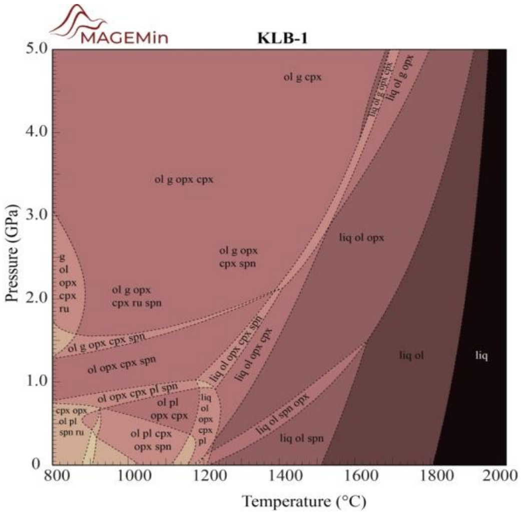
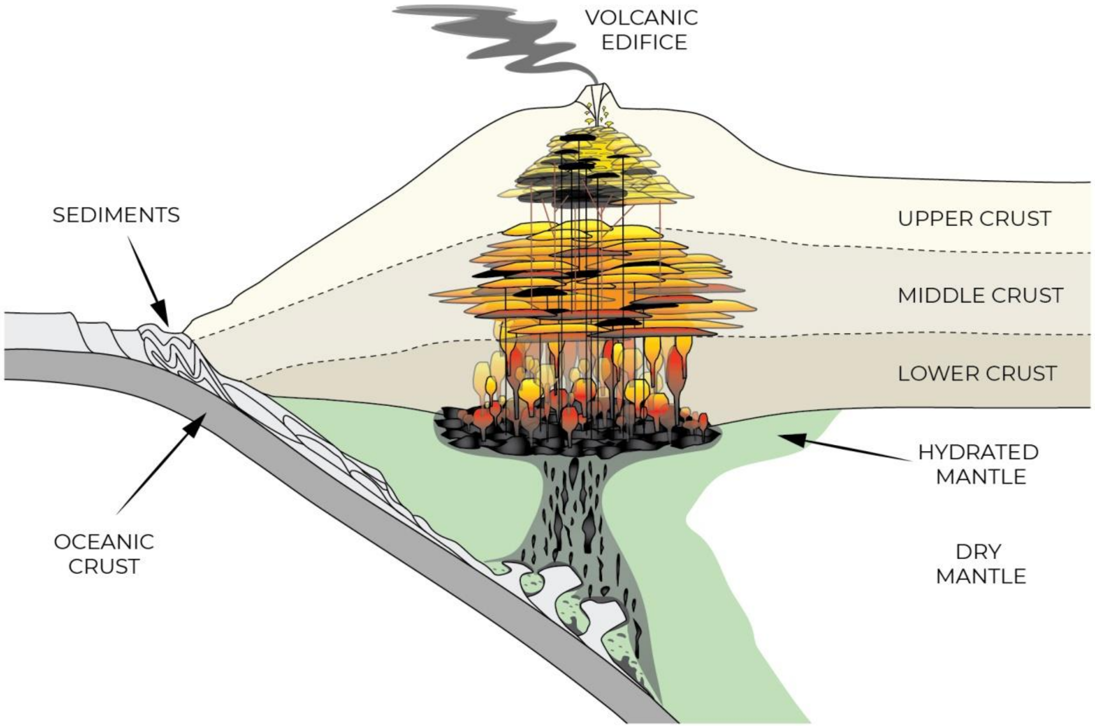
MAGEMin, an efficient Gibbs energy minimizer: application to magmatic systems

Nicolas Riel[1], Boris Kaus[1], Eleanor Green[2] and Nicolas Berlie[1]



1. *Johannes-Gutenberg University Mainz, Germany*
2. *Melbourne University, Melbourne, Australia*

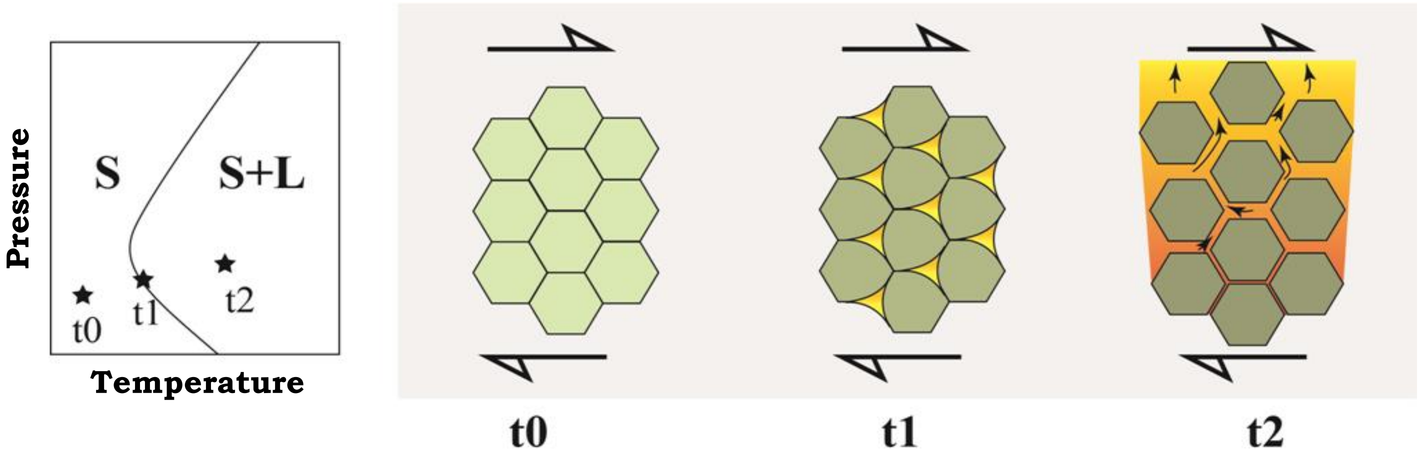
The magmatic refinery



(Modified after J. Cornet, ETH Zürich)

Schematic representation of
the exposed Famatinian magmatic arc
Sierra de Valle Fértil, Argentina

Introduction – Reactive magma transport model



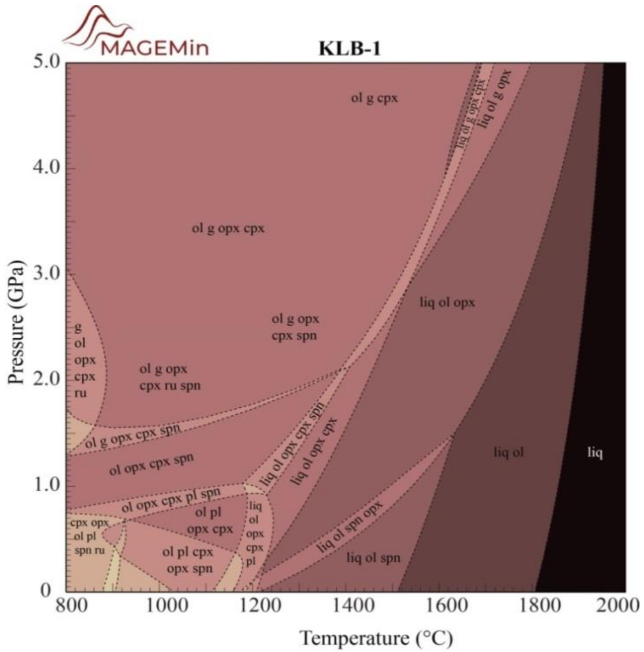
- Thermomechanical deformation (visco-elasto-plastic)
- Two-phase flow (magma segregation)
- **Thermodynamics** **(stable phases)**

