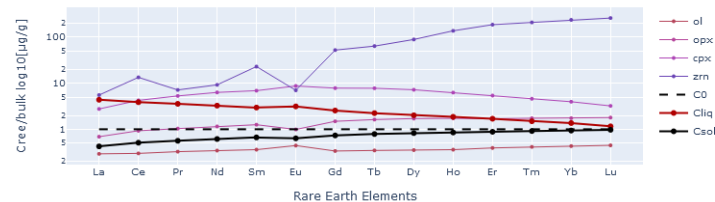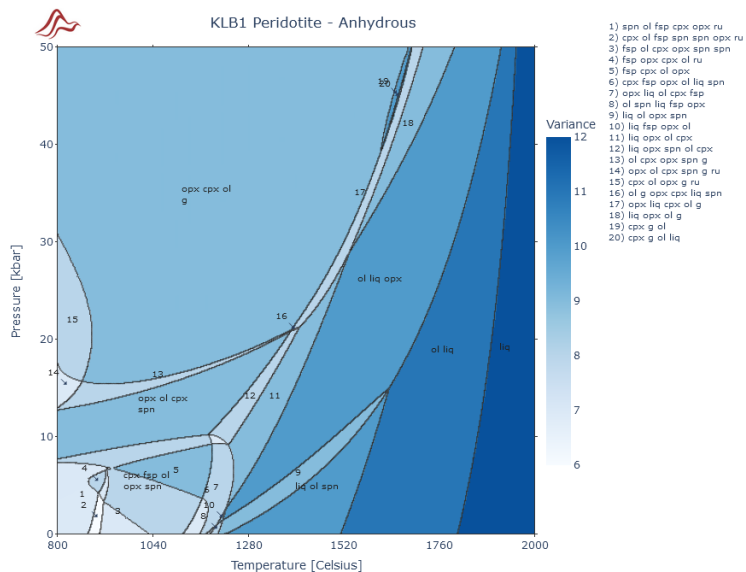# Phase Equilibrium Modelling with MAGEMin

Nicolas Riel - Johannes-Gutenberg University Mainz, Germany   nriel@uni-mainz.de
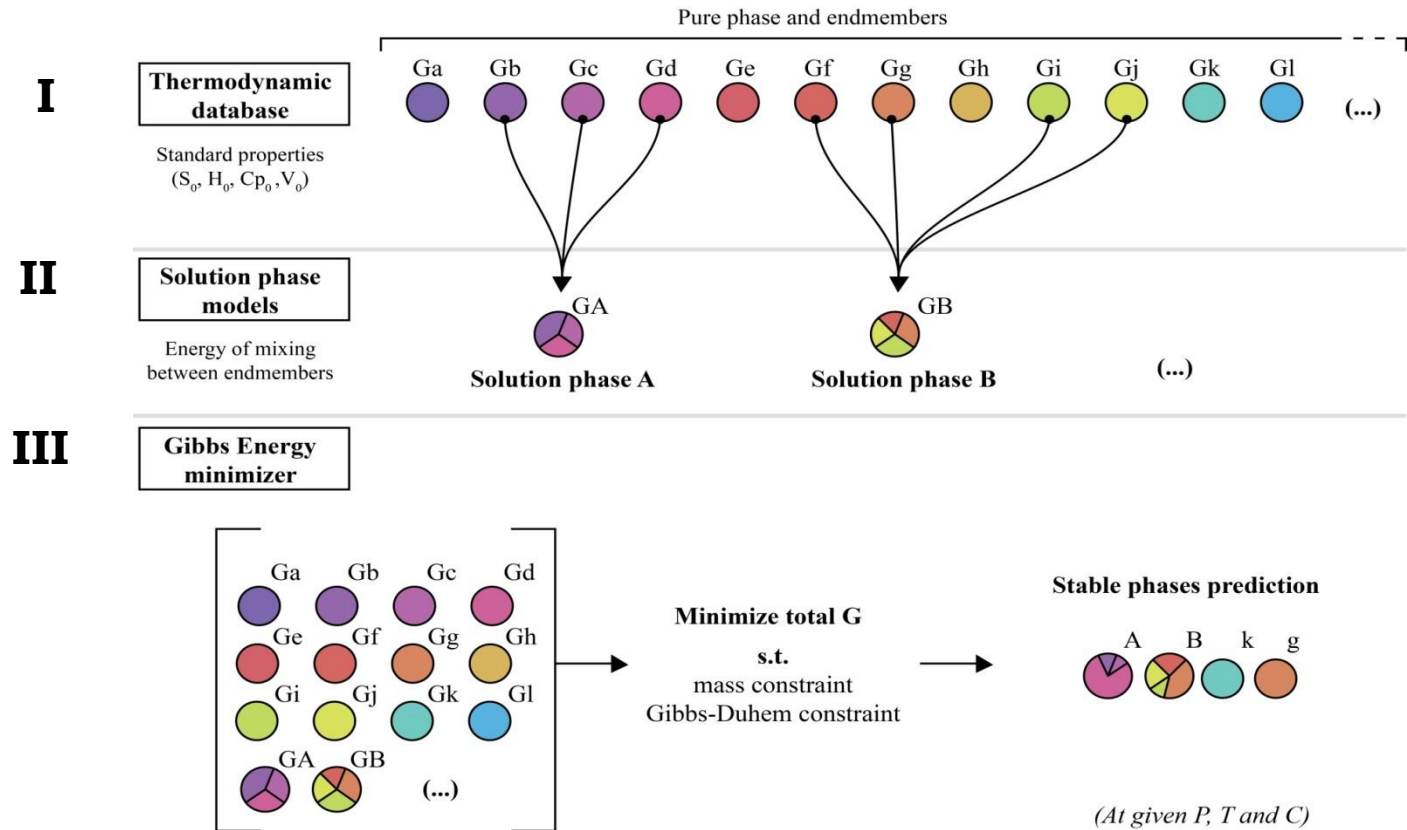
Overview

