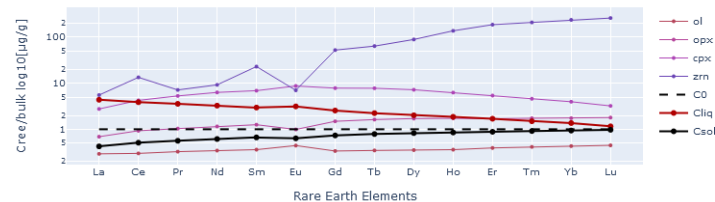
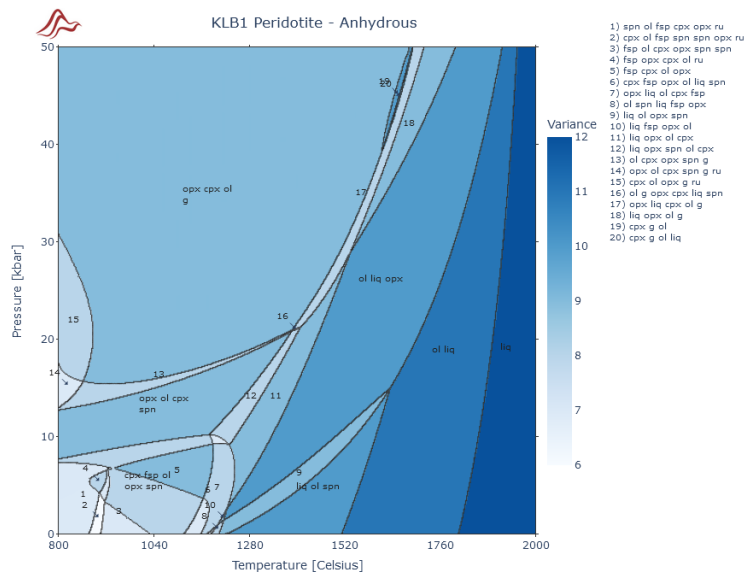


# Phase Equilibrium Modelling with MAGEMin

Nicolas Riel - Johannes-Gutenberg University Mainz, Germany [nriel@uni-mainz.de](mailto:nriel@uni-mainz.de)



# Overview

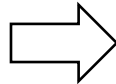
- General introduction and rationales
- The Gibbs free energy minimization problem
- Benchmarks and MAGEMin packages
- MAGEMinApp
- MAGEMin\_C

# Thermodynamic equilibrium – stable phases

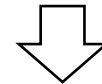
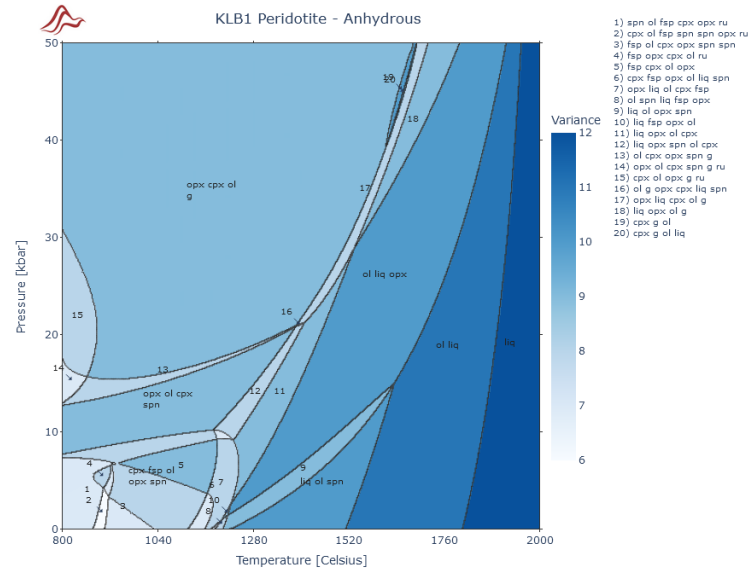
- Pressure
- Temperature
- Composition
- Thermodynamic database (minerals/melt)



