JOHANNES GUTENBERG UNIVERSITÄT MAINZ · MAGMA Consolidator Grant Project · erc European Research Council · Granulites & Granulites 2024 · MAGEMin

Phase Equilibrium Modelling with MAGEMin

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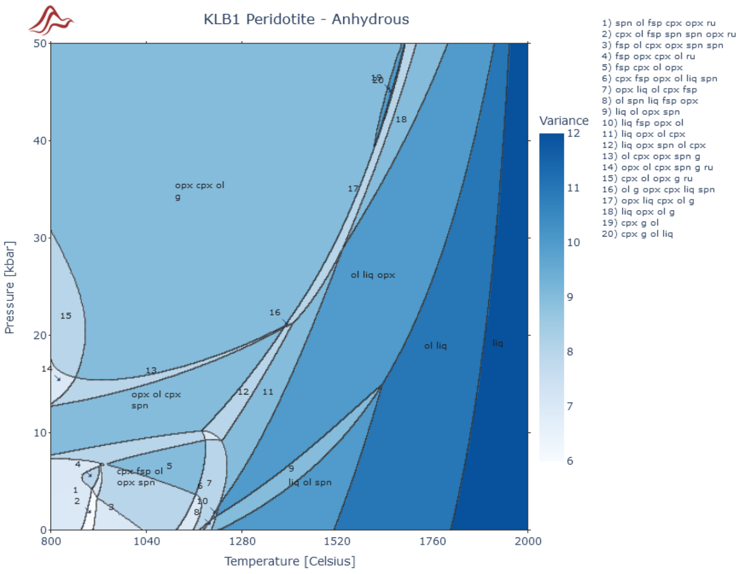
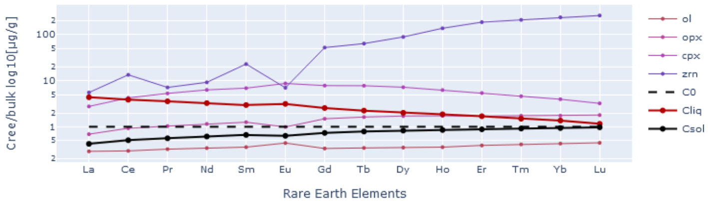
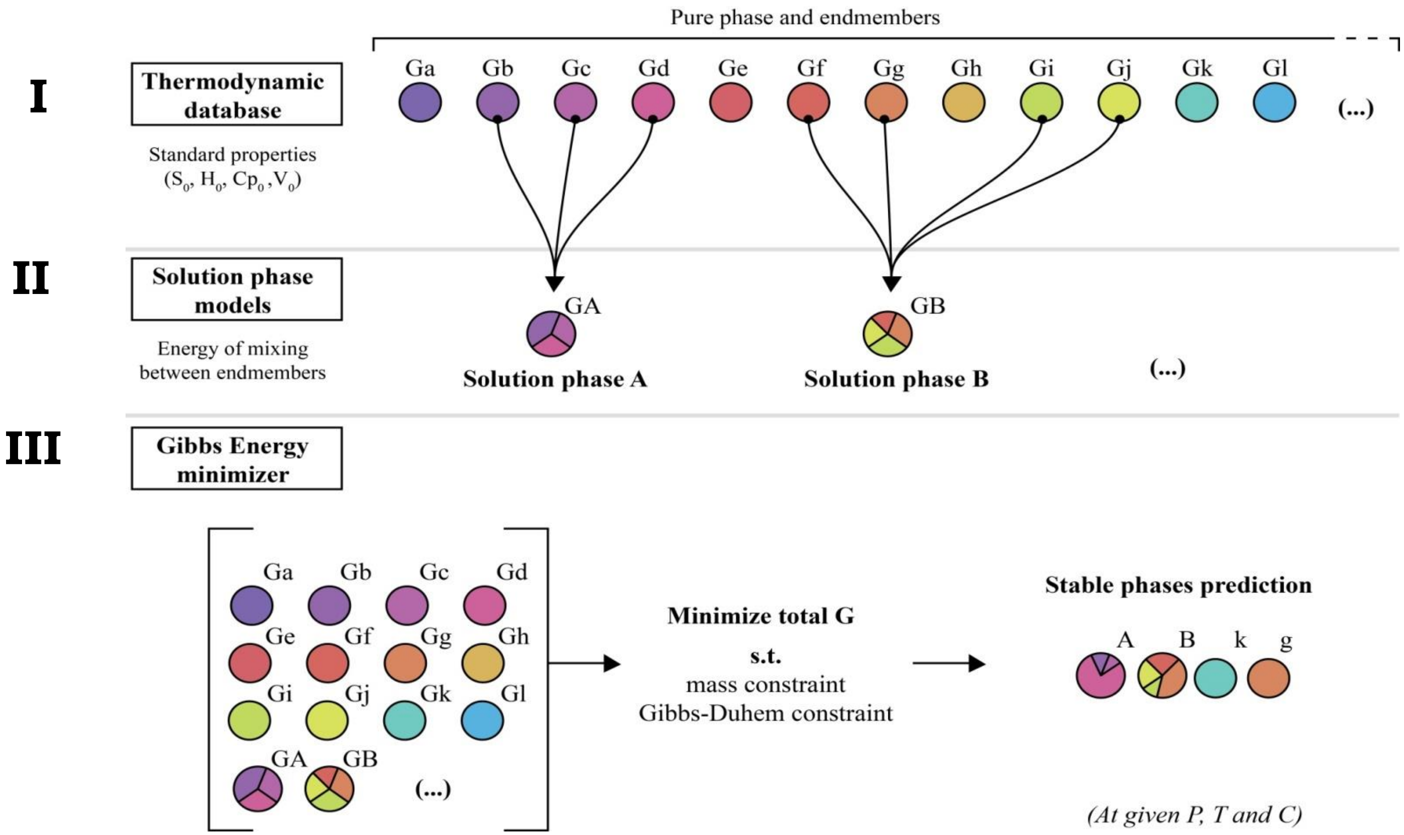