Thermodynamic equilibrium – stable phases

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

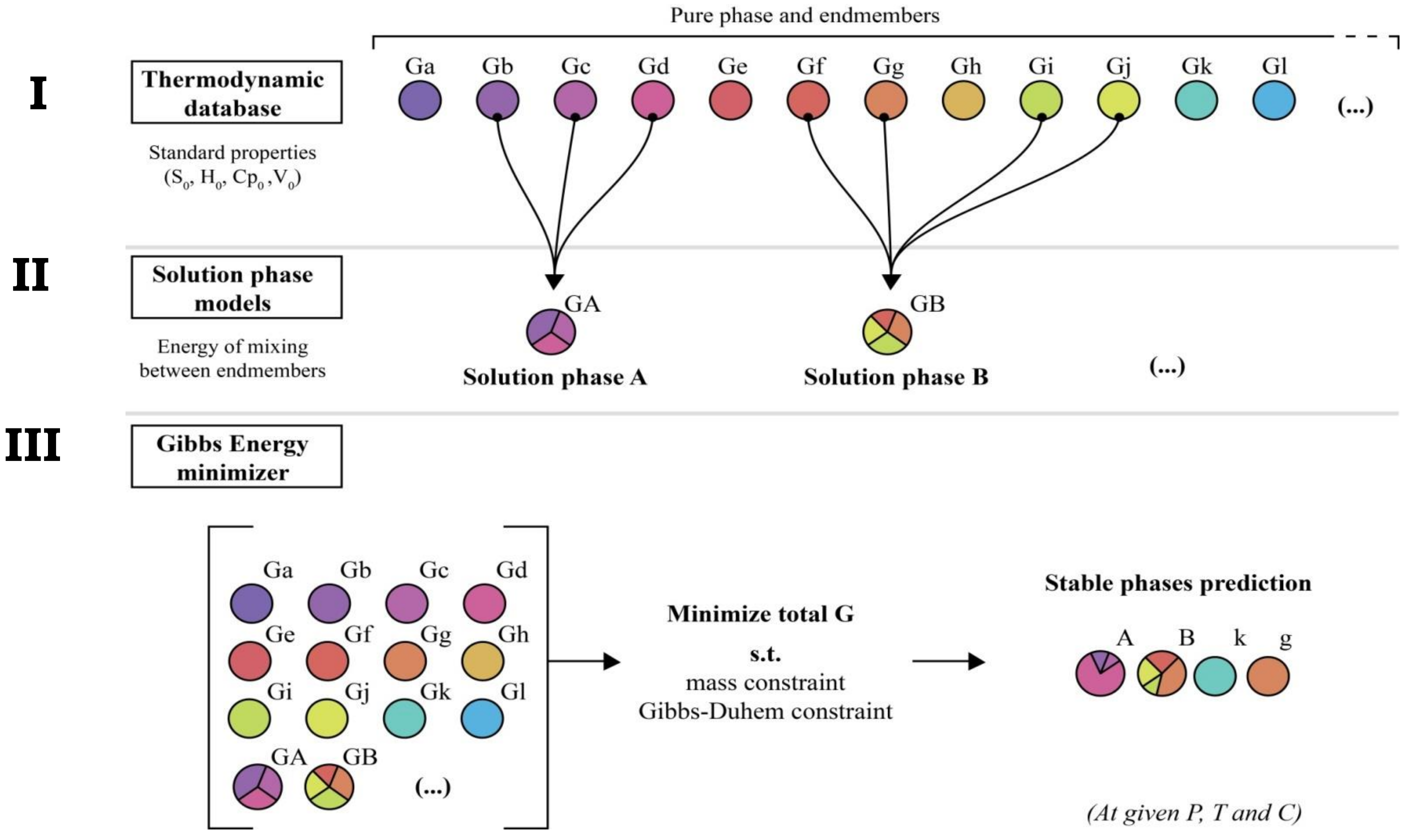
Gibbs free energy minimization

- Perple_X
- MELTS
- Theriak-Domino



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

Components of stable phase prediction



Why another Gibbs energy minimizer?

Available Gibbs energy Minimizer

Perple_X

Theriak-Domino

MELTS

Developed to produce phase diagrams

- Not/partially parallelized
- Relatively slow and/or unstable (often ‘crashes’)
- Cannot be directly coupled to geodynamic simulations
- Not optimized to update solution under slight *P*-*T*-*C* changes
- Lot of work to add new database

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Constraints on a minimizer for magmatic modelling

○ Open source and code efficient	- C language
○ Built-in database	- No input files
○ Fully parallel for scalability	- MPI
○ Easily callable by external software	- Executable or C-wrapper
○ Fast and stable	
○ Incorporate most recent thermodynamic database	- e.g., Holland et al., 2018

Gibbs free energy minimization: a challenging optimization problem

- *Given a set of minerals at given P, T and C*

Minimize
(at fixed P,T,C)

$$G_{\text{sys}} = \underbrace{\sum_{\lambda=1}^{\Lambda} \alpha_\lambda \sum_{i=1}^{N_\lambda} \mu_{i(\lambda)} p_{i(\lambda)}}_{\substack{\textit{Solution phase} \\ \textit{(e.g. olivine)}}} + \underbrace{\sum_{\omega=1}^{\Omega} \alpha_\omega \mu_\omega}_{\substack{\textit{Pure phase} \\ \textit{(e.g. quartz)}}},$$

where

$$\mu_{i(\lambda)} = g^0_{i(\lambda)} + RT \log(idm_{i(\lambda)}) + g^{\text{ex}}_{i(\lambda)}$$

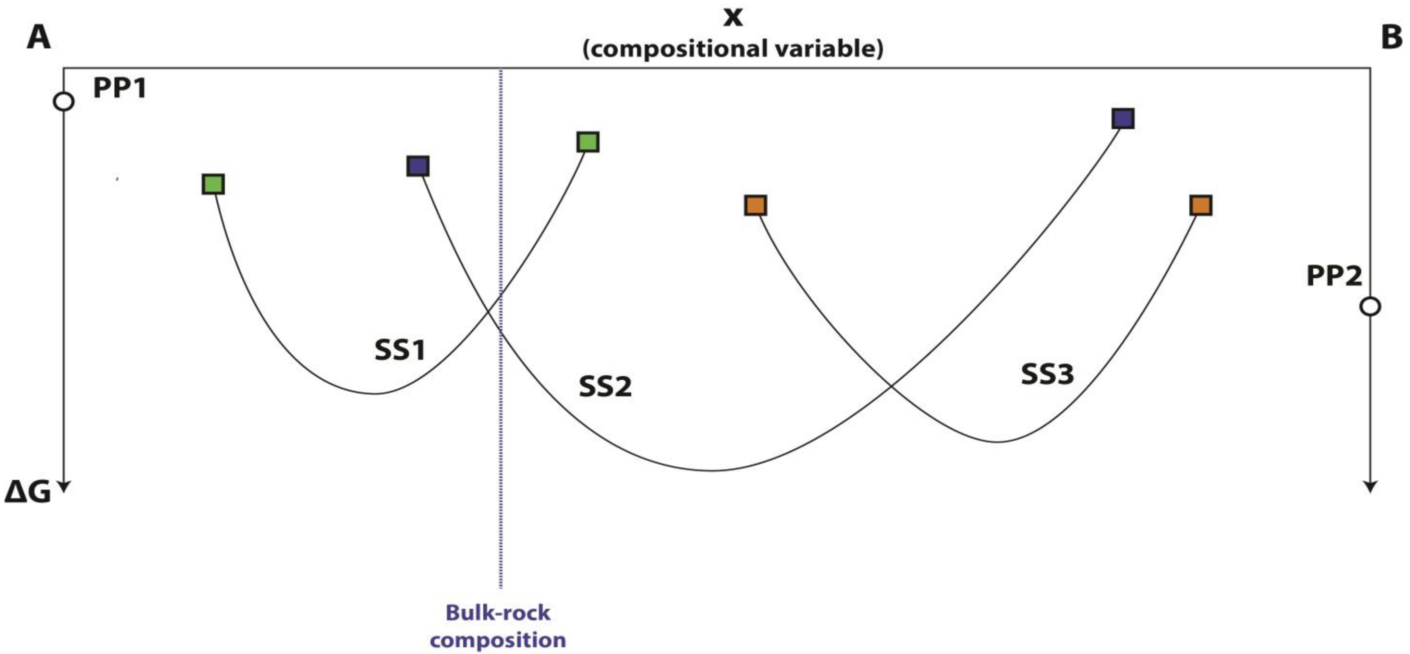
s.t.
Mass constraint

$$\sum_{\lambda=1}^{\Lambda} \alpha_\lambda \sum_{i=1}^{N_\lambda} a_{ij} p_{i(\lambda)} + \sum_{\omega=1}^{\Omega} \alpha_\omega a_{\omega j} - b_j = 0,$$