o General introduction and rationales

o Benchmarks and MAGEMin packages

o MAGEMinApp

o MAGEMin_C

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

How to compute a stable phase equilibrium?

I — Thermodynamic database. Standard properties (S_0, H_0, Cp_0, V_0)

Pure phase and endmembers: Ga, Gb, Gc, Gd, Ge, Gf, Gg, Gh, Gi, Gj, Gk, Gl (...)

e.g.,
tc-ds6xx.txt for TC
hp02ver.dat for Perple_X

II — Solution phase models. Energy of mixing between endmembers

GA — Solution phase A
GB — Solution phase B
(...)

III — Gibbs Energy minimizer

Ga Gb Gc Gd
Ge Gf Gg Gh
Gi Gj Gk Gl
GA GB (...)

Minimize total G
s.t.
mass constraint
Gibbs-Duhem constraint

Stable phases prediction
A   B   k   g

(At given P, T and C)

3

Why a new Gibbs free energy minimizer?

Perple_X

o   Developed (in the 90's) to produce phase diagrams

o   Natively not parallel

o   Minimizations can often fail

o   Not optimized for solution update

o   Difficult to couple to geodynamic codes (written in Fortran)

MAGEMin: current stage and ongoing developments

Current stage

- MPI parallel C-library with several built-in database
(White et al., 2014; Green et al., 2016; Holland et al., 2018; Evans & Forst, 2021)

- Low memory usage < 10 Mb

- Julia wrapper for petrological/geodynamic coupling (MAGEMin_C)

- Parallel web-browser Julia app (MAGEMinApp)

- Single core performance
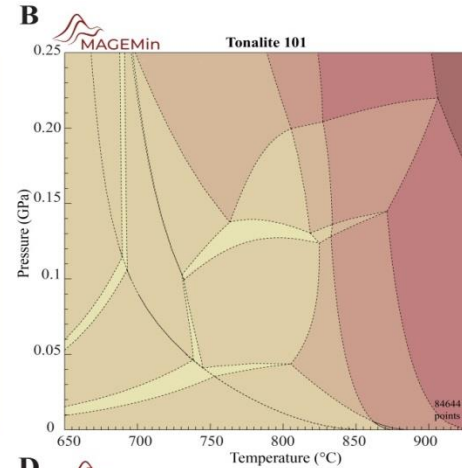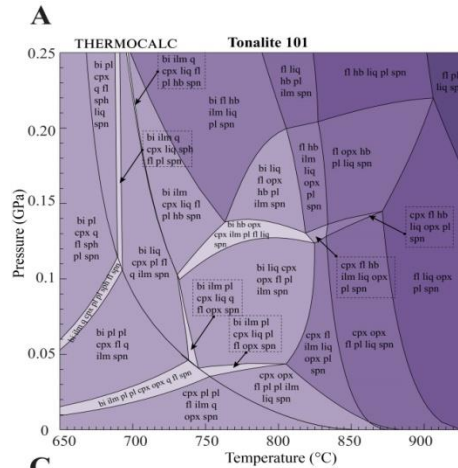 ~10 to 150 ms without initial guess (scales with #oxides and #phases)