Overview

- General introduction and rationales
- Benchmarks and MAGEMin packages
- MAGEMinApp
- MAGEMin_C

How to compute a stable phase equilibrium?



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

Why a new Gibbs free energy minimizer?

Perple_X

Theriak - Domino

MELTS

- Developed (in the 90's) to produce phase diagrams
- Natively not parallel
- Minimizations can often fail
- Not optimized for solution update
- 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)

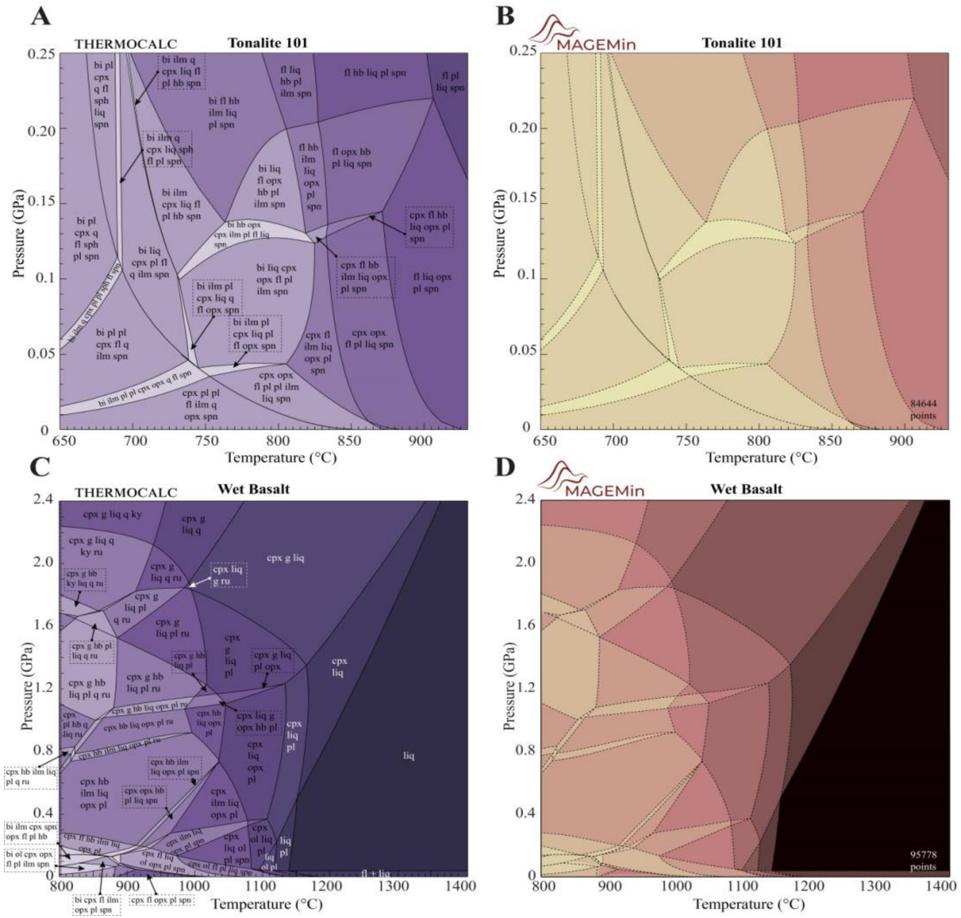
- Full Julia version
  Better performances and flexibity (custom solution phase model, inversion framework for calibration etc.)