And Gibbs-Duhem
constraint

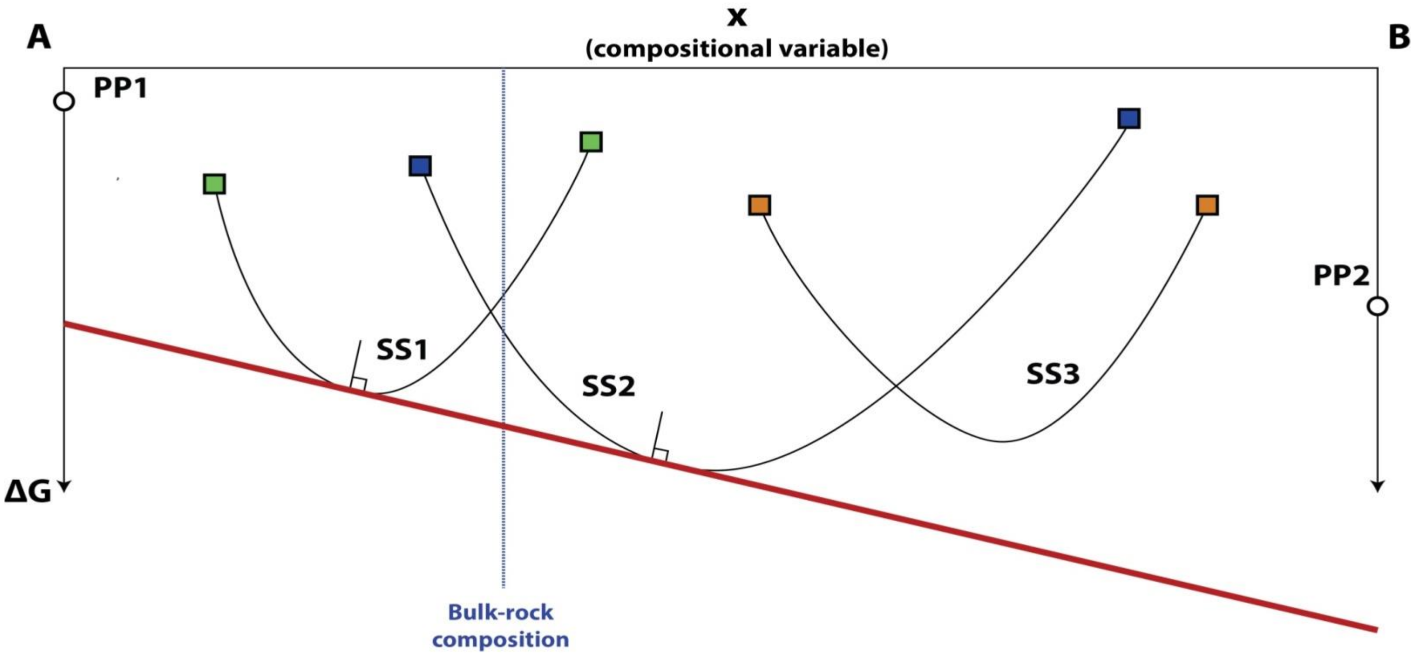
$$\mu_{i(\lambda),\omega} = \sum_{j=1}^{C} a_{i,\omega j} \Gamma_j,$$

Phase equilibria : an optimization problem



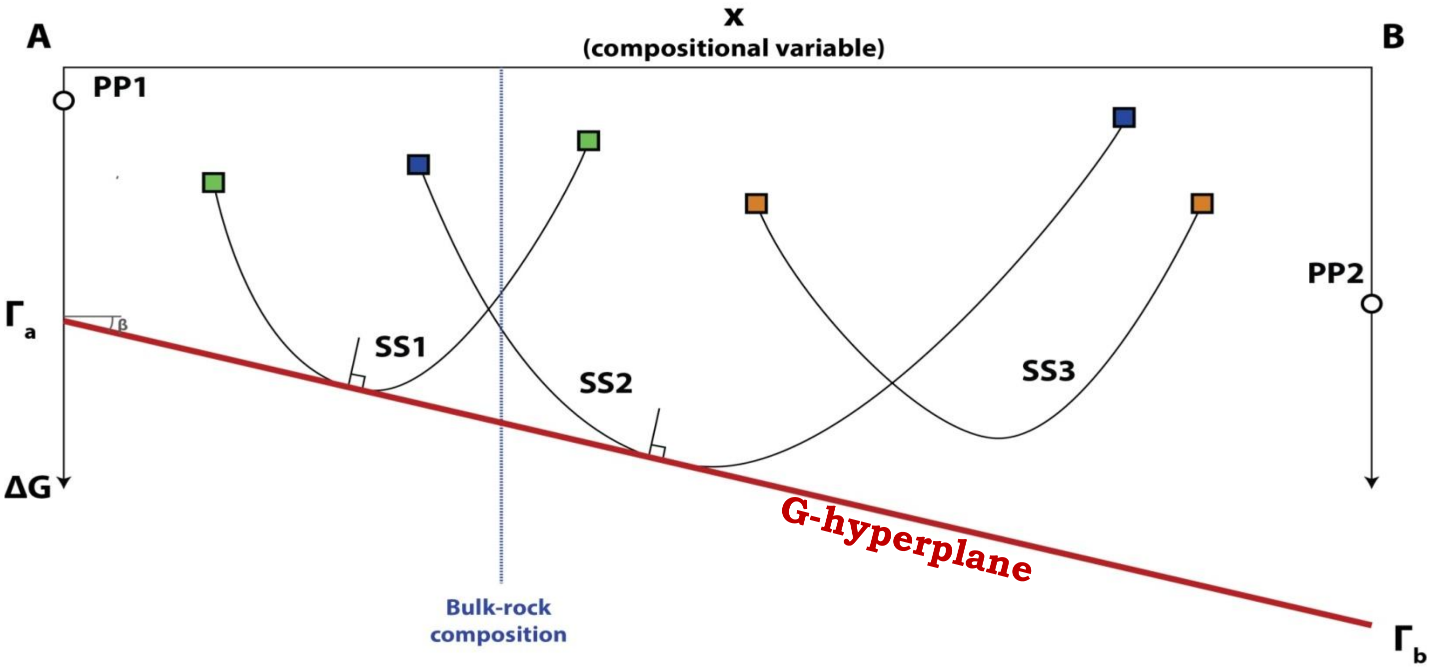
At fixed P-T conditions

Phase equilibria : an optimization problem



At fixed P-T conditions

Phase equilibria : an optimization problem



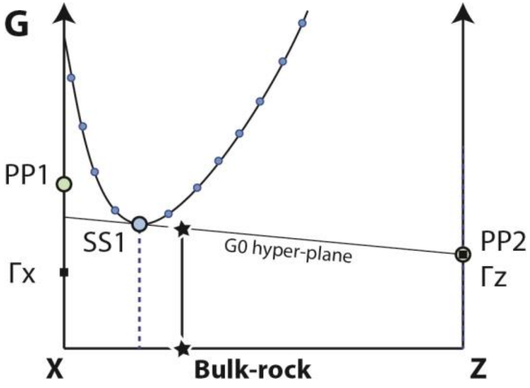
At fixed P-T conditions

Approaches to Gibbs free energy minimization

I. **Pseudocompounds** (Perple_X, Connolly)

- Discretized solution space
  (treat each point as pure phase)

- Simplex linear programming

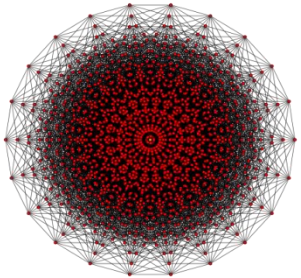


- Avoid local minimum
- Algorithm relatively easy to implement

- Slow for large multicomponent systems
- Massive memory usage

e.g., Amphibole discretization in 11D (10 points/dim)

→ **100 billion** pseudocompounds!