Ongoing development

- Mantle dataset (Stixrude & Lithgow-Bertelloni, 2011)
- Algorithm upgrade to improve performances and stability (paper to be submitted)
- Use of initial guess to drastically improve performance (~ tenfold)

- Full Julia version
  Better performances and flexibity (custom solution phase model,
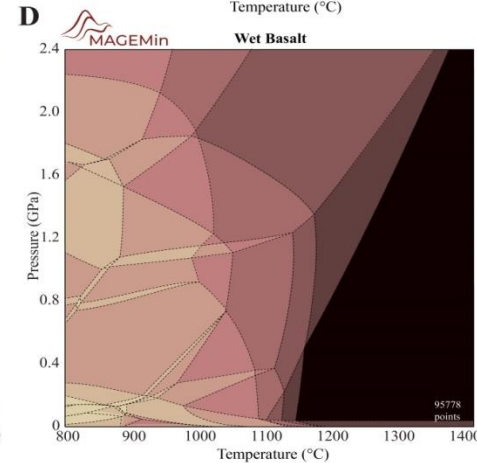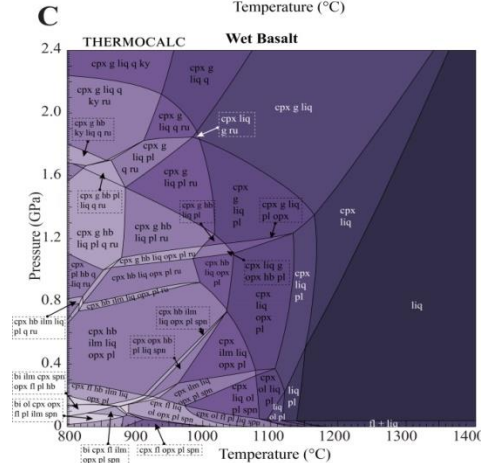 inversion framework for calibration etc.)

o   NCKFMASHTCrO system, using the igneous database of Holland et al. (2018)

Tonalite
fluid oversaturated

Wet Basalt
fluid saturated

(Riel et al., 2022)

o NCKFMASTCrO system, using the igneous database of Holland et al. (2018)

- Computed in parallel on personal laptop
- Using only 3 cores

MAGEMin

- MPI-parallel C code
- Point-wise minimization at given P-T-X

- Metapelite (White et al., 2014)
- Metabasite (Green et al., 2016)
- Igneous (Holland et al., 2018)
- Ultramafic (Evans & Forst, 2021)
- Mantle (Stixude & Lithgrow-Bertelloni, 2010)

(Mineral Assemblage Gibbs Energy Minimization)

MAGEMin_C

- Julia wrapper of the C code
- Flexible programming interface
- Database calibration
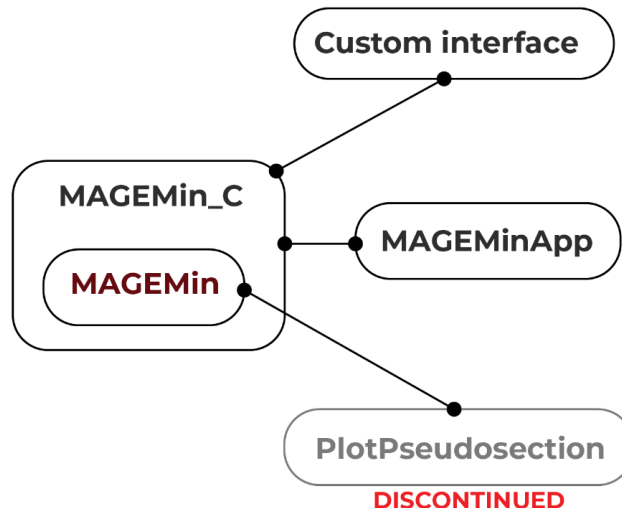- Geodynamic coupling

MAGEMinApp

- Web browser app (graphic user interface)
- Parallel point-wise minimization
- PT, PX, TX and PT-X phase diagrams
- Auto labelling, contouring
- Fractional melting/crystallization paths

PlotPseudosection

- Matlab app (Graphic user interface)
- Parallel point-wise minimization
- PT, PX, TX diagrams
- Contouring
- PT paths
- Trace element partitioning for mafic to ultramafic systems