**Gibbs free energy minimization**

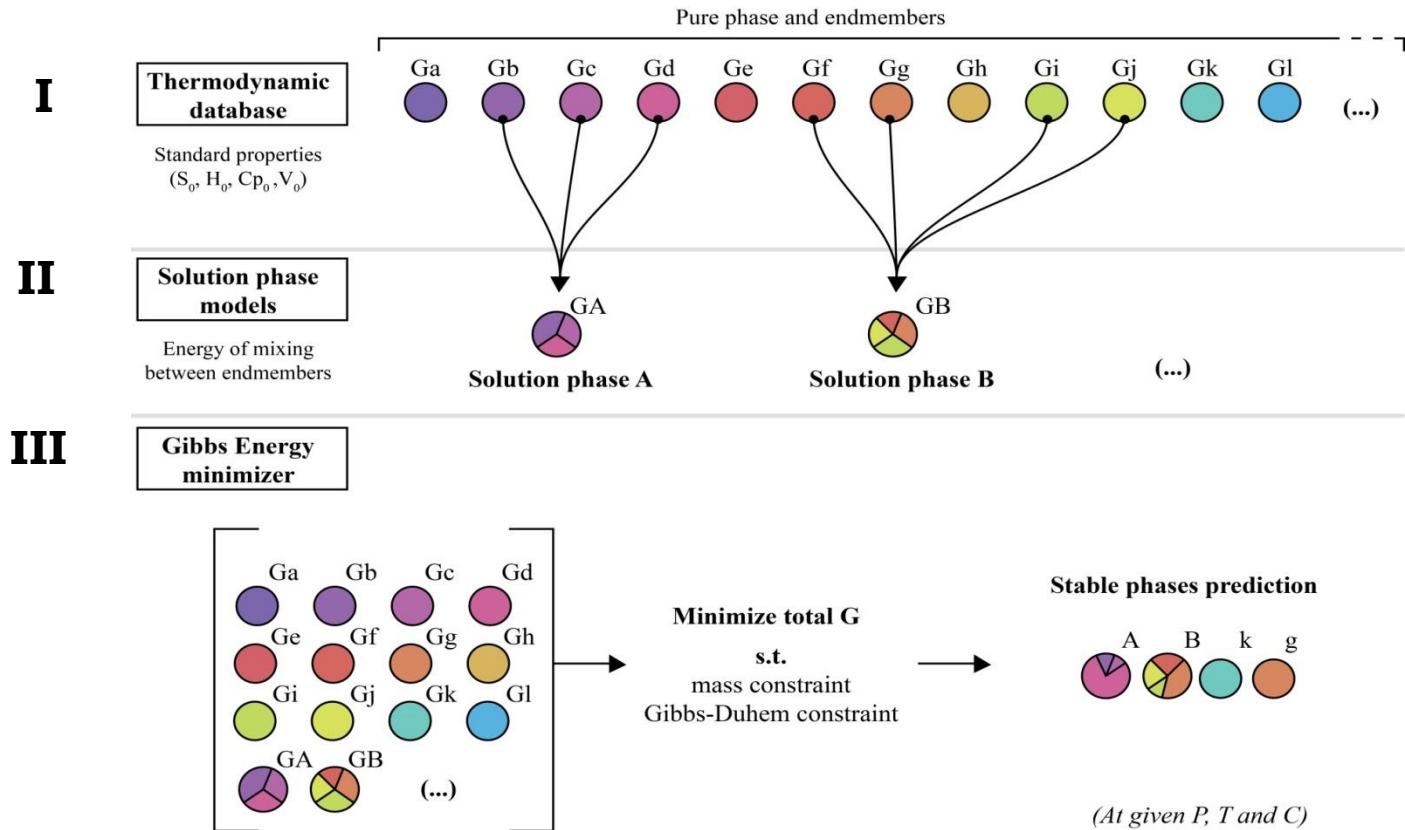


- Perple\_X
- MELTS
- Theriak-Domino
- GeoPS



- Stable phases
- Phase fractions
- Solid/fluid/melt densities
- Seismic velocities, expansivity...