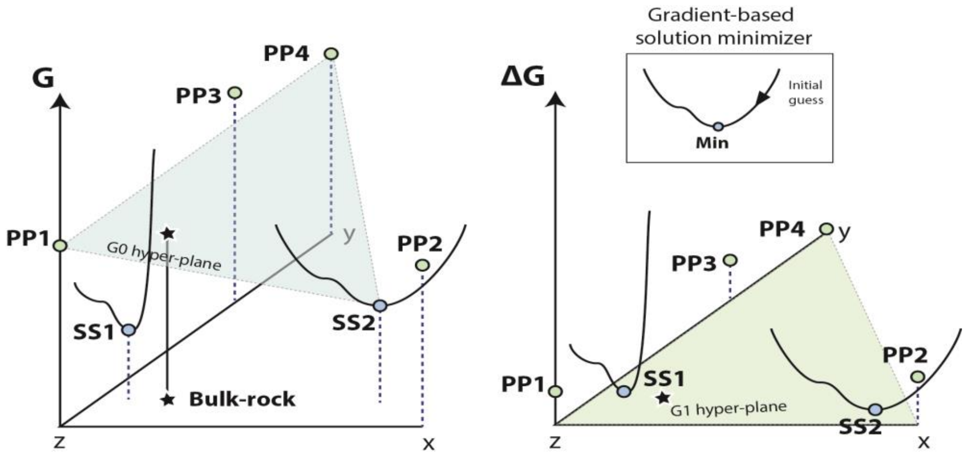


(11D hypercube, after Wikipedia)

II. **Levelling** (Theriak-Domino, de Capitani)

- Consider Endmembers as pure phases
- Simplex approach to estimate Γ
- Minimize solution phases within Γ space

ITERATE



- Gradient based method
- Low memory usage

- Slow for complex systems
- Gibbs-Duhem contraint not coupled with mass constraint

Approaches to Gibbs free energy minimization

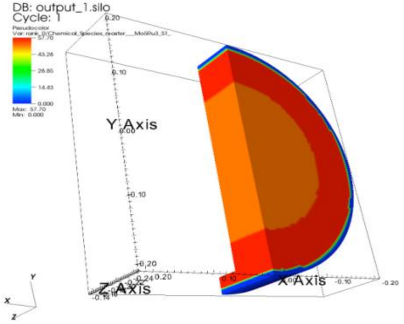
THERMOCHIMICA

III. Partitioning Gibbs energy (Piro et al., 2011, 2013)

- Coupled mass balance and Gibbs-Duhem constraint
- SLE solved with Newton-Raphson method

$$\left.\begin{aligned} \mu_i &= \frac{\tilde{\mu}_i}{RT} = g^{\circ}_{i(l)} + \ln(x_{i(l)}) + g^{\mathrm{ex}}_{i(l)} \\ \mu_i &= \sum_{j=1}^{C} a_{ij}\Gamma_j \end{aligned}\right\} x_{i(l)} = \exp\left(\sum_{j=1}^{C} a_{ij}\Gamma_j - g^{\circ}_{i(l)} - g^{\mathrm{ex}}_{i(l)}\right)$$

$$b_j = \sum_{l=1}^{\mathrm{L}} n_l \sum_{i=1}^{N_l} \exp\left(\sum_{j=1}^{C} a_{ij}\Gamma_j - g^{\circ}_{i(l)} - g^{ex}_{i(l)}\right) a_{ij} + \sum_{k=1}^{K} n_k a_{kj}$$



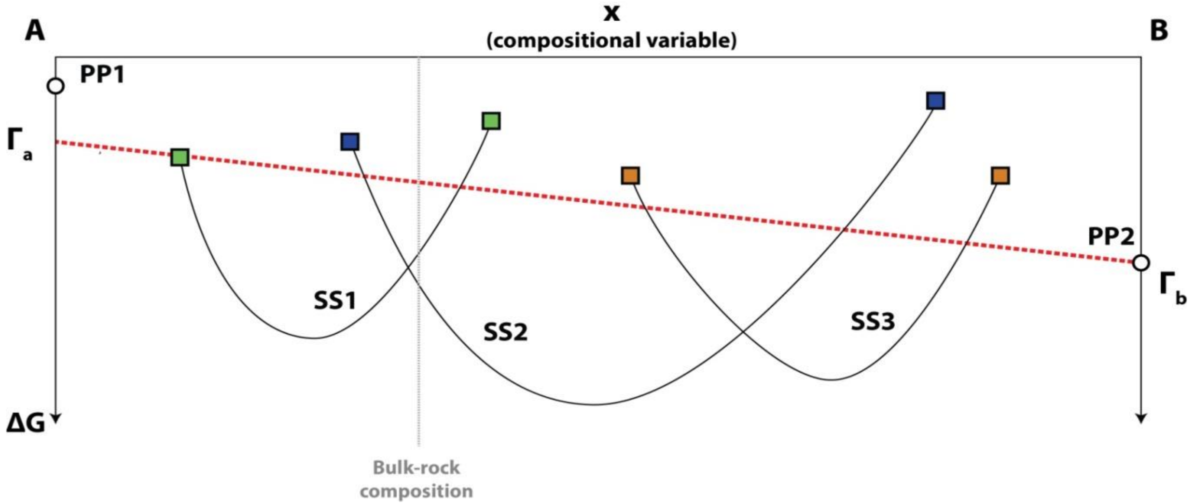
(Distribution of Mo5Ru3(s) in a 3D UO_2 fuel pellet, [Piro, 2011])

- Scales to large multicomponent systems (> 100)
- Mass balance is coupled with chemical potential
- Very efficient (developed for nuclear reactor simulations)
- Easily parallelized and memory efficient

- Cannot deal with complex mineral phases (Site-Fraction based)

MAGEMin: a three step Gibbs energy minimizer

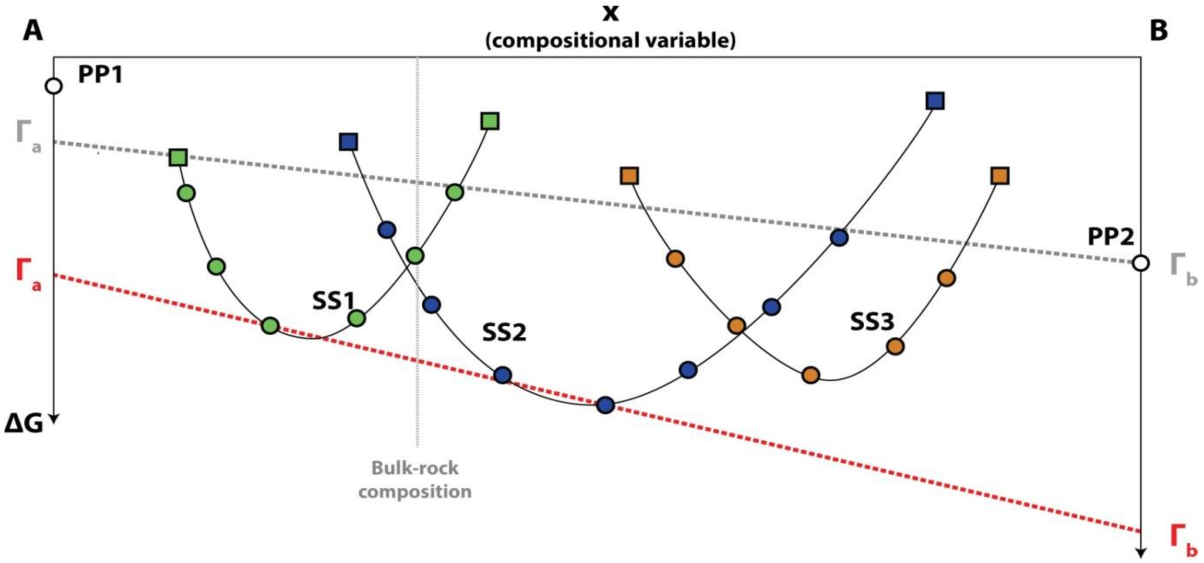
(1) Levelling using pure phases and solution endmembers



