PHASE EQUILIBRIUM MODELLING: APPROACHES AND PITFALLS

THERIAK-DOMINO: Introduction to the toolset

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Day 2 Part 2: Virtual Workshop, May 10-14, 2021

Objective

- Introduce new users to what tools are available in the suite of programs
- Give some examples

Topics Covered

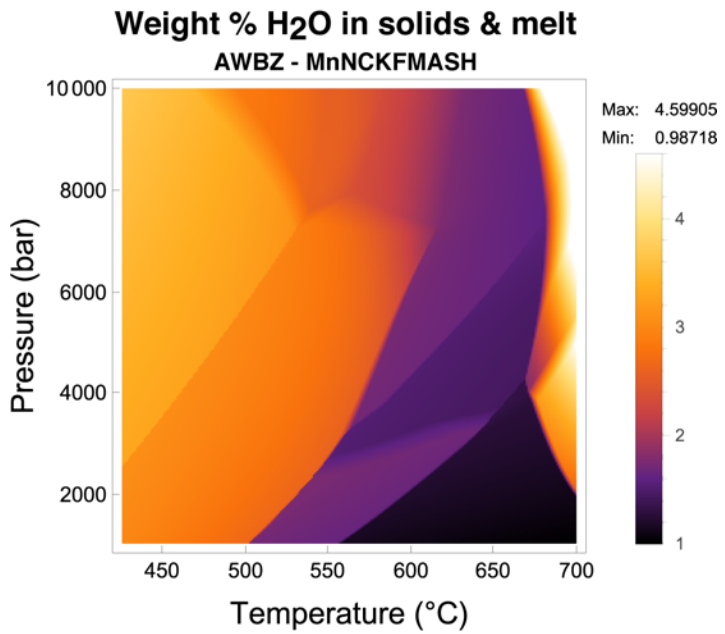
- Theriak-Domino: What it is and where to get it
- Gibbs minimization algorithm
- Input files (databases, solution models) & program Thalia
- Programs Theriak and PlotXY
- Program Domino & pixel maps
- Programs Therter/Therbin (Fe-Ti-O example)
- Pitfalls, pointers, advice

INTRODUCTION TO THERIAK-DOMINO

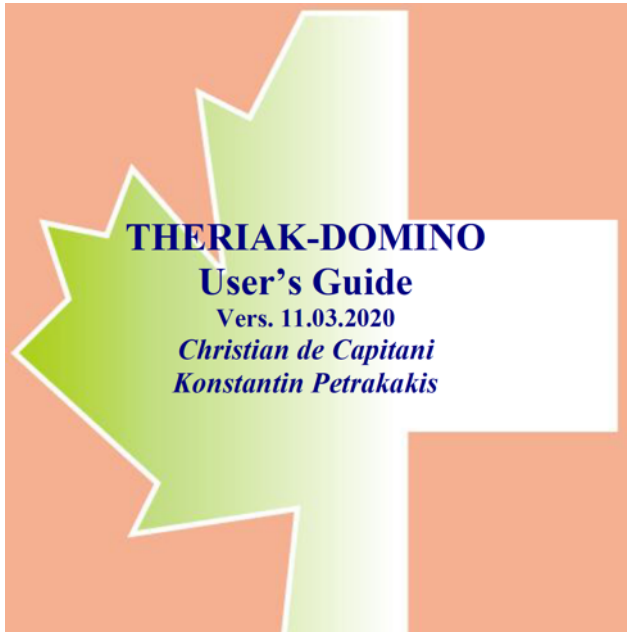
Suite of programs capable of

- Calculating and plotting thermodynamic properties of pure phases and solutions from a thermodynamic database
- Calculating equilibrium assemblages for a given bulk system composition
- Calculating and plotting equilibrium assemblage diagrams for a given bulk or range of bulk compositions
  - P-T, T-X, P-X, X-X diagrams and more
  - Ternary diagrams
  - Contour diagrams for phase composition or mode
  - Contour diagrams for various system/rock properties
  - Pixel maps of system and phase properties
  - It does not calculate petrogenetic grids nor does it do traditional reaction-based thermobarometry like AvePT or winTWQ

pixelmap output from program Domino



INTRODUCTION TO THERIAK-DOMINO



- Written and maintained by Christian de Capitani at the University of Basel, Switzerland
- Equilibrium calculations via Gibbs energy minimization
- Main algorithm is published (de Capitani & Brown, 1987)
- Written in fortran and source code distributed with programs
- Not technically open source (unlicensed), but a statement allowing user modification is provided, and source code is freely available for user modification and customization
- Comprehensive user manual for the main programs included in distribution (read it)
- Distributed with multiple thermodynamic databases and included solution models

Main publications for programs

Geochimica et Cosmochimica Acta Vol. 51, pp. 2639–2652
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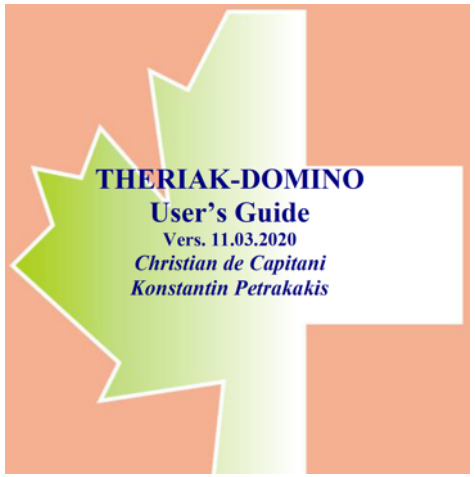
0016-7037/87/$3.00 + .00

The computation of chemical equilibrium in complex systems containing non-ideal solutions

CHRISTIAN DE CAPITANI and THOMAS H. BROWN
Department of Geological Sciences, University of British Columbia, Vancouver, B.C., Canada, V6T 2B4

(*Received October* 2, 1986; *accepted in revised form July* 2, 1987)

Algorithm: de Capitani & Brown (1987), *Geochimica*



User manual: de Capitani

American Mineralogist, Volume 95, pages 1006–1016, 2010

The computation of equilibrium assemblage diagrams with Theriak/Domino software

CHRISTIAN DE CAPITANI[1,*] AND KONSTANTIN PETRAKAKIS[2]

[1]Mineralogisch-Petrographisches Institut, Universität Basel, Bernoullistrasse 30, CH-4056 Basel, Switzerland
[2]Department of Geological Sciences, University of Vienna, Althanstrasse 14, A-1090 Vienna, Austria

Domino: de Capitani & Petrakakis (2010), *Am Min*

THERIAK-DOMINO & ADD-ON PROGRAMS

- **Theriak**: Equilibrium assemblage calculation
- **Domino**: XY and ternary equilibrium assemblage diagram calculations
- **Therbin** & **Therter**: Binary and ternary phase diagrams
- **Guzzler/Explot/PlotXY/Makemap**: Output processors to produce editable graphics files
- **Thermo/Thalia**: Thermodynamic property calculators (pure phases and solutions)
- Others: **Theriaq, Theriak3**
- Add-ons or interfacing programs:
    - **Theria_G** (Gaidies *et al.*, 2008; distributed with Theriak-Domino)
    - **TheriakD** (Duesterhoeft & de Capitani, 2013; distributed with Theriak-Domino)
    - **Bingo-Antidote** (Duesterhoeft & Lanari, 2020; distributed with XMapTools)

DOWNLOADING THERIAK-DOMINO

Official THERIAK-DOMINO distribution site

- https://titan.minpet.unibas.ch/minpet/theriak/theruser.html

Programs and translations of THERMOCALC files also downloadable from

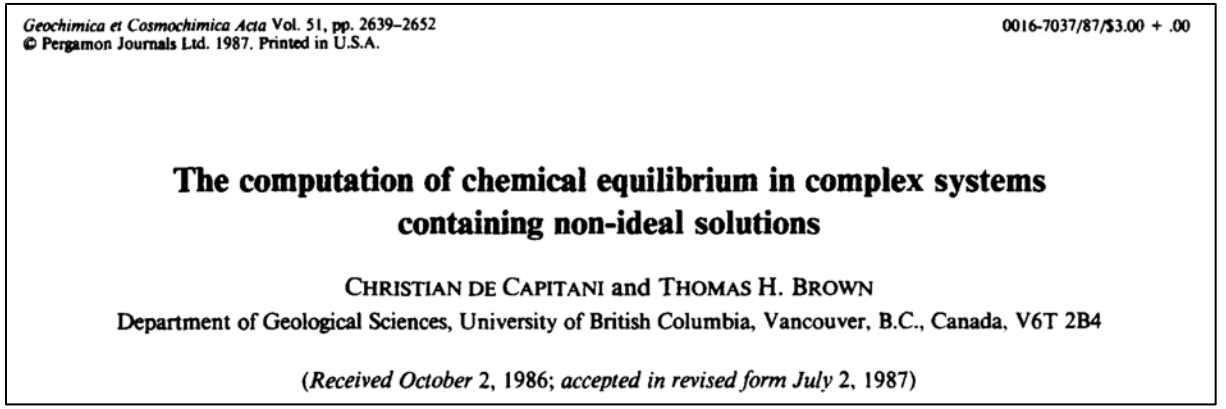
- http://dtinkham.net/peq.html
- **Updates coming with newly formatted files for the Holland & Powell databases**

Programs and databases included with XMapTools distribution

- https://www.xmaptools.com/

Gibbs Minimization Algorithm

- Algorithm published in 1987 (de Capitani & Brown, *Geochimica*)



Geochimica et Cosmochimica Acta Vol. 51, pp. 2639–2652 0016-7037/87/$3.00 + .00
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The computation of chemical equilibrium in complex systems containing non-ideal solutions

CHRISTIAN DE CAPITANI and THOMAS H. BROWN
Department of Geological Sciences, University of British Columbia, Vancouver, B.C., Canada, V6T 2B4

(*Received October* 2, 1986; *accepted in revised form July* 2, 1987)

de Capitani & Brown (1987), *Geochimica*

Algorithmic flow (generalized)

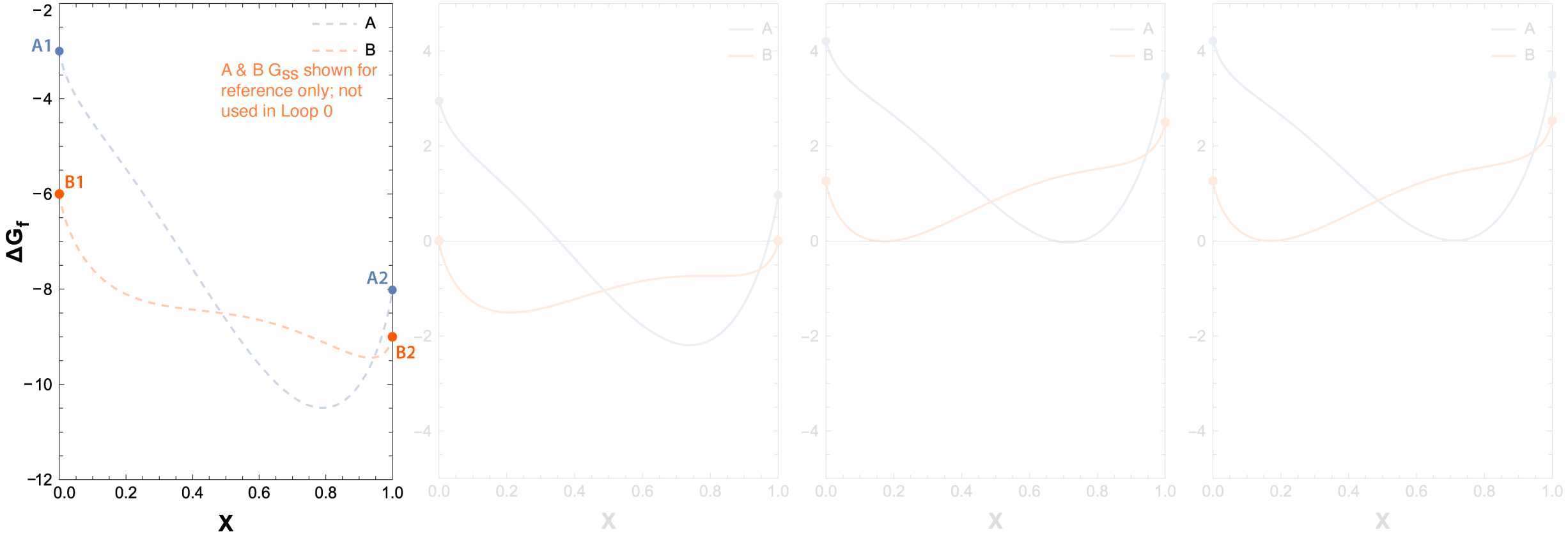
- Find initial minimum G assemblage from the pool of database members (pure phases) and fictive phases with compositions of the system components

