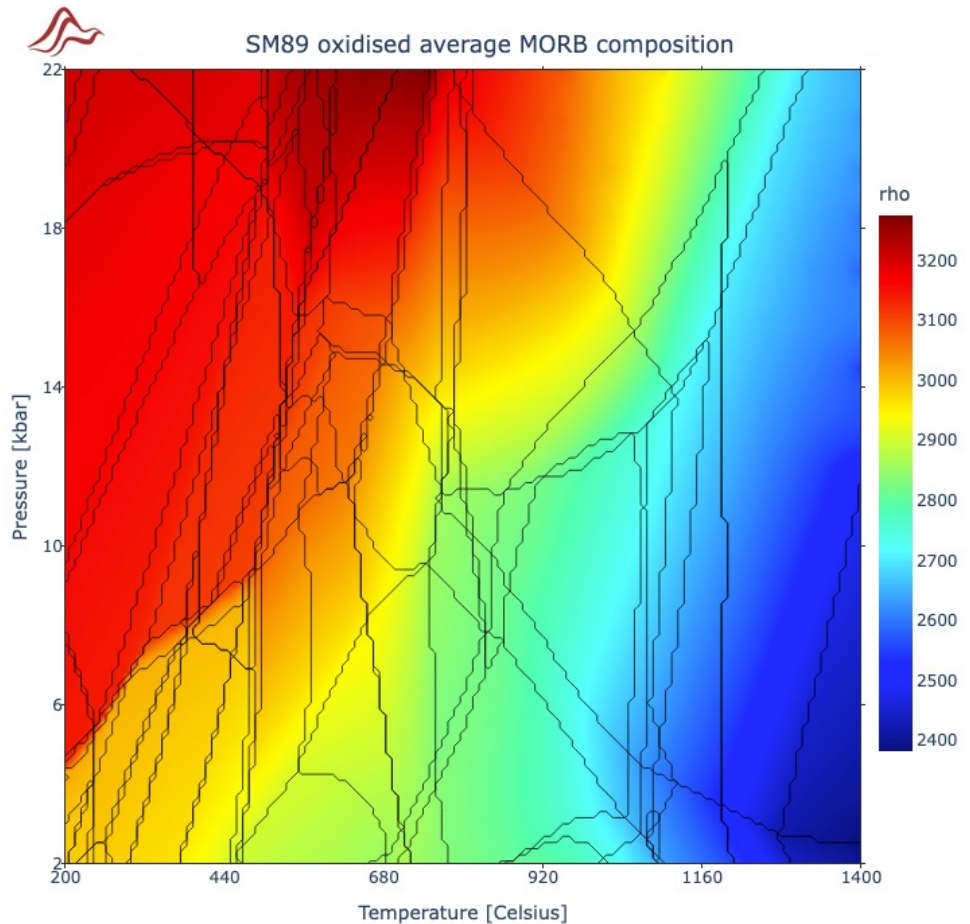
Gives a low-resolution diagram (enough for density)

MAGEMin – phase diagrams

Display options

Show reaction lines	false
Show grid	false
Show stable phases	false
Field	ρ_{system}
Colormap	jet
Smooth colormap	best
Colormap range	1 2 3 4 5 6 7 8 9
Reverse colormap	false

2



Gives a low-resolution diagram (enough for density)

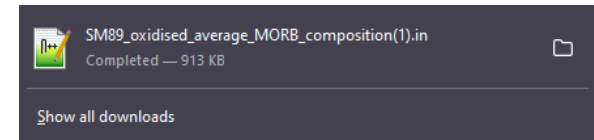
2. Change field to rho and colormap to jet