- Very low computational cost

MAGEMin: a three step Gibbs energy minimizer

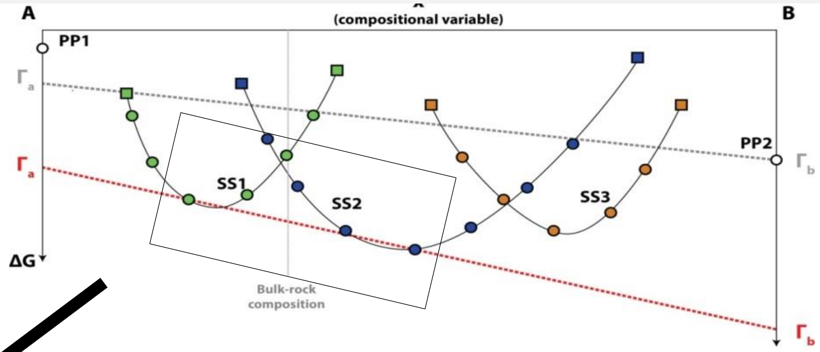
(2) Discretization under the G-hyperplane

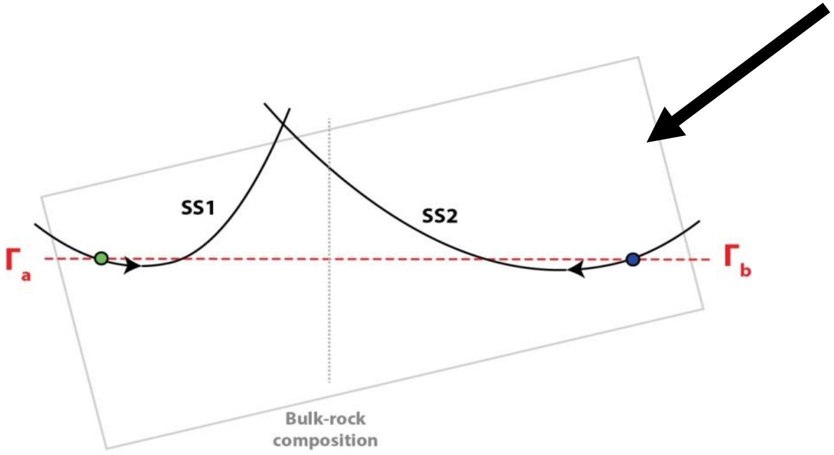


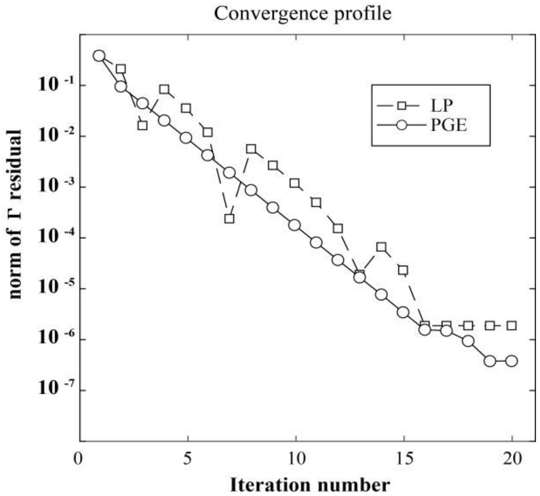
- Discretization under the G-hyperplane guess
- Avoid local minimum and computationally cheap

MAGEMin: a three step Gibbs energy minimizer

(3) Partitioning Gibbs Energy



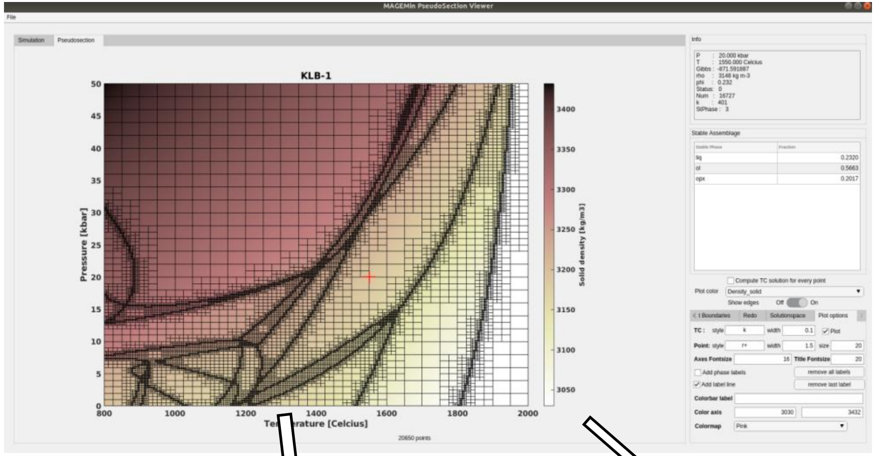


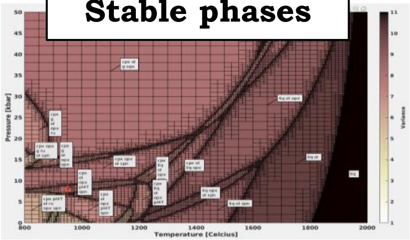


- Quick convergence to arbitrary mass residual
- Decreases oscillation during convergence

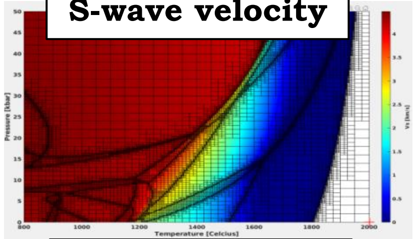
MAGEMin - interface

- Igneous database “from mantle to granite” *(Holland et al., 2018)*
- Command line single/parallel point calculation
- MATLAB based Graphic User Interface