1) Find several local minimums of each solution phase (multiple starting compositions, scans, and refinements), and **add those to pool of fixed phase compositions**; solution phase composition precision nearly at machine precision
2) Try to swap each fixed composition phase from pool into currently stable assemblage to check for new lower-G assemblage; check for convergence and iterate on step 1 or end

Similar to Perple_X in the sense you are minimizing discrete 'fixed-composition' phases in one of the steps, but the pool of fixed-composition phases are drawn from minimizations of solution models over continuous composition space

Gibbs Minimization Algorithm – Loop 0

- Consider pure phases of dataset
- Do not consider solid solution space, just end-members of solution models

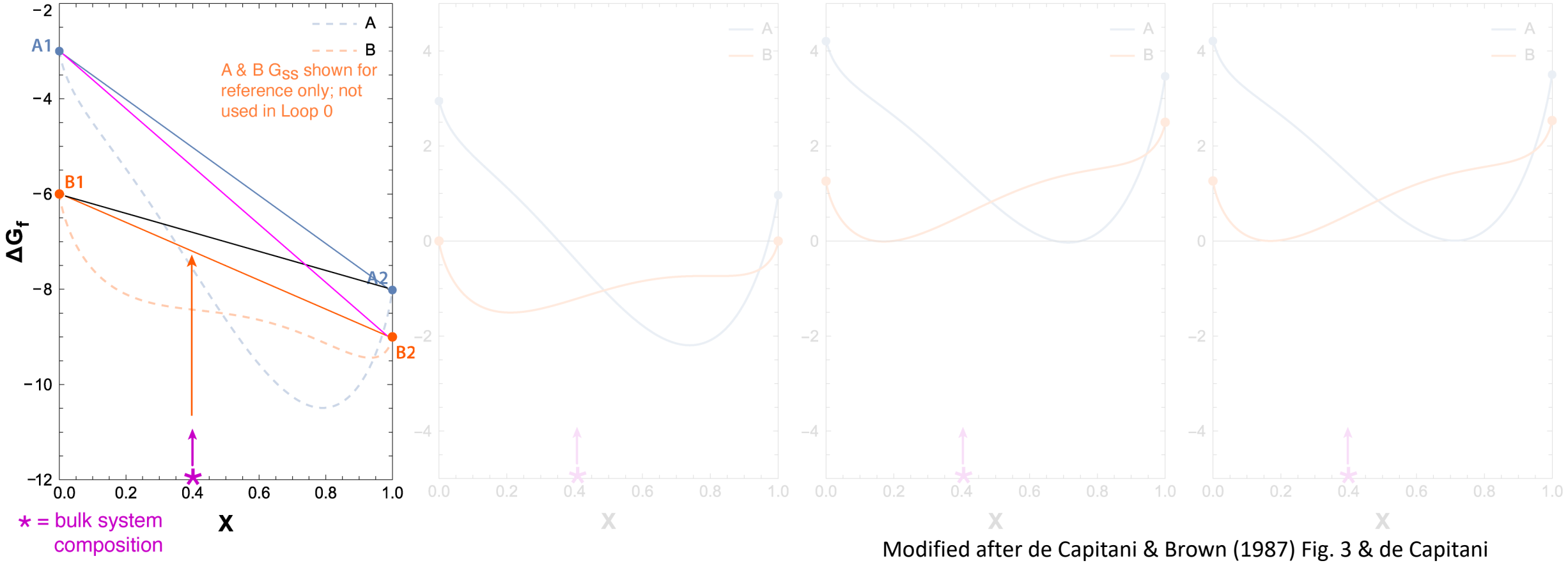


Modified after de Capitani & Brown (1987) Fig. 3 & de Capitani (2010) Univ. Calgary Theriak-Domino short course notes

Gibbs Minimization Algorithm – Loop 0

- Consider pure phases of dataset
- Do not consider solid solution space, just end-members of solution models

- Find combination of pure phases that forms minimum G assemblage for bulk system composition
- B1 + B2 assemblage is most stable



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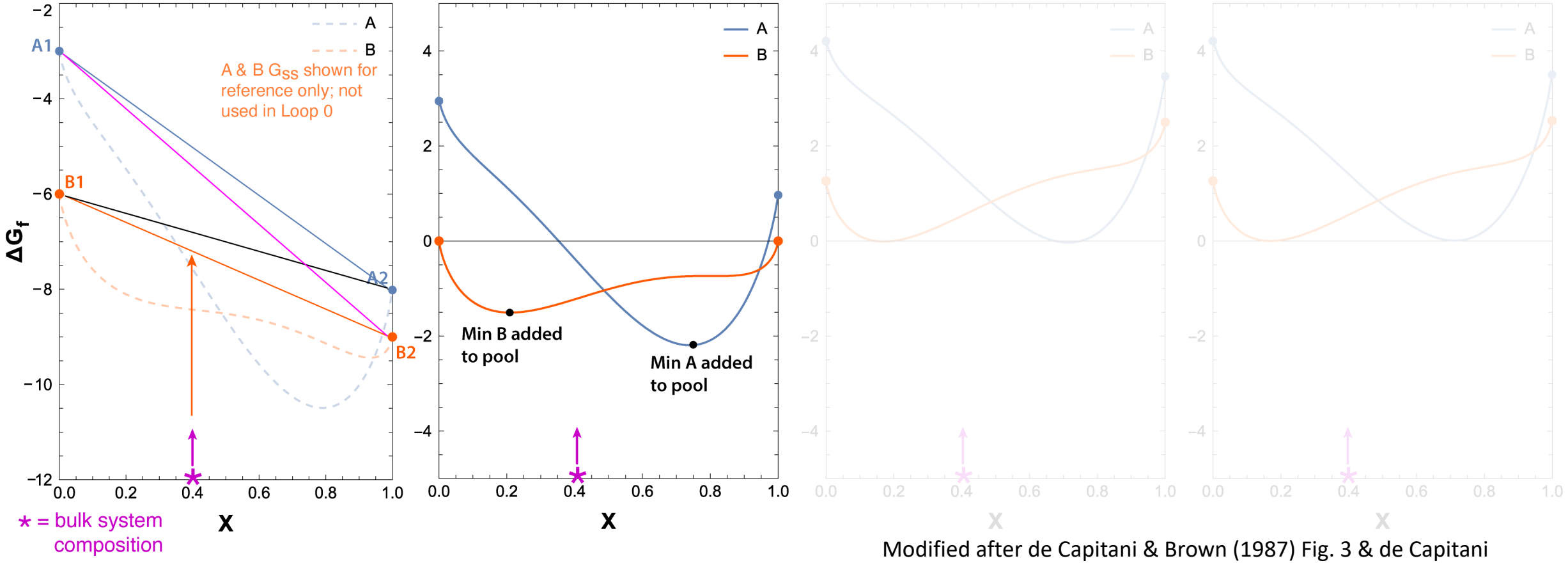
Gibbs Minimization Algorithm - Loop 1

- Do a ‘reference’ base change and translate the current stable hyperplane to G = 0.0
- Consider continuous solution model space, and find new minimum G compositions for all active solution models



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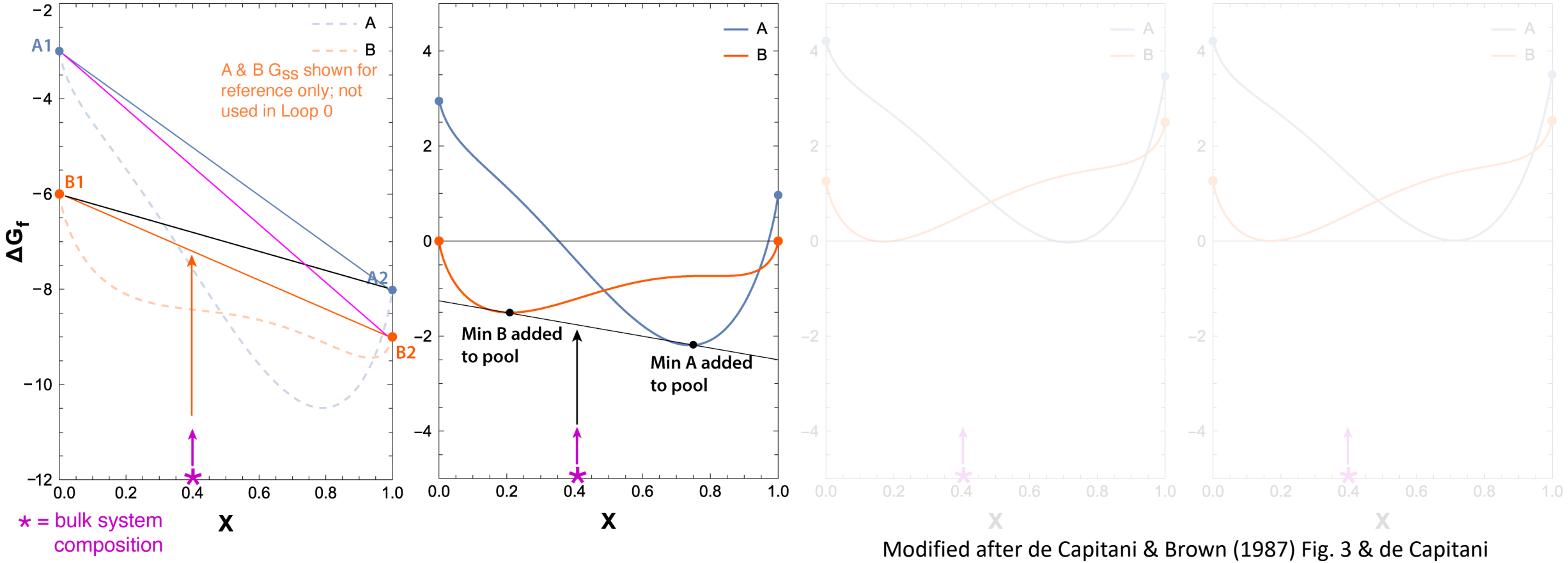
Gibbs Minimization Algorithm – Loop 1

- Consider continuous solution model space, and find new minimum G compositions for all active solution models
- Attempt to add or swap all the new minimum points for each solution into the current minimum assemblage to find a lower G assemblage (negative G)
- Do the change of reference base along the way to get current stable assemblage hyperplane at G = 0.0