# 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**



**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)



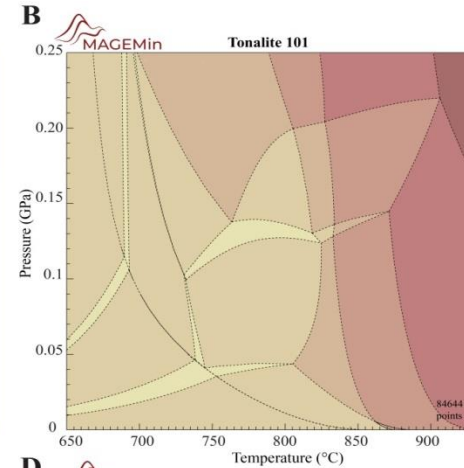
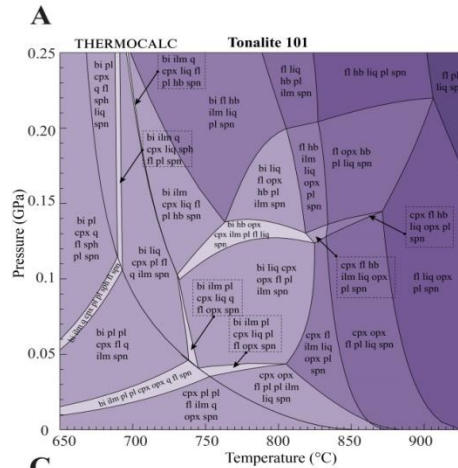
## Ongoing development

- 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 flexibility (custom solution phase model, inversion framework for calibration etc.)

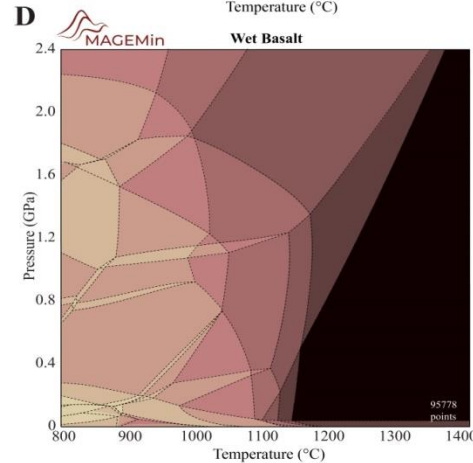
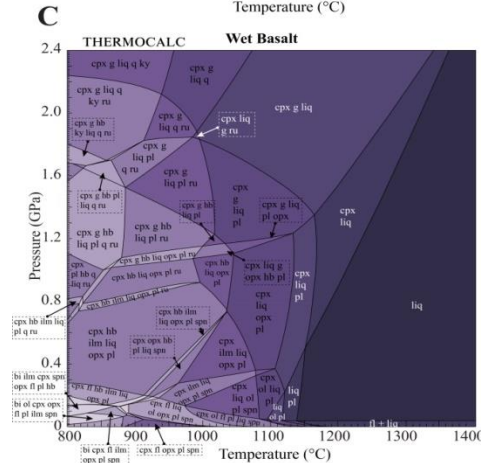
# Application to magmatic system – wet system benchmark