Application to magmatic system – wet system benchmark

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

Tonalite
fluid oversaturated

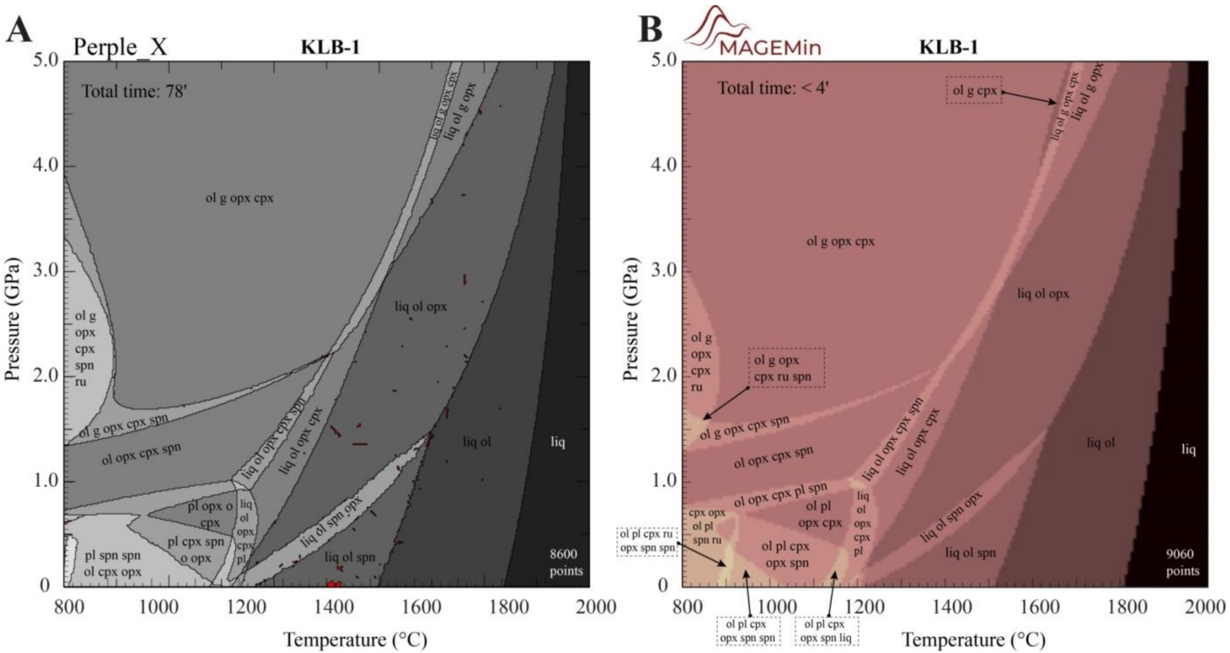
Wet Basalt
fluid saturated



(Riel et al., 2022)

Computational efficiency

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



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

MAGEMin framework

(Mineral Assemblage Gibbs Energy Minimization)

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)