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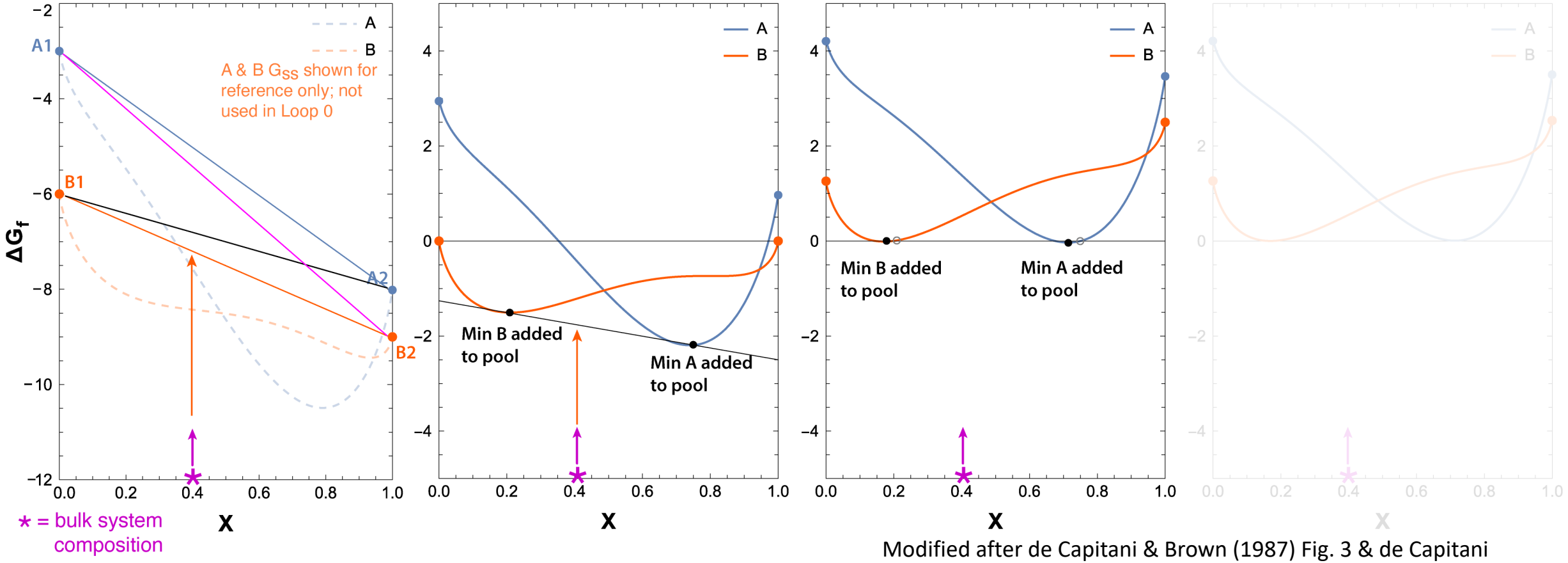
Gibbs Minimization Algorithm – Loop 2

- Minimize each solution model again to find new minimum G compositions
- Attempt to add or swap all the new minimum points of solution models to find a lower G assemblage (negative G)



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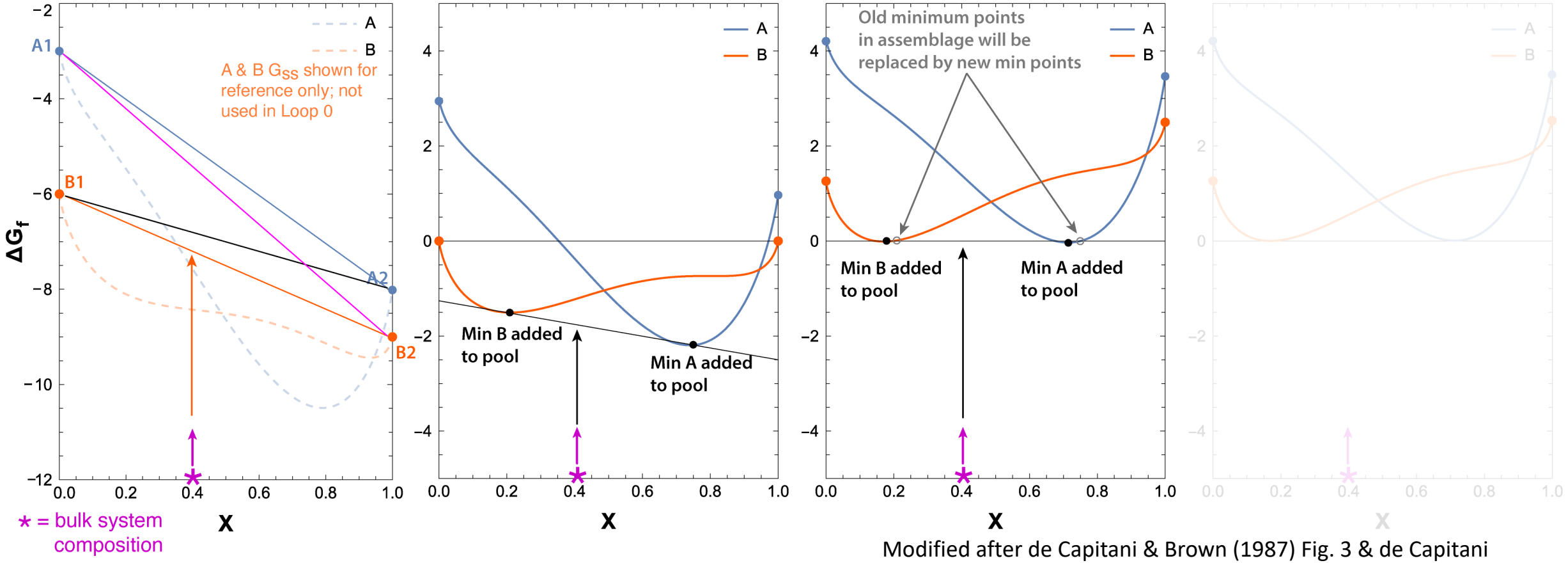
Gibbs Minimization Algorithm

- Attempt to add or swap all the new minimum points of solution models to find a lower G assemblage (negative G)
- Points that were part of the old stable assemblage are replaced if better ones found
- Do the change of reference base along the way to get current stable assemblage hyperplane at G = 0.0



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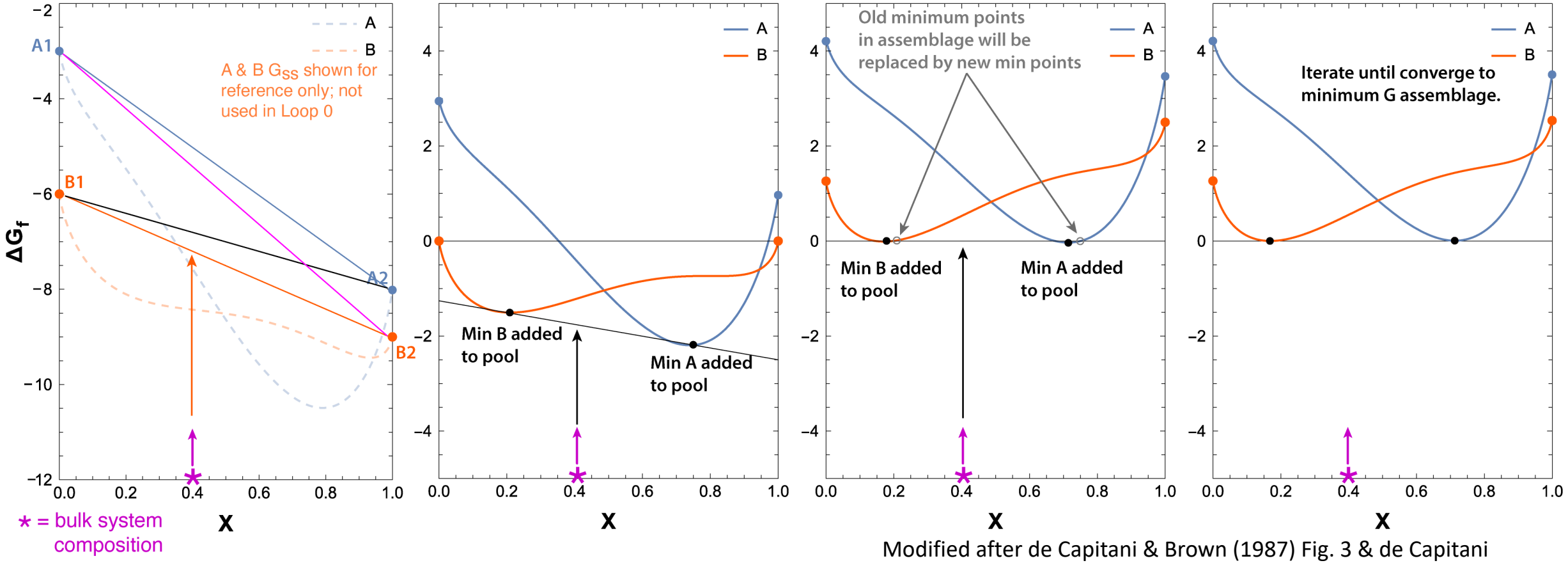
Gibbs Minimization Algorithm

- Iterate until reach convergence (decrease in G is below some threshold)



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Databases and Solution Models

Databases:

- Flexible format that can accommodate multiple databases
- Main databases shipping with program:
  - variants of the Berman database (1988; Jun ‘92 update)
  - variants of the Holland & Powell databases (1998 ds5.5; 2011 ds6.2)
- Database file mixes solution models with the end-member thermodynamic database proper (not a separate file for database and solution models)

Solution Models:

- Accepts a wide variety of models (ideal mixing-on sites and molecular mixing for ideal activity; regular and symmetric formalism symmetric excess mixing; asymmetric-formalism and subregular asymmetric excess mixing; and a within-site excess mixing model)
- Special models that do not conform to the above models can be hard-coded and program recompiled
- Effective program use requires basic familiarity with the format of database files and solution model input format. Read the official user manual and comments in database files.

Database file: database members

- *** denotes a keyword flag
- GAS and MINERAL indicates the following data is for a pure phase/species; the difference controls output, not calculation

```
126  *** GAS DATA ***
127  H2O                    H(2)O(1)                              H2O              code
128   SPC    PS94H2O
129   ST              0.0      -241810.0          188.8          0.0
130   C3             40.1       0.008656       487500.0       -251.2              0.00
131  CO2                    C(1)O(2)                              CO2              code
132   SPC    PS94CO2
133   ST              0.0      -393510.0          213.7          0.0
134   C3             87.8       -0.002644       706400.0       -998.9              0.00
135  *** MINERAL DATA ***
136  and                    AL(2)SI(1)O(5)                        and              code
137   ST              0.0     -2588670.0           92.7          5.153
138   C3            277.3       -0.006588      -1914100.0      -2265.6              0.00
139   V11      0.0000181          1442.0            6.89         -0.0048             0.00
140  ky                     AL(2)SI(1)O(5)                        ky               code
141   ST              0.0     -2592970.0           83.5          4.414
142   C3            279.4       -0.007124      -2055600.0      -2289.4              0.00
143   V11      0.0000192          1601.0            4.05         -0.0025             0.00
```

Database file: database members

- SPC indicated the thermodynamic properties are calculated by a special routine specific to that phase (PS94H2O & PS94CO2)

- ST, C3 and V11 indicate specific types of thermodynamic values follow on that line
  - ST: reference state G,H,S,V
  - C3: particular grouping of heat capacity coefficients
  - V11: data go with a specific EOS, in this case HP ‘11 dataset

```
126  *** GAS DATA ***
127  H2O                    H(2)O(1)                              H2O              code
128   SPC    PS94H2O
129   ST                0.0      -241810.0          188.8          0.0
130   C3               40.1       0.008656       487500.0       -251.2          0.00
131  CO2                    C(1)O(2)                              CO2              code
132   SPC    PS94CO2
133   ST                0.0      -393510.0          213.7          0.0
134   C3               87.8       -0.002644      706400.0       -998.9          0.00
135  *** MINERAL DATA ***
136  and                    AL(2)SI(1)O(5)                        and              code
137   ST                0.0     -2588670.0           92.7          5.153
138   C3              277.3       -0.006588     -1914100.0      -2265.6          0.00
139   V11        0.0000181         1442.0           6.89         -0.0048         0.00
140  ky                     AL(2)SI(1)O(5)                        ky               code
141   ST                0.0     -2592970.0           83.5          4.414
142   C3              279.4       -0.007124     -2055600.0      -2289.4          0.00
143   V11        0.0000192         1601.0           4.05         -0.0025         0.00
```