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

**Tonalite**  
fluid oversaturated



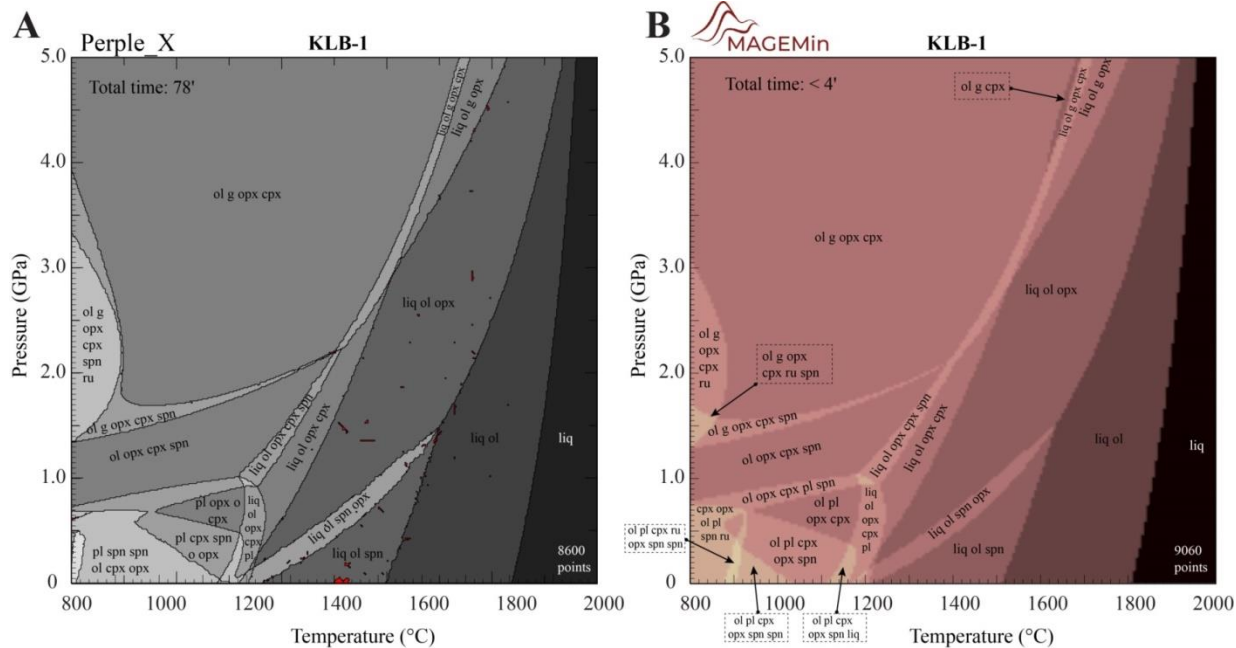
**Wet Basalt**  
fluid saturated



(Riel et al., 2022)

# Computational efficiency

- NCKFMASCrO 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 & Lithgow-Bertelloni, 2010)

## MAGEMin\_C



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

## MAGEMinApp



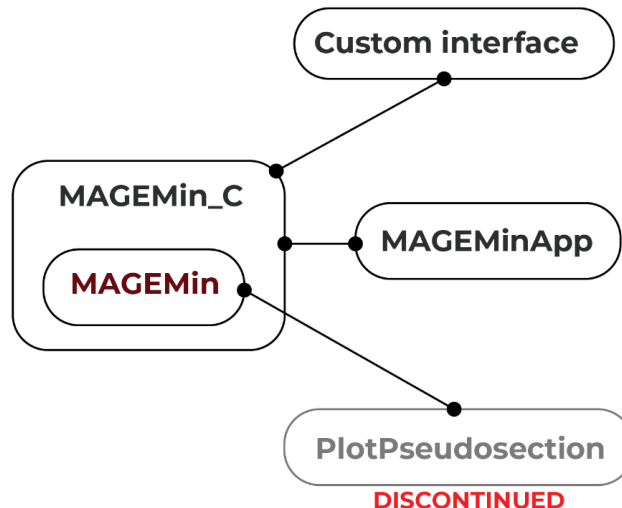
- Web browser app (graphic user interface)
- Parallel point-wise minimization
- PT, PX, TX and PT-X phase diagrams
- Auto labelling, contouring
- Fractional melting/crystallization paths