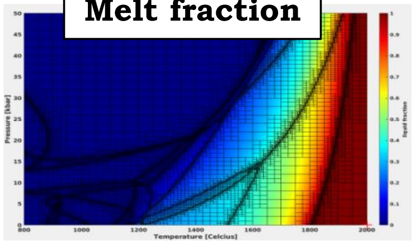




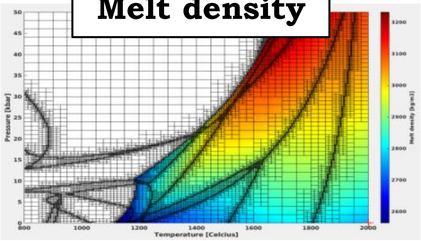
Stable phases



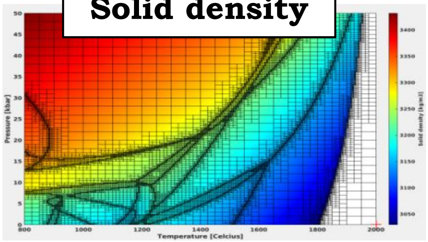
S-wave velocity



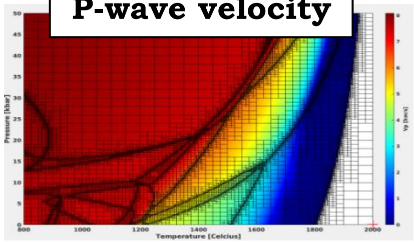
Melt fraction



Melt density



Solid density



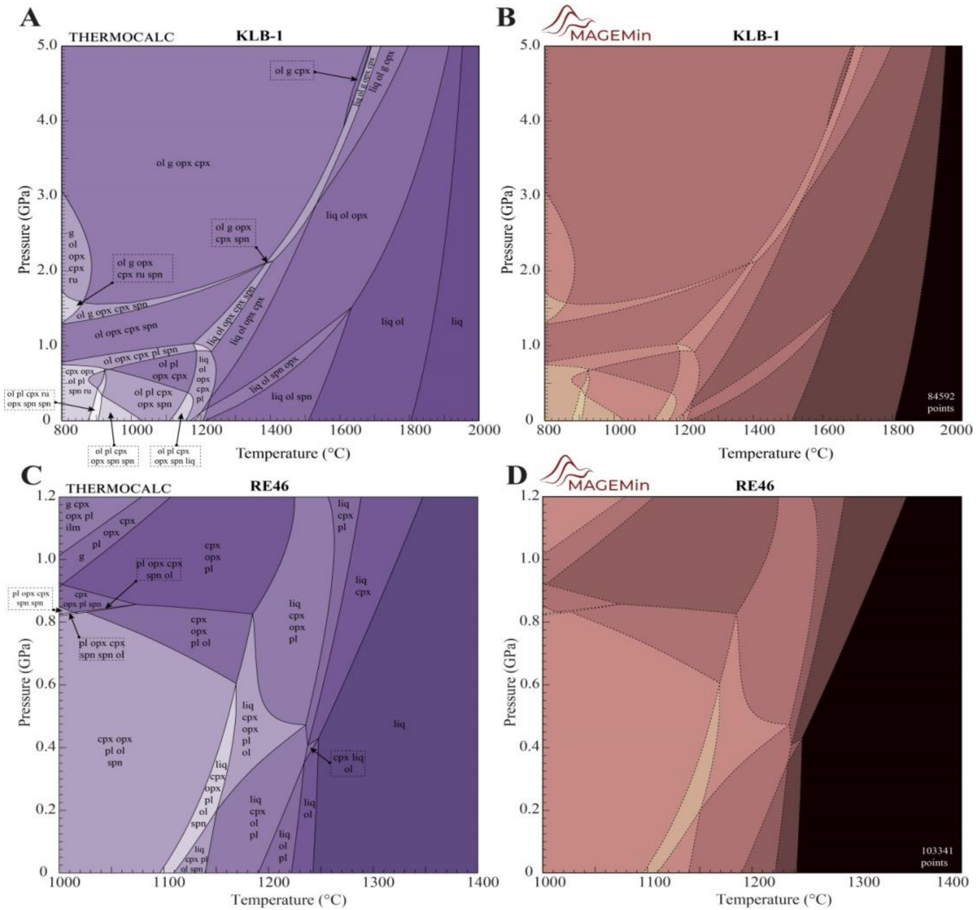
P-wave velocity

Application to magmatic system – dry system benchmark

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

Peridotite

Basalt



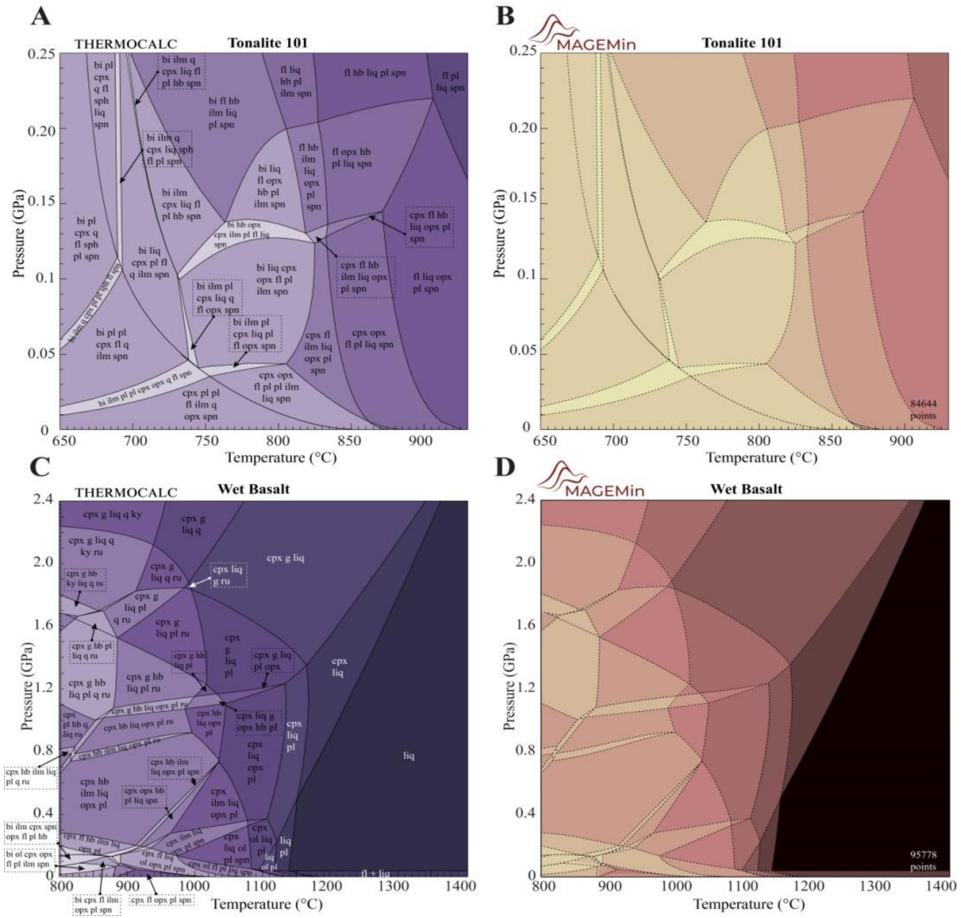
(Riel et al., 2022)

Application to magmatic system – wet system benchmark

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

Tonalite
fluid oversaturated

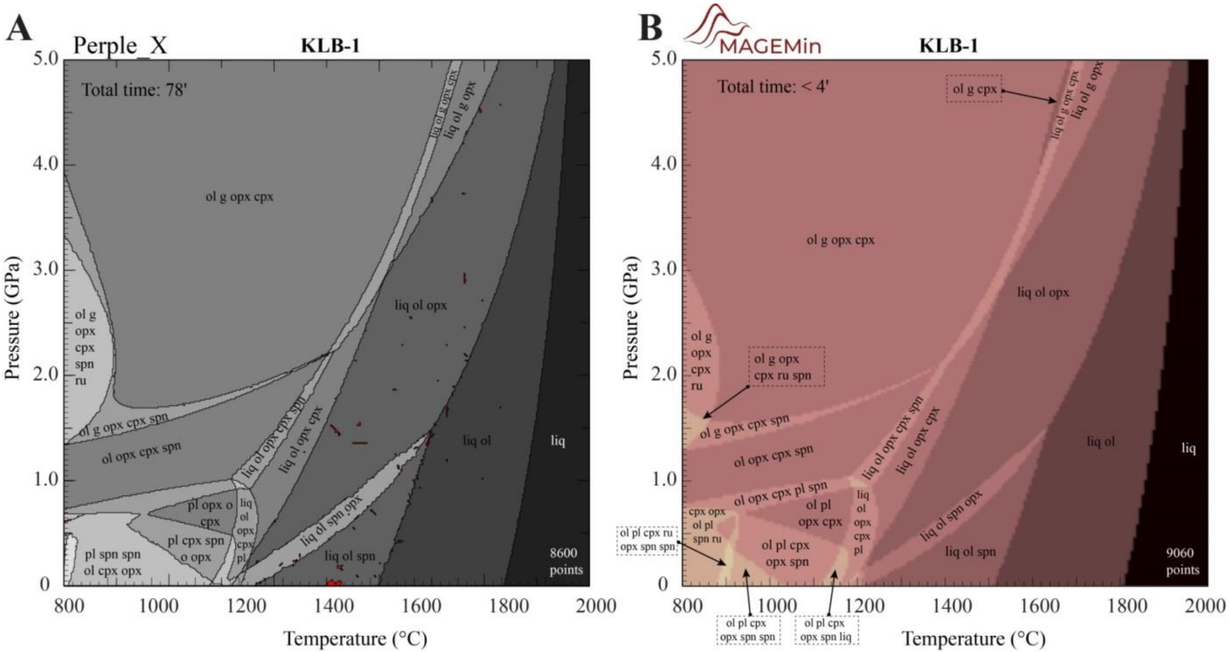
Wet Basalt
fluid saturated



(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 6 threads

MAGEMin: current stage and ongoing developments

Current stage

- MPI parallel C-library with built-in igneous database (*Holland et al., 2018*)
- Combines the best of available methods and further extend them
- Accounts for solvus
- Low memory usage < 5 Mb
- Matlab GUI
- Julia wrapper for geodynamic coupling (MAGEMin_C)
- Single core performance