Database: solution model format

- *** SOLUTION indicates the following data describes mixing of phase components of a solution model
- (-SITE,MARGULES) indicates mixing is described by mixing on sites, and that the phase exhibits non-ideal mixing, defined by interaction parameters (between phase components)
- “SITE” would indicate all phase component proportions are restricted to be > 0
- “-SITE” indicates phase components proportions can be negative

```
929  *** SOLUTION DATA ***
930  BI14    (-SITE,MARGULES)   M3(1):Mg,Fe,Al,Ti,F3,Mn - M12(2):Mg,Fe,Mn - T(2):Si,Al - V(2):OH,O
931    phl           Mg - Mg,Mg - Si,Al - OH,OH
932    annm          Fe - Fe,Fe - Si,Al - OH,OH
933    obi           Fe - Mg,Mg - Si,Al - OH,OH
934    east          Al - Mg,Mg - Al,Al - OH,OH
935    tbi           Ti - Mg,Mg - Si,Al - O,O
936    fbi           F3 - Mg,Mg - Al,Al - OH,OH
937    mmbi          Mn - Mn,Mn - Si,Al - OH,OH
938  *** MARGULES PARAMETERS ***
939  phl - annm
940  12          12000        0        0
941  phl - obi
942  12           4000        0        0
943  phl - east
944  12          10000        0        0
```

Database: solution model format – site mixing

- M3(1), M12(2), T(2), V(2): Arbitrary names of sites, with site multiplicity indicated
- T(2):Si,Al simply means a site multiplicity of 2, and the entities that can mix on site T are denoted by the names Si and Al. Note that the names of entities mixing on the site is arbitrary (could be anything else that makes sense)
- tbi Ti – Mg,Mg – Si,Al – O,O Site composition of phase component tbi

```
929  *** SOLUTION DATA ***
930  BI14    (-SITE,MARGULES)   M3(1):Mg,Fe,Al,Ti,F3,Mn - M12(2):Mg,Fe,Mn - T(2):Si,Al - V(2):OH,O
931    phl           Mg - Mg,Mg - Si,Al - OH,OH
932    annm          Fe - Fe,Fe - Si,Al - OH,OH
933    obi           Fe - Mg,Mg - Si,Al - OH,OH
934    east          Al - Mg,Mg - Al,Al - OH,OH
935    tbi           Ti - Mg,Mg - Si,Al - O,O
936    fbi           F3 - Mg,Mg - Al,Al - OH,OH
937    mmbi          Mn - Mn,Mn - Si,Al - OH,OH
938  *** MARGULES PARAMETERS ***
939  phl - annm
940  12          12000        0        0
941  phl - obi
942  12           4000        0        0
943  phl - east
944  12          10000        0        0
```

Database: solution model format – excess energy

- *** MARGULES Indicates data for interaction parameters between phase components follows next
- phl – obi & 12 4000 0 0 specifies a binary interaction parameter to describe excess energy of mixing

```
929  *** SOLUTION DATA ***
930  BI14    (-SITE,MARGULES)   M3(1):Mg,Fe,Al,Ti,F3,Mn - M12(2):Mg,Fe,Mn - T(2):Si,Al - V(2):OH,O
931    phl           Mg - Mg,Mg - Si,Al - OH,OH
932    annm          Fe - Fe,Fe - Si,Al - OH,OH
933    obi           Fe - Mg,Mg - Si,Al - OH,OH
934    east          Al - Mg,Mg - Al,Al - OH,OH
935    tbi           Ti - Mg,Mg - Si,Al - O,O
936    fbi           F3 - Mg,Mg - Al,Al - OH,OH
937    mmbi          Mn - Mn,Mn - Si,Al - OH,OH
938  *** MARGULES PARAMETERS ***
939  phl - annm
940  12            12000          0          0
941  phl - obi
942  12             4000          0          0
943  phl - east
944  12            10000          0          0
```

Comparing TD and TC AX File Formats

White et al. (2000) FTO Ilmenite model & Holland & Powell (2011) ds6.2 update

The model has 3 phase components (ordered ilmenite, disordered ilmenite, and hematite)

involves ordering of Fe & Ti across sites

The TD equivalent of TC ‘make’ is ‘COM’.

TC makes the new dataset member oilm from the existing dataset member ilm by stripping off the Landau ordering contributions at reference conditions, and does not add the Landau contributions at elevated P & T.

The TD entry for the member ilmD- has the Landau contribution removed at reference conditions by the file author, and does not add Landau ordering contributions at elevated P & T (it should match what the TC command “make 1 disordered ilm” does).

Both programs then adjust the Gibbs energy by:

-13607.5 + 9.426 * Tk (j/mol)

Formatted for use in Theriak-Domino

```
!------------------------------------------------------------------------------
*** MINERAL DATA ***
ilmD-                FE(1)TI(1)O(3)                          ilmD-          -c
 ST              0.0  -1215398.4244   120.51831967   3.1873638661
 C3            138.9       0.005081    -1288800.0        -463.7          0.00
 V11        0.000024         1700.0           8.3        -0.0049          0.00
hemD-                FE(2)O(3)                               hemD-          -c
 ST              0.0   -816087.2292   100.33766837         3.027
 C3            163.9            0.0    -2257200.0        -657.6          0.00
 V11       0.0000279         2230.0          4.04        -0.0018          0.00
!==============================================================================
!================================================================ AX MODEL ILM00
! ref 0,-3
!         Converted from HPx-eos website files
!         tc-mp50MnNCKFMASHTO.txt & tc-ds62.txt (ds62a)
! note:   This version does not contain Mn & Mg members, so it may not be the
!         best choice at lower T's if your ilm has a significant amount of Mn.
! entry:  D.K. Tinkham. Sun 11 Apr 2021 19:33:10 (via dsaxcnvrt.wl)
!. . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .
*** MINERAL DATA ***
!  Required dataset phase components for COM's: {ilmD-, hemD-}
oilm1                FE(1)TI(1)O(3)                          oilm1          code
 ST              0.0       -13607.5         -9.426              0
 COM       ilmD-[1]
dilm1                FE(1)TI(1)O(3)                          dilm1          code
 ST              0.0         1992.8            2.1              0
 COM       ilmD-[1]
dhem1                FE(2)O(3)                               dhem1          code
 ST              0.0            0.0            0.0            0.0
 COM       hemD-[1]
!. . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .
*** SOLUTION DATA ***
ILM00     (-SITE,MARGULES)1/2      A(2):Fe,Ti,F3 - B(2):Ti,Fe,F3
  oilm1          Fe,Fe - Ti,Ti
  dilm1          Fe,Ti - Fe,Ti
  dhem1          F3,F3 - F3,F3
*** MARGULES PARAMETERS ***
oilm1 - dilm1
12         15600.0        0        0
oilm1 - dhem1
12         26600.0        0        0
dilm1 - dhem1
12           11000        0        0
!END AX MODEL ILM00
!------------------------------------------------------------------------------
```

THERMOCALC tc-mp50MnNCKFMASHTO.txt ax file. HPx-eos website

```
% ============================================================
% Ilmenite: FTO
% White, RW, Powell, R, Holland, TJB & Worley, BA (2000) The effect of TiO2 and
% Fe2O3 on metapelitic assemblages at greenschist and amphibolite facies conditio
% mineral equilibria calculations in the system K2O-FeO-MgO-Al2O3-SiO2-H2O-TiO2-F
% Journal of Metamorphic Geology, 18, 497-511.
%
% E-m   Formula    Mixing sites
%                      A          B
%                   Fe2 Ti Fe3  Fe2 Ti Fe3
% oilm  FeTiO3       1   0   0   0   1   0     - ordered ilm
% dilm  FeTiO3      1/2 1/2  0  1/2 1/2  0     - disordered ilm
% dhem  Fe2O3        0   0   1   0   0   1     - disordered hem
%
% x(ilm) = 1 - xFe3A
% Q(ilm) = x(Fe2,A) - x(Fe2,B)    - order variable
% NOTE: Q(ilm) must have a range of -x to +x
% ------------------------------------------------------------
verbatim
 x(ilm) 0.80
 Q(ilm) 0.55   range -0.99 0.99
% ------------------------------------------------------------
% psub = {ph -> 1 - x, po -> Q, pd -> x - Q};
  p(oilm)  1 1    0  1  1  Q
  p(dilm)  1 1    0  2  1  x -1  Q
  p(dhem)  1 1    1  1 -1  x
% ------------------------------------------------------------
 sf
  W(oilm,dilm)   15.6  0  0
  W(oilm,dhem)   26.6  0  0
  W(dilm,dhem)     11  0  0
% ------------------------------------------------------------
  6     % site fractions
  xFe2A  1 1    0  2  1/2  x  1/2  Q
  xTiA   1 1    0  2  1/2  x -1/2  Q
  xFe3A  1 1    1  1 -1  x
  xFe2B  1 1    0  2  1/2  x -1/2  Q
  xTiB   1 1    0  2  1/2  x  1/2  Q
  xFe3B  1 1    1  1 -1  x
% ------------------------------------------------------------
   oilm      1  2    xFe2A  1  xTiB  1
         make  1 disordered ilm  1
         delG(od)  -13.6075 0.009426 0  % delG - dH + R Log[4]; dH = 15.6
         check 1 1
   dilm      4  4    xFe2A  1/2   xTiA  1/2   xFe2B  1/2   xTiB  1/2
         make  1 disordered ilm  1
         delG(od)    1.9928 -0.0021 0    % delG = G(equil,Landau) - G(equil,SF)
         check 1 0
   dhem      1  2    xFe3A  1  xFe3B  1
         check 0 0
         make 1 disordered  hem 1
```