## 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



# MAGEMin framework

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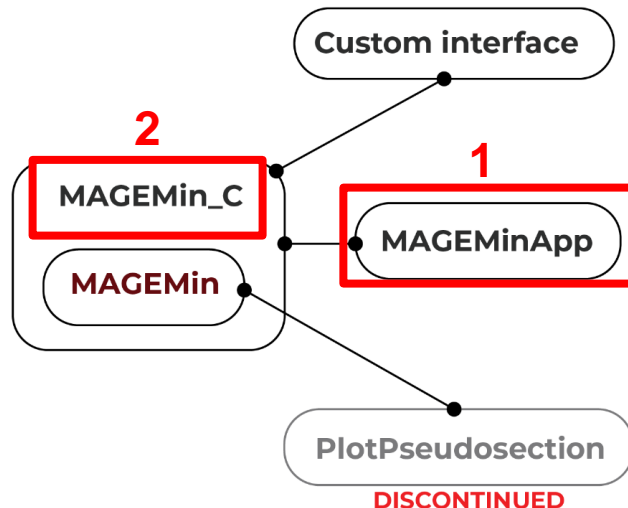
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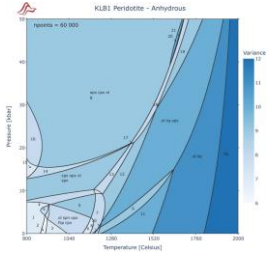


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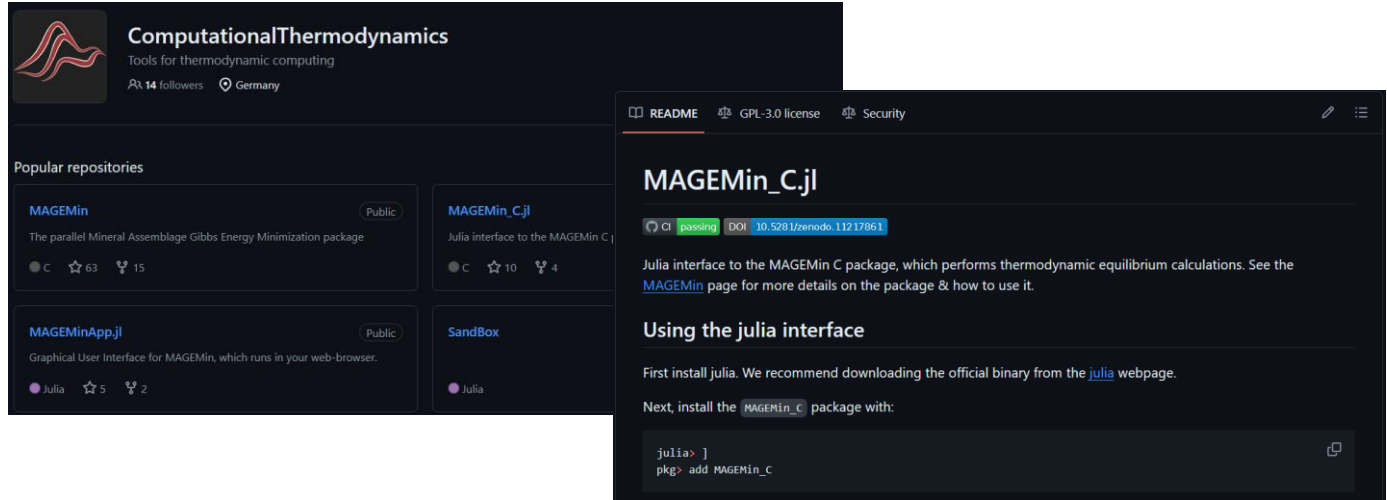
E.G., GEODYNAMIC COUPLING



# MAGEMin Github: ComputationalThermodynamics



nriel@uni-mainz.de



<https://github.com/ComputationalThermodynamics>

[https://github.com/ComputationalThermodynamics/MAGEMin\\_C.jl](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!**