E.G., GEODYNAMIC COUPLING

Custom interface

MAGEMin_C

MAGEMin

MAGEMinApp

PlotPseudosection

DISCONTINUED

MAGEMin framework

MAGEMin

- MPI-parallel C code
- Point-wise minimization at given P-T-X

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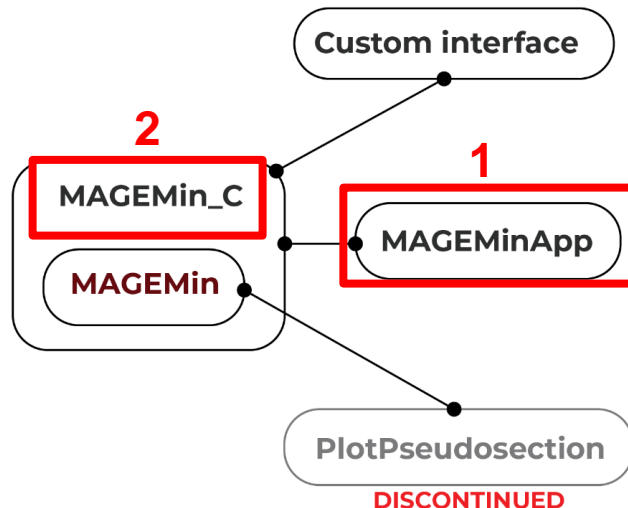- Database calibration
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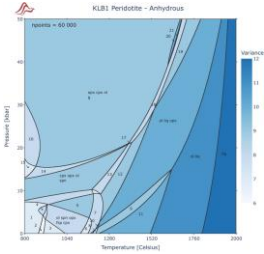
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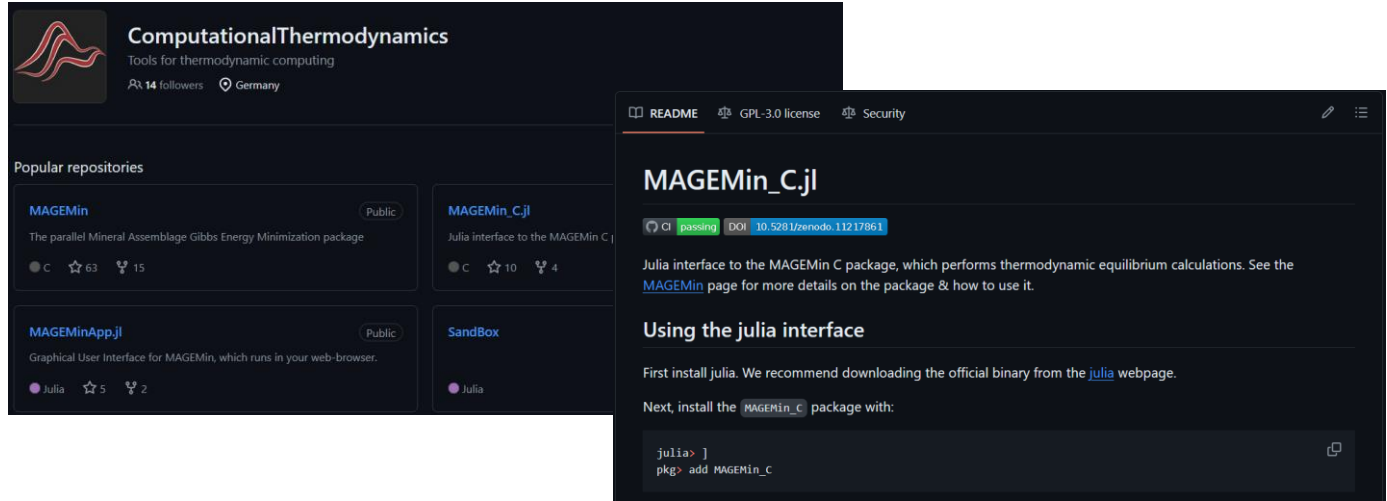 mafic to ultramafic systems

E.G., GEODYNAMIC COUPLING

Custom interface

2

MAGEMin_C

1

MAGEMin   **MAGEMinApp**

PlotPseudosection

DISCONTINUED

nriel@uni-mainz.de

https://github.com/ComputationalThermodynamics
https://github.com/ComputationalThermodynamics/MAGEMin_C.jl
https://github.com/ComputationalThermodynamics/MAGEMinApp.jl
https://github.com/ComputationalThermodynamics/Resources/GG2024

- **Do not hesitate to contact me if anything is wrong/broken or needs to be added**
  I cannot correct bugs or add new options if I am unaware of them!

- **Everything is open source: you can contribute by creating pull-requests on Github!**