MAGEMin – phase diagrams

Export to LaMEM



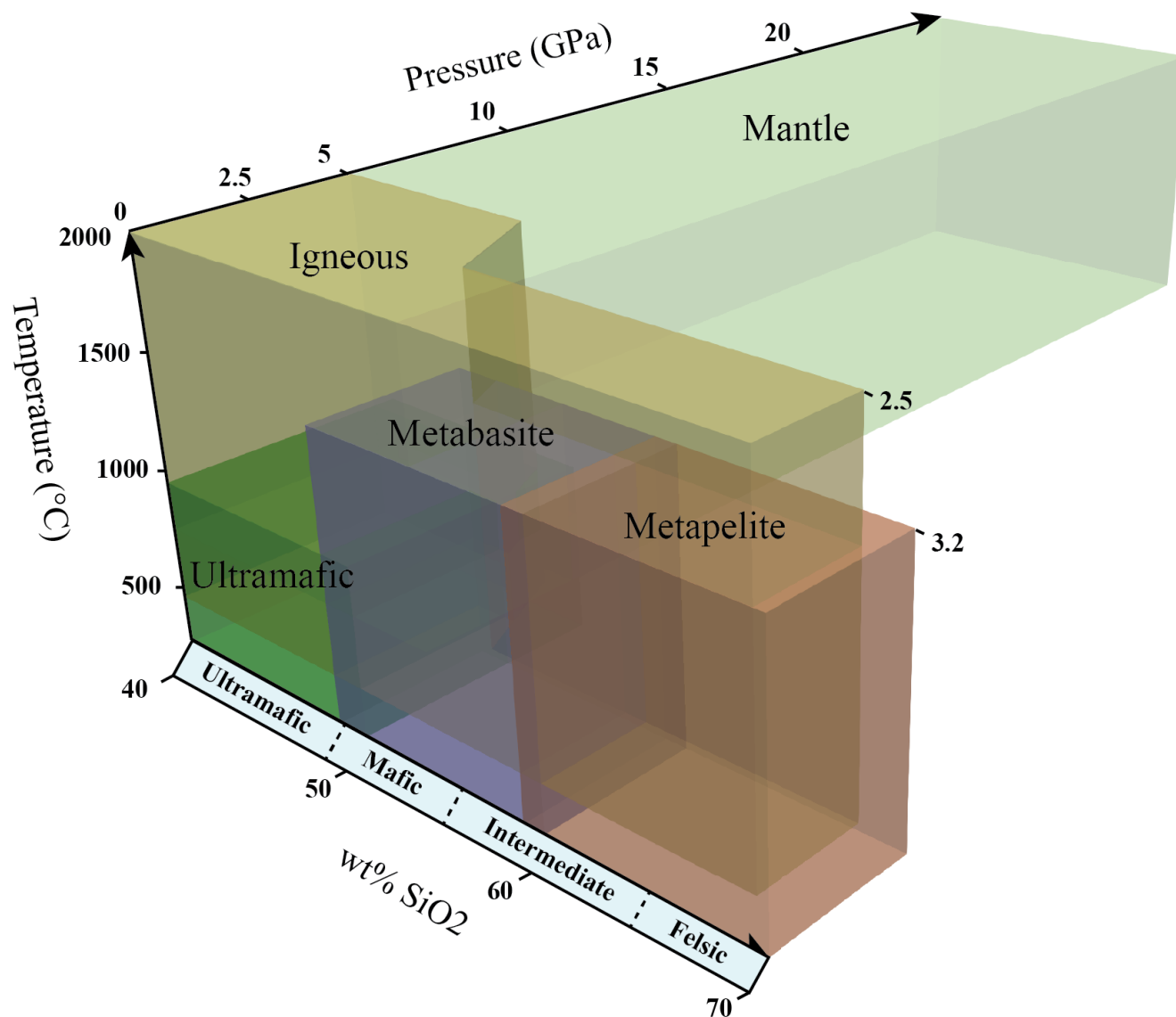
In the top-left
→ “export for LaMEM”



Now it can be added to your LaMEM julia script as `rho_ph = “SM89_oxidised...”`

- 3-4 refinements are enough for a LaMEM density diagram
- Can be done for any custom rock composition and PT conditions
- Make sure you use the right database
- Set minimum pressure > 0.0, e.g. 0.01!
- If your LaMEM simulation goes outside the computed diagram range, it will extrapolate the density from the used phase diagram

MAGEMin – how to choose database



Upper mantle density diagram (Peridotite.in)