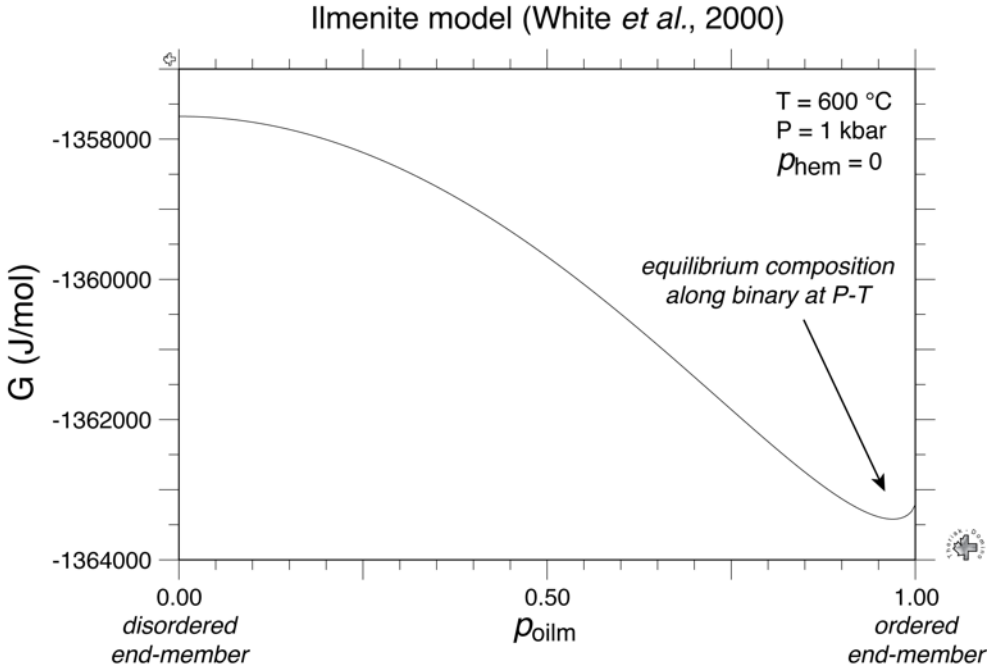
Program Thalia

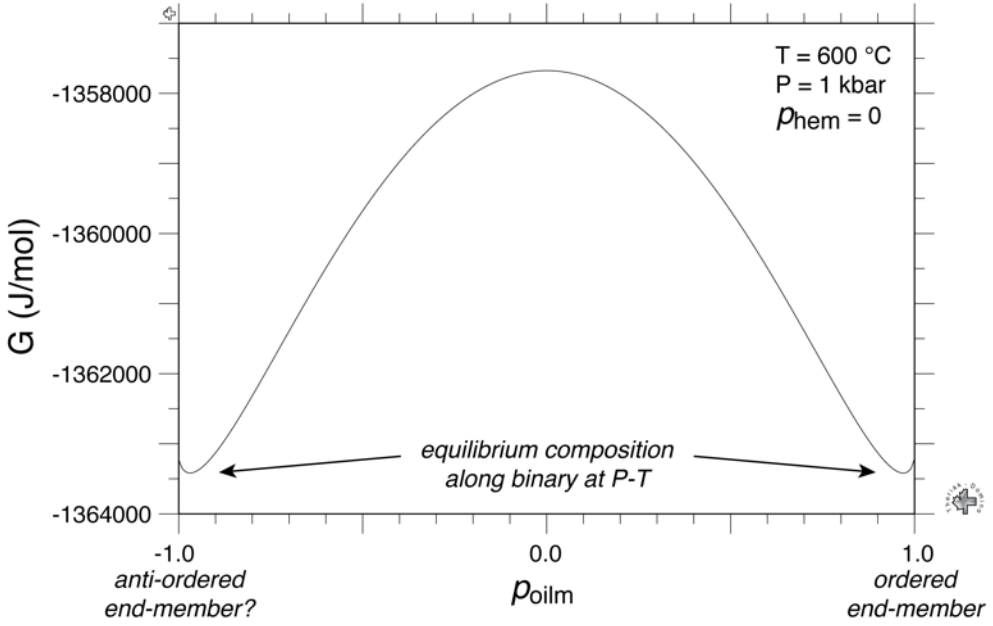
Calculates thermodynamic properties of both pure phases and solution models at P & T

Can plot properties across solution model binaries:

- chemical potential
- G (mech, ideal mix, excess mix, etc.)
- Activities of phase components

- The plot of Gibbs energy across the disordered-ordered binary of ilmenite (White et al. 2000) shows our calculated proportion of the ordered member should be very high or low (close to 1 or -1)
- Thalia is useful for looking at other solution models (amphiboles, pyroxenes, etc.)



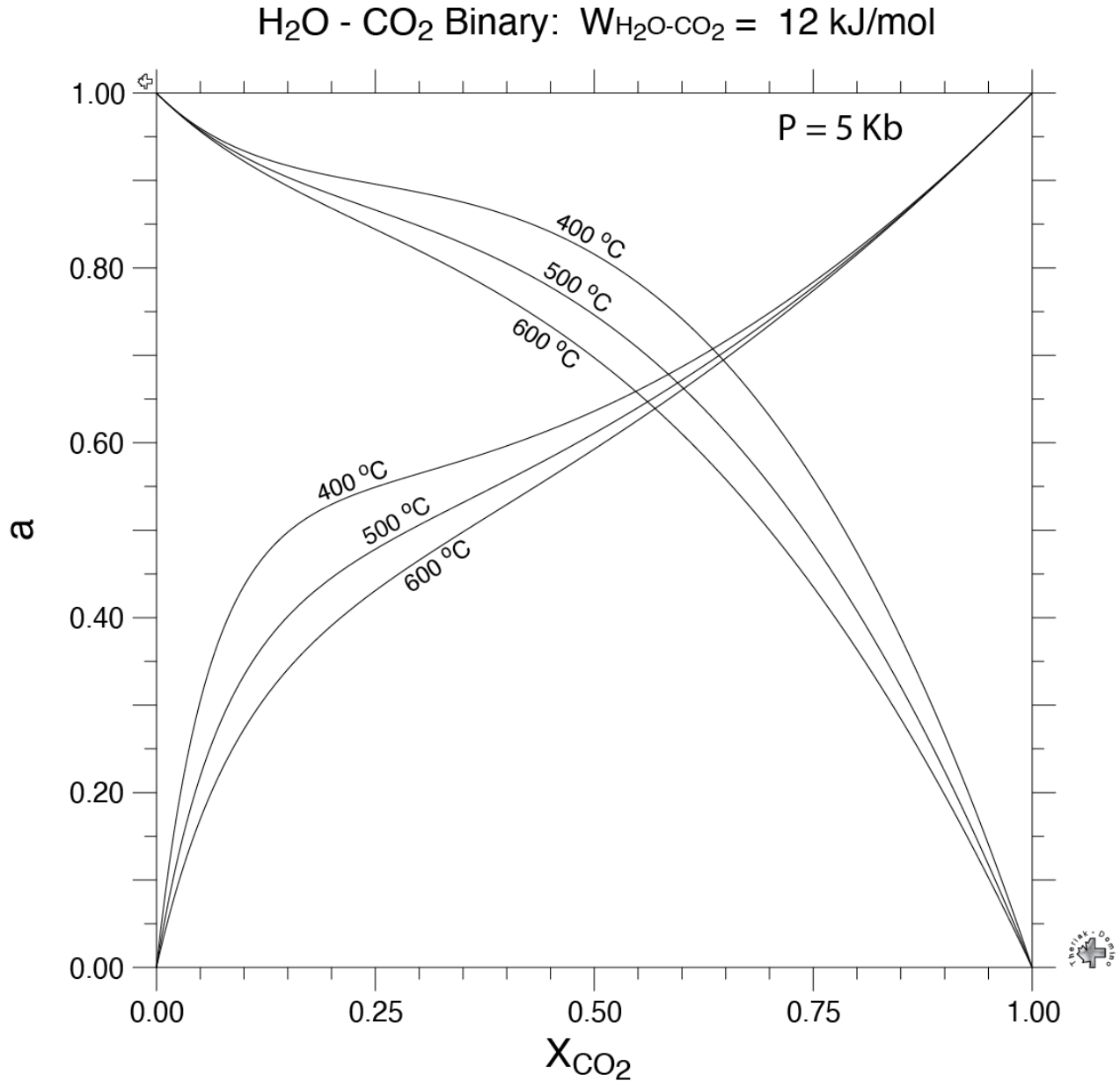


Program Thalia

Calculates thermodynamic properties of both pure phases and solution models at P & T

Can plot properties across solution model binaries:

- chemical potential
- G (mech, ideal mix, excess mix, etc.)
- Activities of phase components



Program Theriak

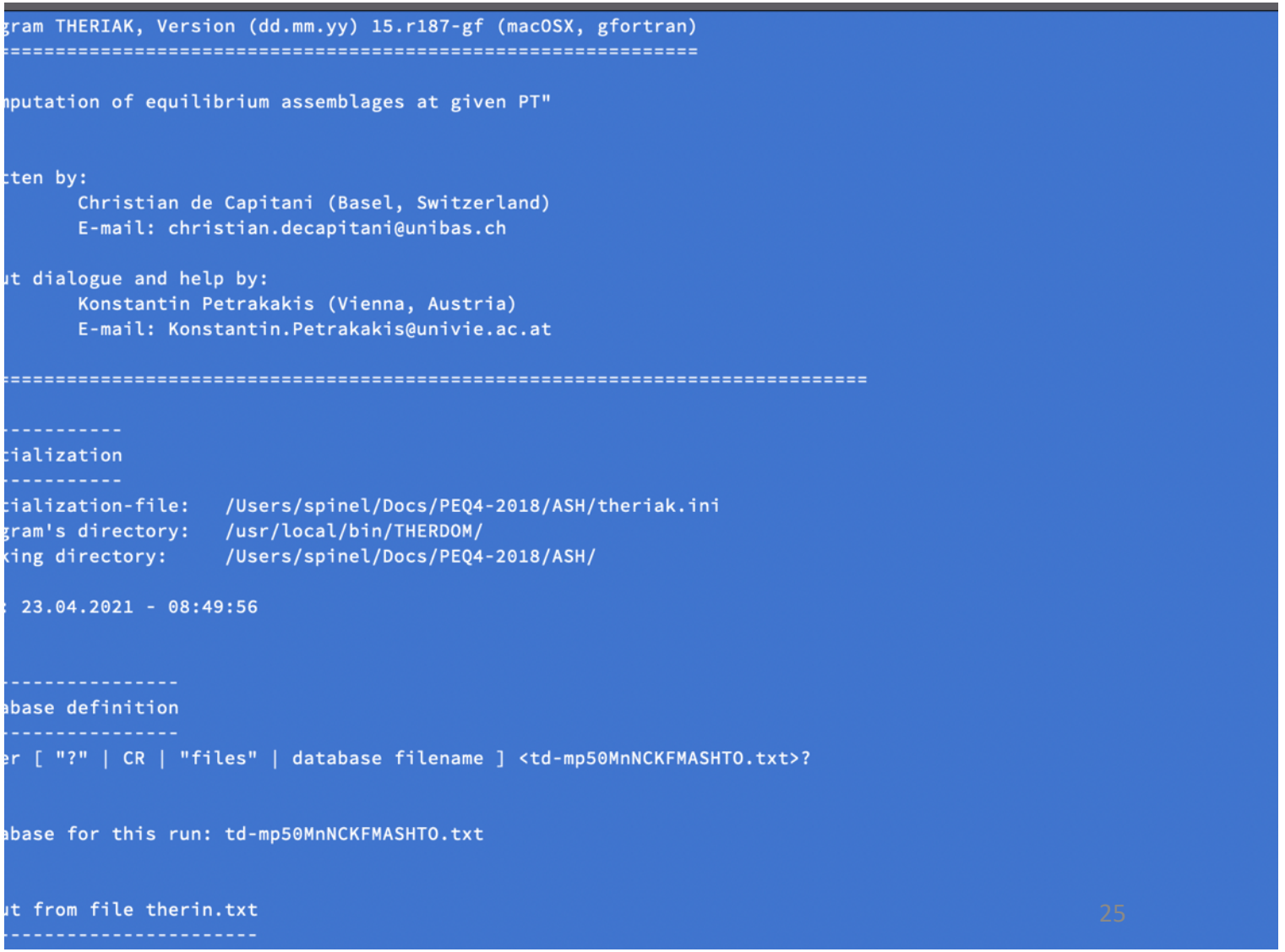
Calculates equilibrium assemblage for a fixed bulk composition

Loops over several input P & T

Output includes phase and system properties for each input P & T

Can plot results easily, in spreadsheet or using the plotxy program

Can pass arguments on the command line to automate calculations and interface with your own programs (written in different languages); see add-on program Theriak_D (Duesterhoeft & de Capitani, 2013) for examples



Theriak: assemblage output

Lists abundance of stable phases

Lists the phase composition (proportions of components and site composition)

Look for ** in output beneath the activity columns; if you see them it indicates the calculation failed to converge to a proper solution