    ~70 to 200 ms with no initial guess (dry-wet cases)

Ongoing development

- Algorithm upgrade to improve performances and stability
- Reduced chemical systems
- More options for the GUI (e.g., isopleth)
- Matlab wrapper (T. Keller)

Possible upcoming additions

- Adding other thermodynamic database

Contact: nriel@uni-mainz.de

https://github.com/ComputationalThermodynamics/MAGEMin

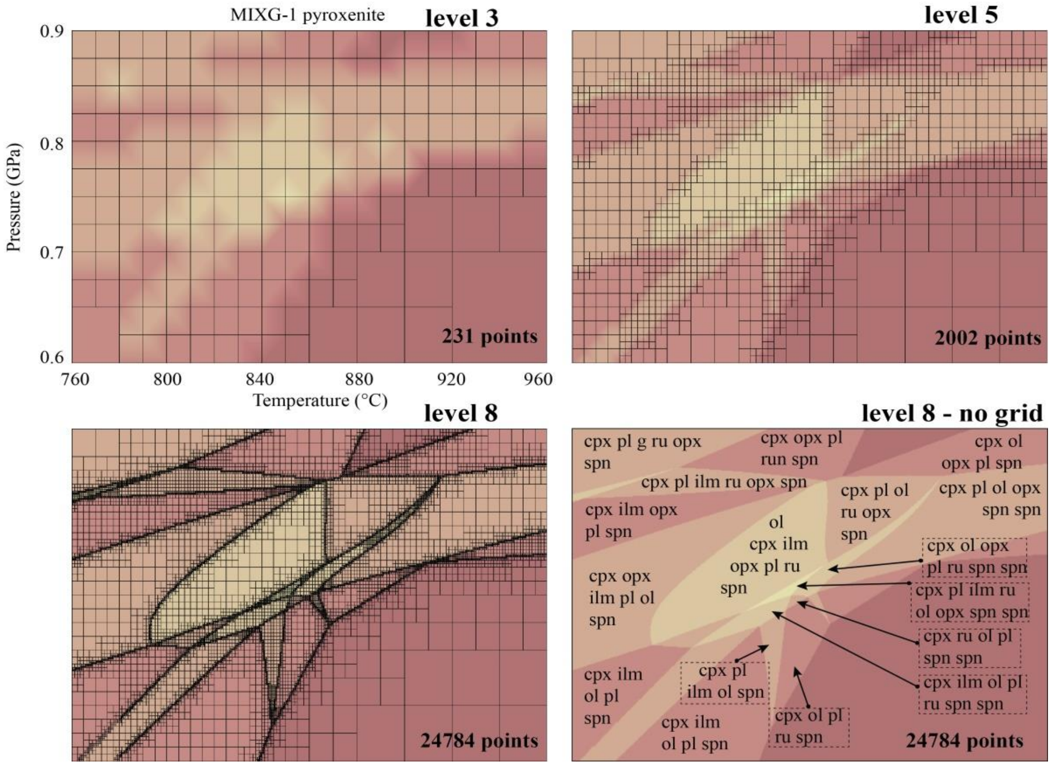
Install MAGEMin_C

```
julia> ]                                                # opens the package manager
pkg> add MAGEMin_C                                      # MAGEMin_C
```

Compute equilibrium

```
julia> using MAGEMin_C                                  # load MAGEMin_C package
julia> gv, DB = init_MAGEMin();                         # initializes MAGEMin
julia> P_kbar,T_C = 8.0, 800.0;
julia> bulk_rock = get_bulk_rock(gv, 0);                # bulk-rock (KLB-1 peridotite)
julia> gv.verbose = -1;                                 # switch off run-time verbose
julia> out = point_wise_minimization(P_kbar,T_C, bulk_rock, gv, DB);
julia> print_info(out);                                 # full display of the minimized point
```

Thank you!


MIXG-1 pyroxenite
level 3
0.9
0.8
0.7
0.6
Pressure (GPa)
760
800
840
880
920
960
Temperature (°C)
231 points
level 5
2002 points
level 8
24784 points
level 8 - no grid
cpx pl g ru opx spn
cpx opx pl run spn
cpx ol opx pl spn
cpx pl ilm ru opx spn
cpx pl ol ru opx spn
cpx pl ol opx spn spn
cpx ilm opx pl spn
ol cpx ilm opx pl ru spn
cpx ol opx pl ru spn spn
cpx opx ilm pl ol spn
cpx pl ilm ru ol opx spn spn
cpx ru ol pl spn spn
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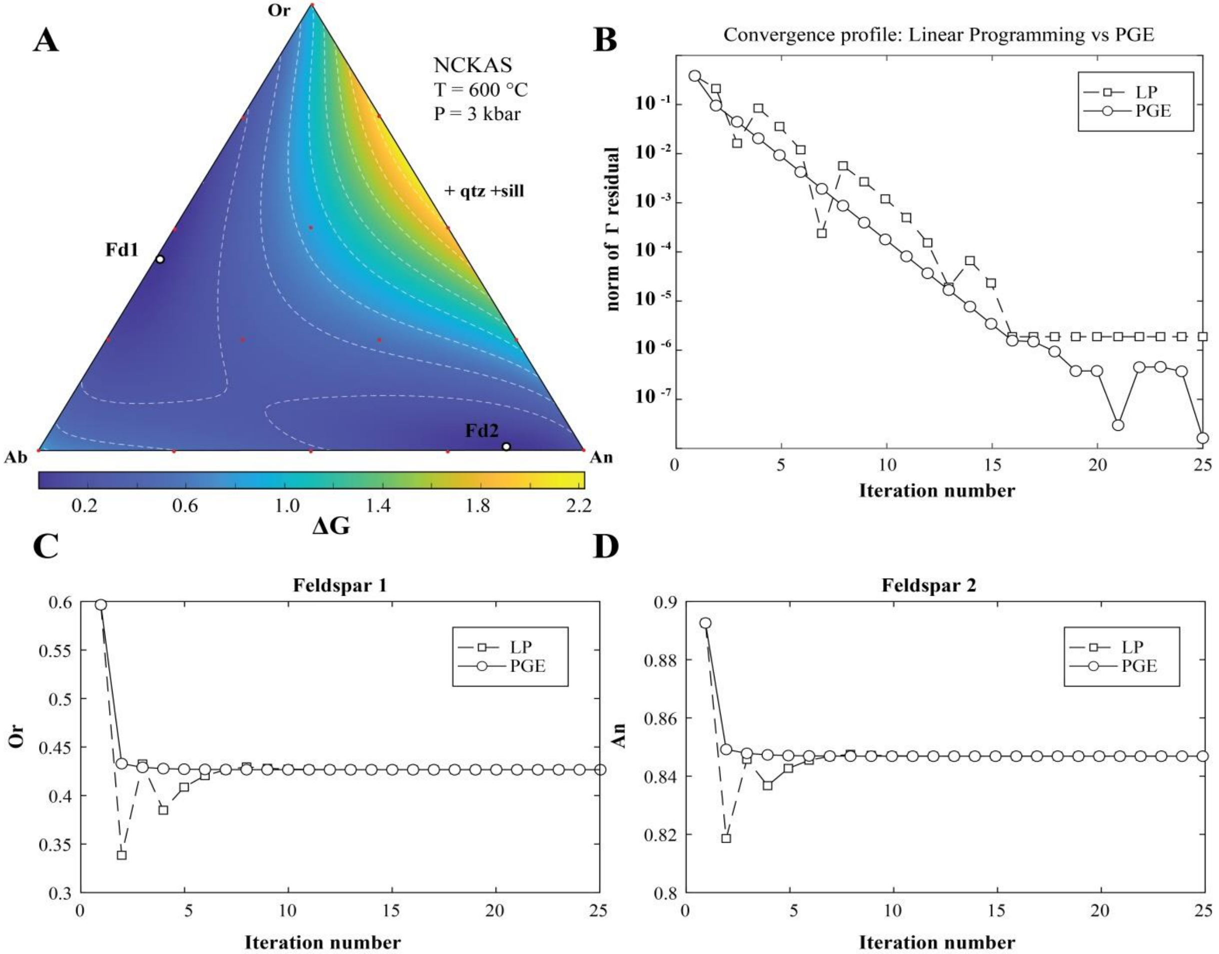
cpx ol pl ru spn
24784 points