MAGEMin_C

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

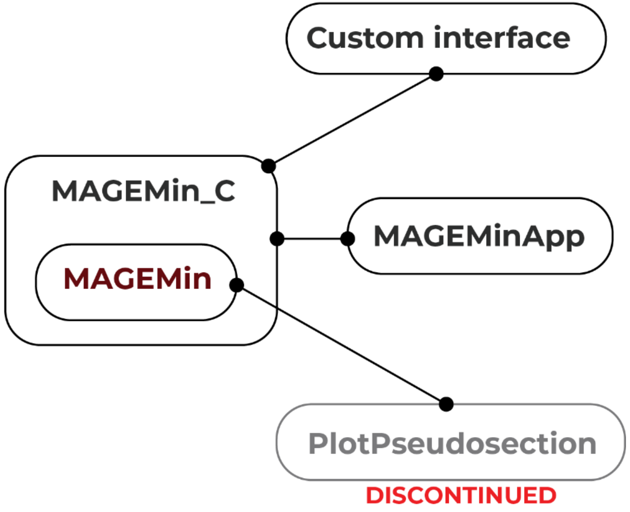
MAGEMinApp

- 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



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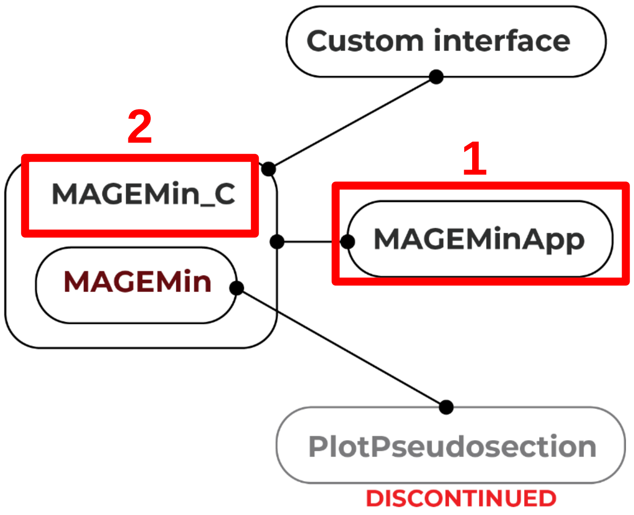
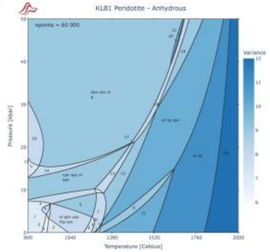


MAGEMin Github: ComputationalThermodynamics



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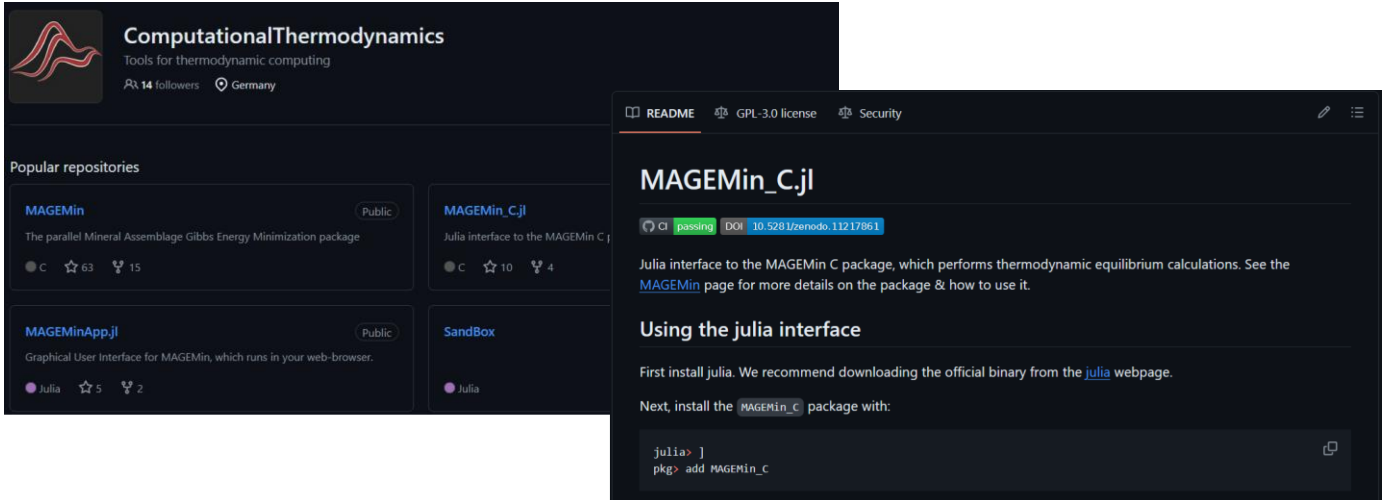

https://github.com/ComputationalThermodynamics
https://github.com/ComputationalThermodynamics/MAGEMin_C.jl
https://github.com/ComputationalThermodynamics/MAGEMinApp.jl
https://github.com/ComputationalThermodynamics/Resources/GG2024

- **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!**