Columns x & x indicate the proportion (or mole fraction) of each phase component

Columns activity and act.(x) lists the activity of each phase component calculated in 2 ways; they should be very close to one another but are rarely identical

```
-----------------
ibrium assemblage:
-----------------

 5000.00 bar       P(Gas) =  5000.00 bar     T =  550.00 C    =  823.15 K

le phases:   11    loop =  69     loop2 =   1     max.phases =      1640     gcalc =   1934771       blkshift = 3.12250E-15
estions:  24530    ridiculous phases:    1125     non-ideal min.:   4845     newton:      2298       ideal min.:          0
  = 2.11135E-12    G(System) =  -132423807.28     stepsize = 0.00000E+00     R =     8.3144100       MaxG(-)  = 0.00000E+00


   phase                 N         mol%                                    x             x          activity       act.(x)
   -----                 -         ----                                    -             -          --------       -------
1  PO_trov             5.140287    2.822664        trot              0.066571     6.65707E-02   5.88502E-01   5.88502E-01
                                                   trov              0.933429     9.33429E-01   9.97608E-01   9.97608E-01

                     [Fe(M)]     = 8.83321E-01     [v(M)]      = 1.16679E-01

2  FLUID3_H2O         94.983537   52.157911        H2O               0.984071     9.84071E-01   9.84732E-01   9.84732E-01
                                                   H2S               0.005305     5.30537E-03   1.19971E-02   1.19970E-02
                                                   CH4               0.000087     8.66262E-05   6.43936E-04   6.43832E-04
                                                   CO2               0.010435     1.04354E-02   4.87212E-02   4.87213E-02
                                                   O2                0.000000     6.76935E-27   2.66117E-26   6.53412E-27
                                                   S2                0.000000     1.72511E-08   1.67080E-08   1.66788E-08
                                                   H2                0.000095     9.54989E-05   6.62743E-04   6.62767E-04
                                                   CO                0.000006     6.15911E-06   5.43405E-05   5.43240E-05

                     [h2o(M)]    = 9.84071E-01     [h2s(M)]    = 5.30537E-03     [ch4(M)]    = 8.66262E-05
                     [co2(M)]    = 1.04354E-02     [s2(M)]     = 1.72511E-08     [o2(M)]     = 6.76935E-27
                     [h2(M)]     = 9.54989E-05     [co(M)]     = 6.15911E-06

3  GRT_spss            0.004862    0.002670        py                0.139167     1.39167E-01   4.69940E-03   4.69940E-03
                                                   alm               0.082306     8.23057E-02   6.80192E-04   6.80192E-04
                                                   spss              0.704593     7.04593E-01   3.35855E-01   3.35855E-01
                                                   gr                0.073167     7.31667E-02   7.30673E-04   7.30673E-04
                                                   kho               0.000768     7.67967E-04   2.45168E-08   2.45168E-08

                     [Mg(X)]     = 1.39935E-01     [Fe(X)]     = 8.23057E-02     [Mn(X)]     = 7.04593E-01
                     [Ca(X)]     = 7.31667E-02
                     [Al(Y)]     = 9.99232E-01     [F3(Y)]     = 7.67967E-04
```

Theriak: assemblage output

Below the phase composition output on the last slide, a nice data table with the main assemblage information appears

Phase abundance (moles, volume, weight), density and H2O content is listed

I typically look at vol% on a first pass

All of the information seen on screen appears in a simple text log file

~/Docs/PEQ4-2018/ASH — theriak-20-010-3if

```
--------------------------------------
volumes and densities of stable phases:
--------------------------------------

 solid phases          N       volume/mol  volume[ccm]    vol%  |    wt/mol      wt [g]      wt %  | density [g/ccm]
 ------------                                                    |
 PO_trov            5.1403       18.0263      92.6603    3.9306 |    81.3941     418.3889    6.4302 |     4.515297
 GRT_spss           0.0049       118.8915      0.5780    0.0245 |    479.1731      2.3297    0.0358 |     4.030340
 MRG_ma             0.1786       131.6385     23.5100    0.9973 |    396.6954     70.8479    1.0889 |     3.013520
 WM_mu              2.1203       141.6728    300.3942   12.7424 |    397.4061    842.6351   12.9504 |     2.805098
 CHL14_ames         0.9253       211.0187    195.2491    8.2823 |    565.8082    523.5248    8.0460 |     2.681318
 ky                 1.8769        44.5727     83.6606    3.5488 |    162.0456    304.1513    4.6745 |     3.635538
 q                 72.1245        22.9979   1658.7158   70.3611 |     60.0843   4333.5508   66.6023 |     2.612594
 ru                 0.1400        19.0341      2.6648    0.1130 |     79.8658     11.1812    0.1718 |     4.195934
                                             ----------  -------- |             ----------  -------- |   ----------
 total of solids                            2357.4328  100.0000 |             6506.6098  100.0000 |     2.760040


 gases and fluids      N       volume/mol  volume[ccm]             wt/mol      wt [g]             density [g/ccm]
 ---------------
 FLUID3_H2O        94.9835       21.8768    2077.935               18.3701   1744.8605                0.839709
 QFM-BUFFER         2.5412       19.0511      48.412               31.9988     81.3146                1.679627
 -PPS-BUFFER        2.0721      -10.7346     -22.243              -64.1300   -132.8842                5.974121


----------------------------
H2O content of stable phases:
----------------------------

                                                                |  wt% of     wt% of     wt% of
 solid phases          N      H2O[pfu]    H2O[mol]     H2O [g]  |  phase      solids     H2O.solid
 ------------                                                   |
 MRG_ma             0.1786      1.000       0.1786       3.2174 |  4.54134    0.04945     2.9766
 WM_mu              2.1203      1.000       2.1203      38.1985 |  4.53322    0.58707    35.3389
 CHL14_ames         0.9253      4.000       3.7011      66.6759 | 12.73596    1.02474    61.6845
                                        --------    ---------- |             --------
 total H2O in solids                        6.0000     108.0918 |             1.66126

                                                                |  wt% of
 gases and fluids      N      H2O[pfu]    H2O[mol]     H2O [g]  |  phase
 ---------------                                                |
 FLUID3_H2O        94.9835      0.990      94.0000    1693.4362 |  97.05281
```

Theriak – Loop Tables

Theriak can automatically loop over a sequence of P-T and save hundreds of system and phase properties to a text file (comma-delimited)

System Properties:

U, G, H, S, V, TS, PV

System composition (for fractionation)

Volume and density of solids

Moles, weight, and weight % H2O in solids

- **Fractionation calculations (can remove variable percentages of any phase produced at each step)**
- **Can manually specify changes in bulk composition at each step**
- **Program plotxy reads and plots loop table output from theriak**

Phase Properties:

Abundance (moles and volume)

Density and molar volume

Mg# (Mg / (Mg+Fe_T)

Si p.f.u., Al p.f.u.

Moles of H2O and weight of H2O in each phase

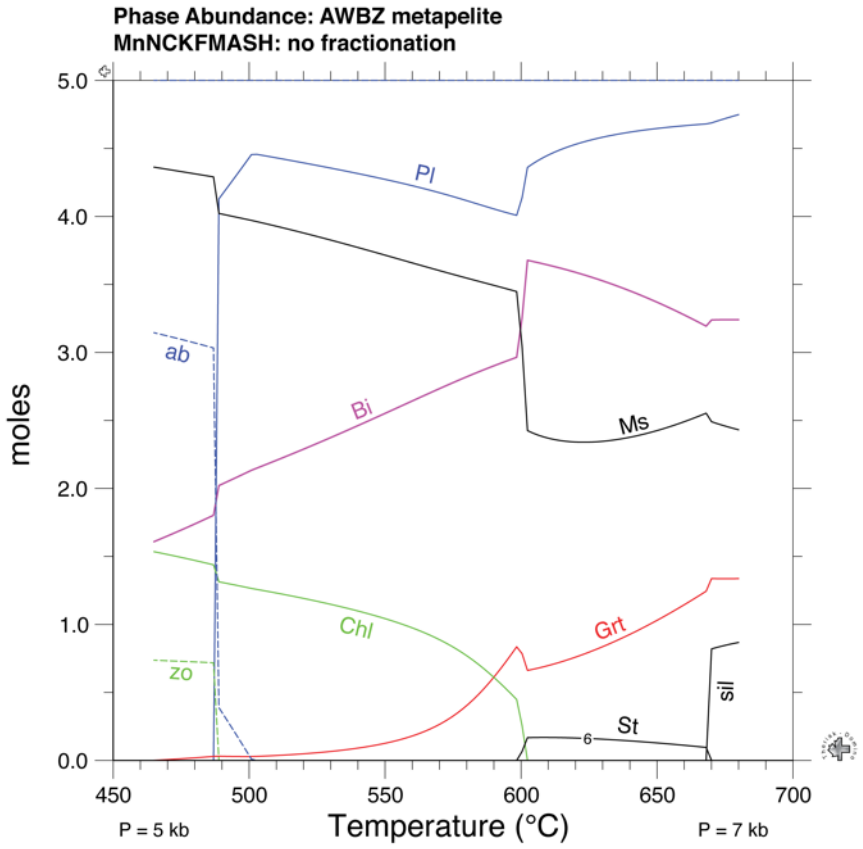
Moles, proportion, & activity of each phase component

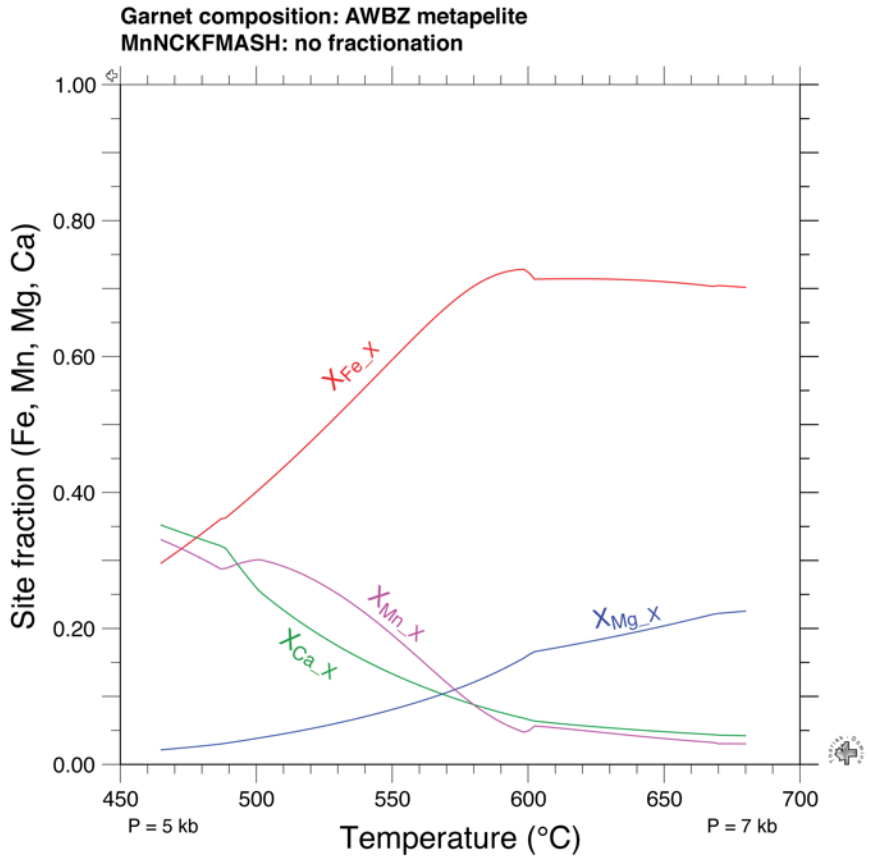
All site fractions

Theriak & PlotXY – Phase abundance & Grt chemistry

Predicted mineral abundance and garnet composition: 465 °C @ 5 kb to 680 °C @ 7kb

- Calculated using theriak driver file to generate loop table in 100 increments up T
- File setup time: 5 min; Calculation time: 1 min 1.8 sec; Plotting and drafting time: 30-45 min
- Postscript plots generated using program plotxy shown below, with manual touch up of labels and coloring