A
Or
NCKAS
T = 600 °C
P = 3 kbar
+ qtz +sill
Fd1
Fd2
Ab
An
0.2
0.6
1.0
1.4
1.8
2.2
ΔG
B
Convergence profile: Linear Programming vs PGE
LP
PGE
norm of Γ residual
Iteration number
C
Feldspar 1
Or
Iteration number
D
Feldspar 2
An
Iteration number

Mineral Assemblage Gibbs Energy Minimization: MAGEMin

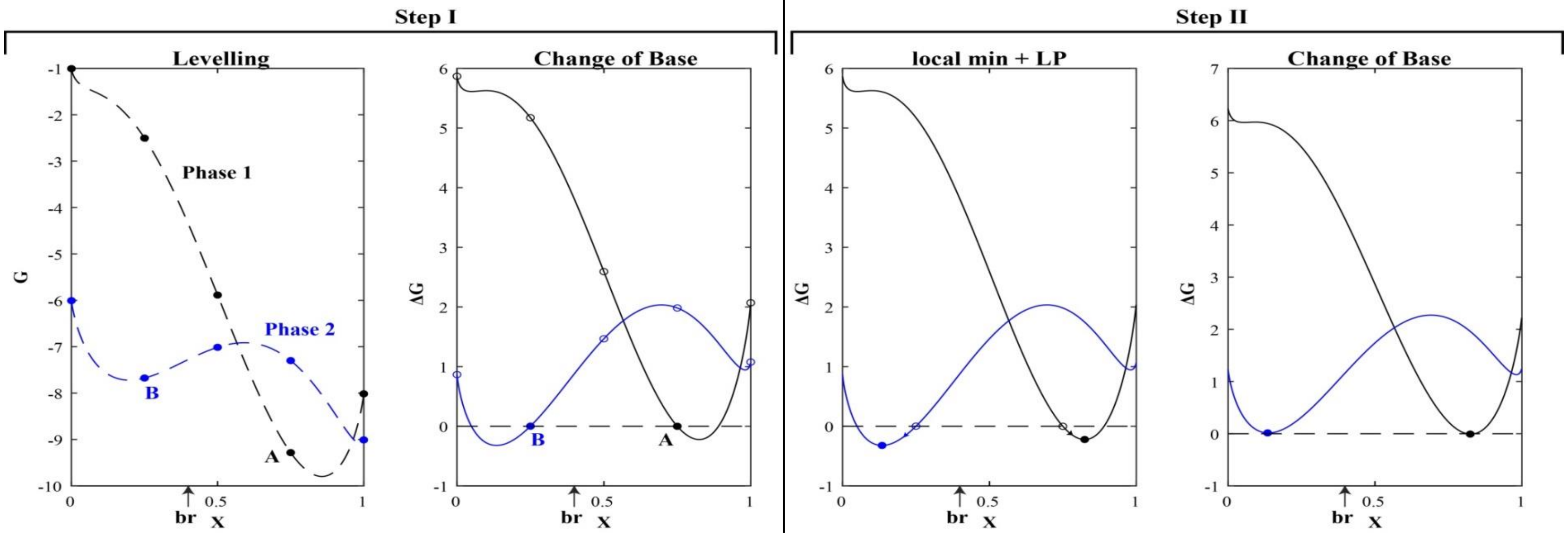
- MAGEMin: a two steps Gibbs energy minimizer

I. Levelling

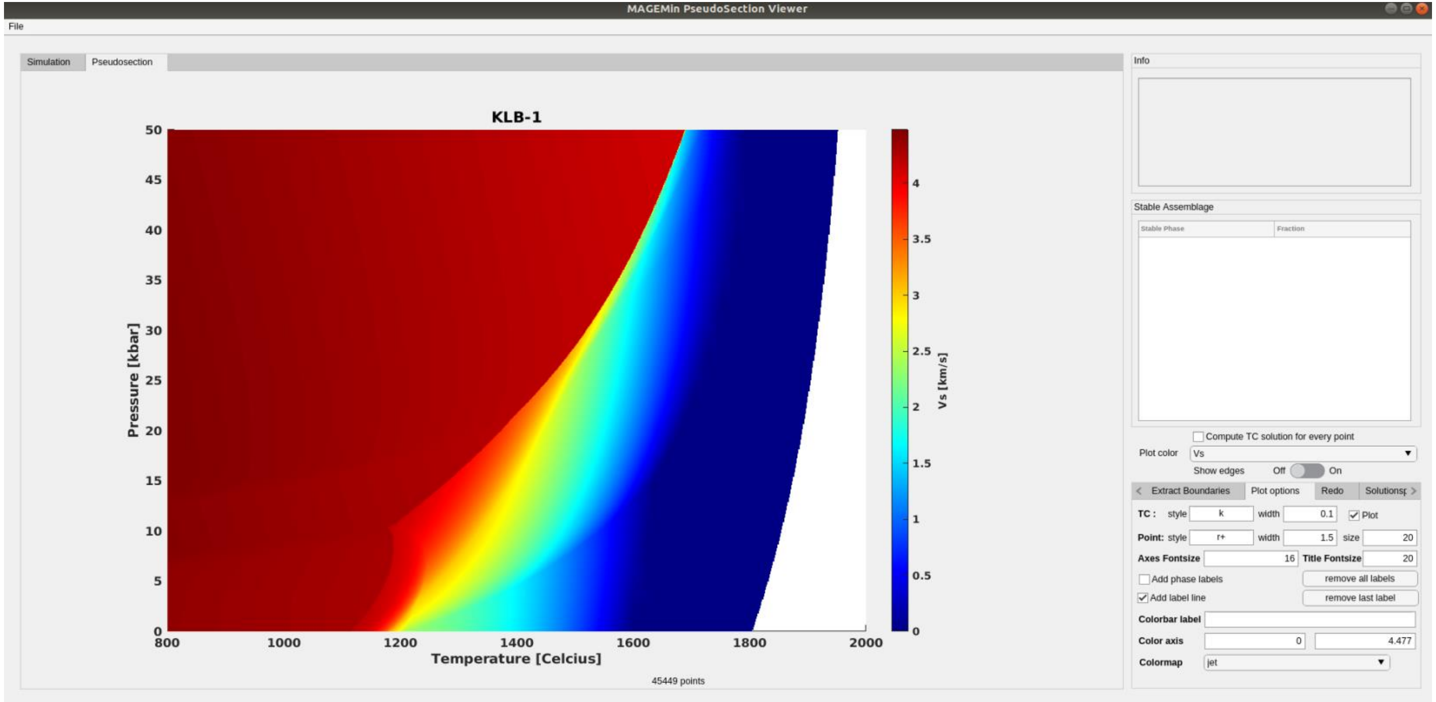
Using solution model discretization

II. Partitioning Gibbs energy

contrained Gibbs-hyperplane rotation



MAGEMin - Vs


MAGEMin PseudoSection Viewer
File
Simulation
Pseudosection
KLB-1
Pressure [kbar]
Temperature [Celcius]
Vs [km/s]
45449 points
Info
Stable Assemblage
Stable Phase
Fraction
Compute TC solution for every point
Plot color
Vs
Show edges
Off
On
Extract Boundaries
Plot options
Redo
TC : style k width 0.1 Plot
Point: style r+ width 1.5 size 20
Axes Fontsize 16 Title Fontsize 20
Add phase labels
remove all labels
Add label line
remove last label
Colorbar label
Color axis 0 4.477
Colormap jet