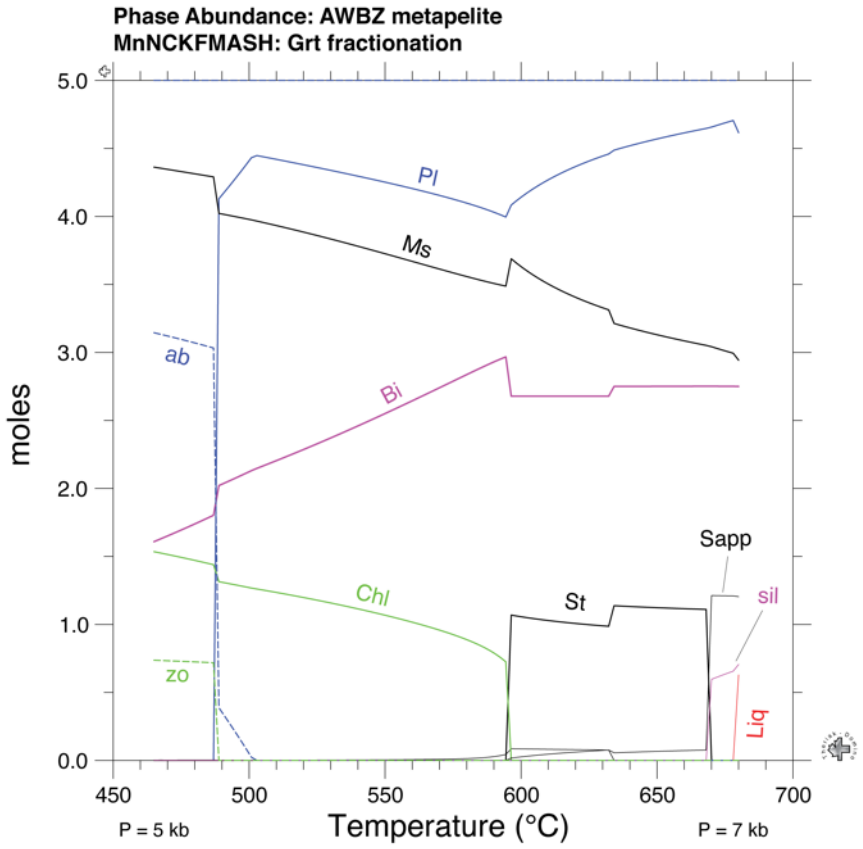


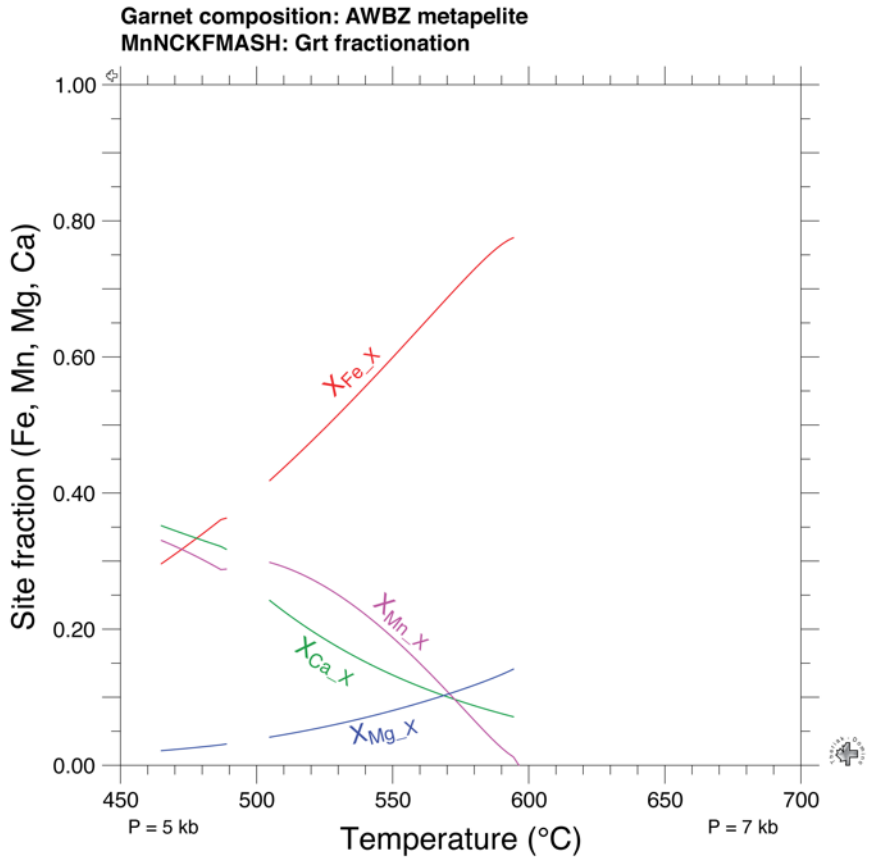


Theriak & PlotXY – Simple garnet fractionation

Predicted mineral abundance and garnet composition: 465 °C @ 5 kb to 680 °C @ 7kb

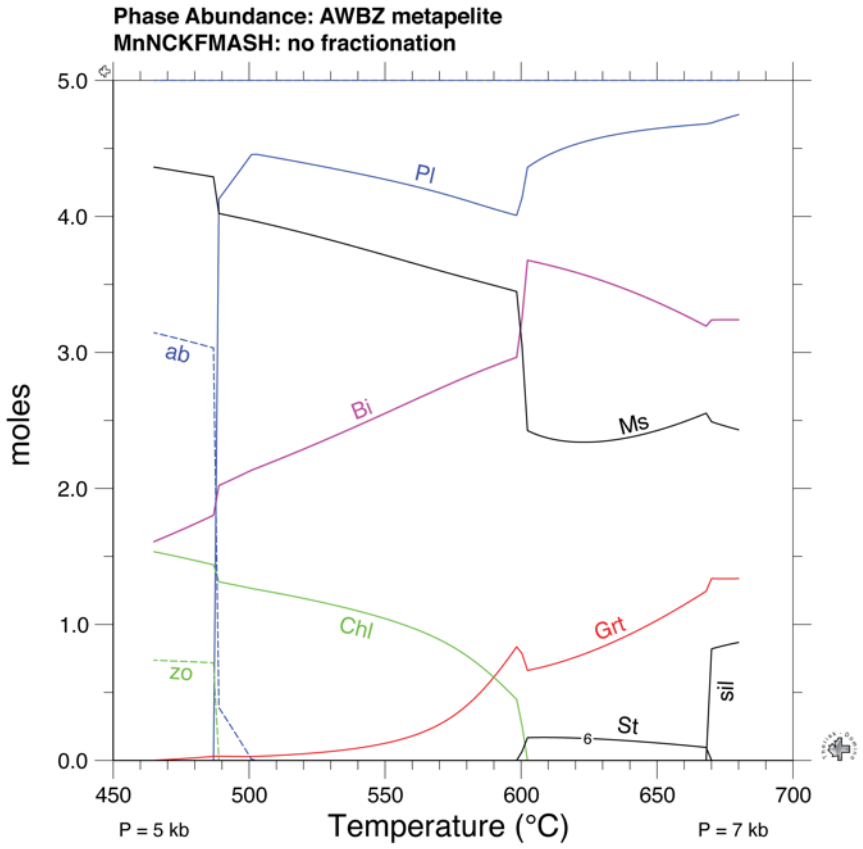
- 100 increments up T, 98% of all garnet removed from system at each step
- Grt production stops by 600 °C along this P-T vector

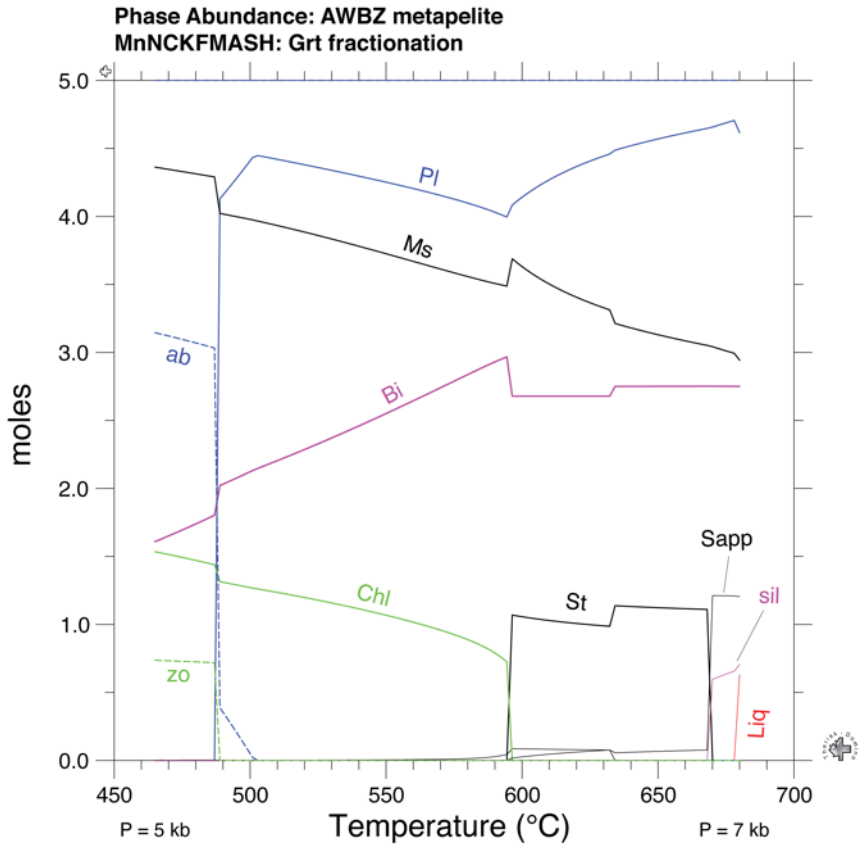




Constant bulk vs garnet fractionation

- St > 4x more abundant in Grt fractionating case
- Bt consumed & Ms produced in fractionating case; opposite in non-fractionation run

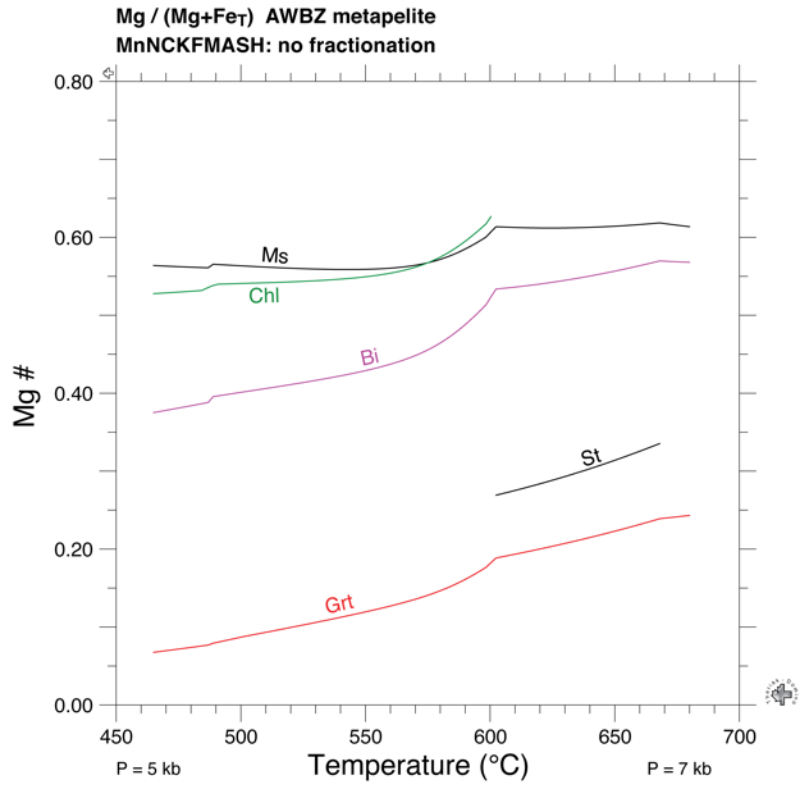




Program PlotXY

- Generates quality output in postscript and svg format
- Can plot all variables saved in loop table during run
- Need to add or subtract variables at times

103+107 = n_[alm] + n_[gr] = total moles of garnet



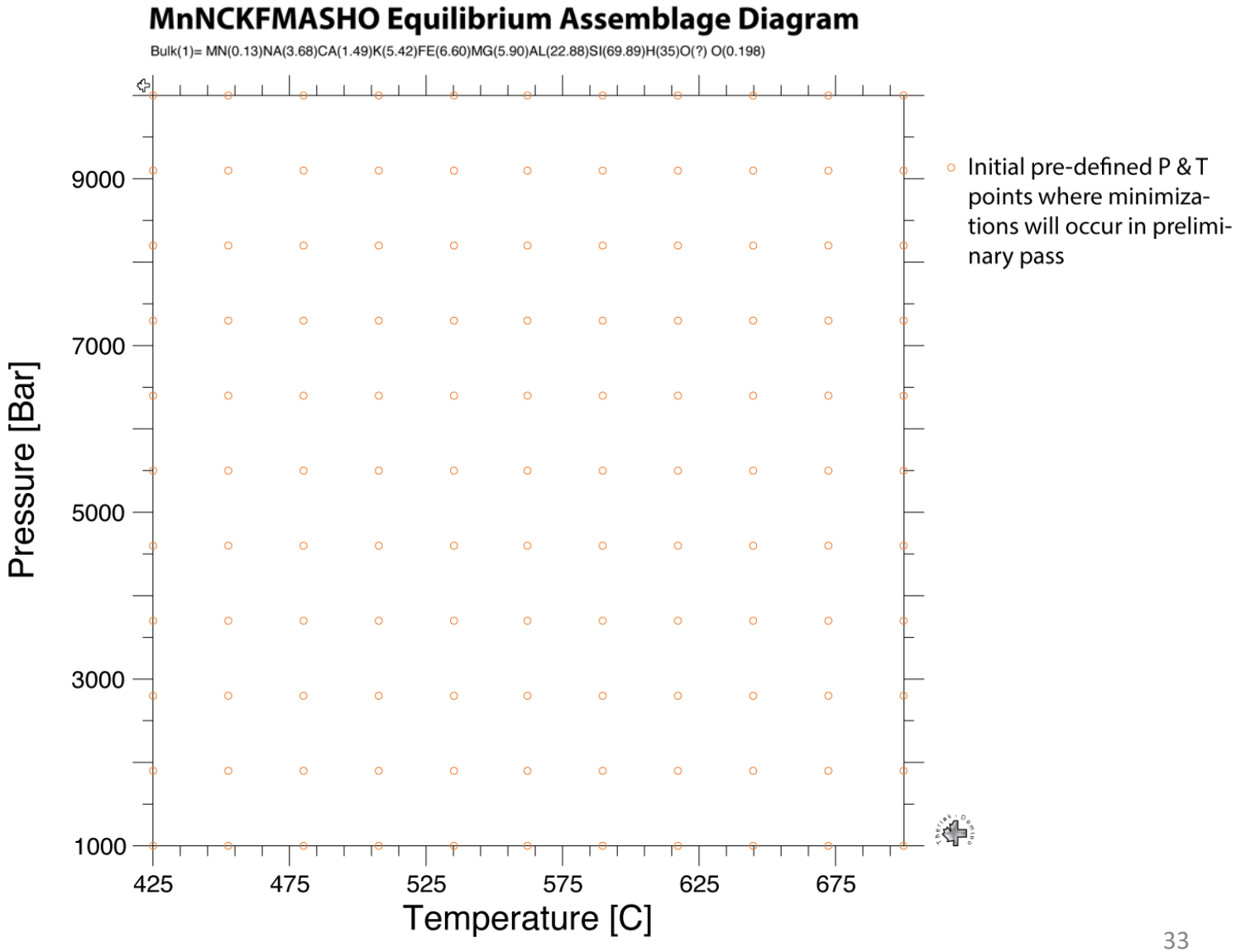
~/Docs/PEQ-2021/AWBZ/PT-MnNCKFMASH-ds62a/wo-mic/Frac — plotxy-20-010if

~/MYCODE/GITLAB_SpinelDev/TD/tddev — -zsh | ...Z/PT-MnNCKFMASH-ds62a/wo-mic/Frac — plotxy-20-010if

```
 Enter [ "?" | CR | "files" | filename ] < >?
thktab.tab

 Variables available:

[b]: b-rich solution  a : activity    blk: bulk     Mg# : Mg/(Mg+Fe)    mvol: molar volume
n  : mass [mol]       pc: percent     wt : weight   x   : mole fraction

   1: NR(step)           2: Pressure           3: Temperature        4: Al_pfu_[abh]       5: Al_pfu_[annm]
   6: Al_pfu_[daph]      7: Al_pfu_[mu]        8: G_overstep         9: G_system          10: G_tot
  11: H_tot             12: Mg#_[alm]         13: Mg#_[annm]        14: Mg#_[daph]       15: Mg#_[fst]
  16: Mg#_[gr]          17: Mg#_[mu]          18: PV-_tot           19: S_tot            20: Si_pfu_[abh]
  21: Si_pfu_[annm]     22: Si_pfu_[daph]     23: Si_pfu_[mu]       24: TS_tot           25: U_tot
  26: V_H2O             27: V_[abh]           28: V_[alm]           29: V_[annm]         30: V_[daph]
  31: V_[fst]           32: V_[gr]            33: V_[mu]            34: V_ab             35: V_q
  36: V_sill            37: V_solids          38: V_tot             39: V_zo             40: a_abh_[abh]
  41: a_afchl_[daph]    42: a_alm_[alm]       43: a_alm_[gr]        44: a_ames_[daph]    45: a_anC_[abh]
  46: a_annm_[annm]     47: a_cel_[mu]        48: a_clin_[daph]     49: a_daph_[daph]    50: a_east_[annm]
  51: a_fcel_[mu]       52: a_fst_[fst]       53: a_gr_[alm]        54: a_gr_[gr]        55: a_mat_[mu]
  56: a_mmbi_[annm]     57: a_mmchl_[daph]    58: a_mnstm_[fst]     59: a_mstm_[fst]     60: a_mu_[mu]
  61: a_obi_[annm]      62: a_ochl1_[daph]    63: a_ochl4_[daph]    64: a_pa_[mu]        65: a_phl_[annm]
  66: a_py_[alm]        67: a_py_[gr]         68: a_san_[abh]       69: a_spss_[alm]     70: a_spss_[gr]
  71: blk_AL            72: blk_CA            73: blk_E             74: blk_FE           75: blk_H
  76: blk_K             77: blk_MG            78: blk_MN            79: blk_NA           80: blk_O
  81: blk_SI            82: mvol_H2O          83: mvol_[abh]        84: mvol_[alm]       85: mvol_[annm]
  86: mvol_[daph]       87: mvol_[fst]        88: mvol_[gr]         89: mvol_[mu]        90: mvol_ab
  91: mvol_q            92: mvol_sill         93: mvol_zo           94: n_H2O            95: n_H2O_H2O
  96: n_H2O_[annm]      97: n_H2O_[daph]      98: n_H2O_[fst]       99: n_H2O_[mu]      100: n_H2O_solids
 101: n_H2O_zo         102: n_[abh]          103: n_[alm]          104: n_[annm]        105: n_[daph]
 106: n_[fst]          107: n_[gr]           108: n_[mu]           109: n_ab            110: n_abh_[abh]
 111: n_afchl_[daph]   112: n_alm_[alm]      113: n_alm_[gr]       114: n_ames_[daph]   115: n_anC_[abh]
 116: n_annm_[annm]    117: n_cel_[mu]       118: n_clin_[daph]    119: n_daph_[daph]   120: n_east_[annm]
 121: n_fcel_[mu]      122: n_fst_[fst]      123: n_gr_[alm]       124: n_gr_[gr]       125: n_mat_[mu]
 126: n_mmbi_[annm]    127: n_mmchl_[daph]   128: n_mnstm_[fst]    129: n_mstm_[fst]    130: n_mu_[mu]
 131: n_obi_[annm]     132: n_ochl1_[daph]   133: n_ochl4_[daph]   134: n_pa_[mu]       135: n_phl_[annm]
 136: n_py_[alm]       137: n_py_[gr]        138: n_q              139: n_san_[abh]     140: n_sill
 141: n_spss_[alm]     142: n_spss_[gr]      143: n_zo             144: pcH2O_solids    145: rho_H2O
 146: rho_[abh]        147: rho_[alm]        148: rho_[annm]       149: rho_[daph]      150: rho_[fst]
 151: rho_[gr]         152: rho_[mu]         153: rho_ab           154: rho_q           155: rho_sill
 156: rho_solids       157: rho_zo           158: wt_H2O_H2O       159: wt_H2O_[annm]   160: wt_H2O_[daph]
 161: wt_H2O_[fst]     162: wt_H2O_[mu]      163: wt_H2O_solids    164: wt_H2O_zo       165: x_Al(M1)_[daph]
 166: x_Al(M2A)_[mu]   167: x_Al(M3)_[annm]  168: x_Al(M4)_[daph]  169: x_Al(T)_[annm]  170: x_Al(T1)_[mu]
 171: x_Al(T2)_[daph]  172: x_Ca(A)_[abh]    173: x_Ca(A)_[mu]     174: x_Ca(X)_[alm]   175: x_Ca(X)_[gr]
 176: x_Fe(M1)_[daph]  177: x_Fe(M12)_[annm] 178: x_Fe(M23)_[daph] 179: x_Fe(M2A)_[mu]  180: x_Fe(M3)_[annm]
 181: x_Fe(M4)_[daph]  182: x_Fe(X)_[alm]    183: x_Fe(X)_[fst]    184: x_Fe(X)_[gr]    185: x_K(A)_[abh]
 186: x_K(A)_[mu]      187: x_Mg(M1)_[daph]  188: x_Mg(M12)_[annm] 189: x_Mg(M23)_[daph] 190: x_Mg(M2A)_[mu]
 191: x_Mg(M3)_[annm]  192: x_Mg(M4)_[daph]  193: x_Mg(X)_[alm]    194: x_Mg(X)_[fst]   195: x_Mg(X)_[gr]
 196: x_Mn(M1)_[daph]  197: x_Mn(M12)_[annm] 198: x_Mn(M23)_[daph] 199: x_Mn(M3)_[annm] 200: x_Mn(X)_[alm]
 201: x_Mn(X)_[fst]    202: x_Mn(X)_[gr]     203: x_Na(A)_[abh]    204: x_Na(A)_[mu]    205: x_Si(T)_[annm]
 206: x_Si(T1)_[mu]    207: x_Si(T2)_[daph]  208: x_abh_[abh]      209: x_afchl_[daph]  210: x_alm_[alm]
 211: x_alm_[gr]       212: x_ames_[daph]    213: x_anC_[abh]      214: x_annm_[annm]   215: x_cel_[mu]
 216: x_clin_[daph]    217: x_daph_[daph]    218: x_east_[annm]    219: x_fcel_[mu]     220: x_fst_[fst]
 221: x_gr_[alm]       222: x_gr_[gr]        223: x_mat_[mu]       224: x_mmbi_[annm]   225: x_mmchl_[daph]
 226: x_mnstm_[fst]    227: x_mstm_[fst]     228: x_mu_[mu]        229: x_obi_[annm]    230: x_ochl1_[daph]
 231: x_ochl4_[daph]   232: x_pa_[mu]        233: x_phl_[annm]     234: x_py_[alm]      235: x_py_[gr]
 236: x_san_[abh]      237: x_spss_[alm]     238: x_spss_[gr]

definition example for axes: 3,5,6+7,8+9
```

Program Domino - Methodology

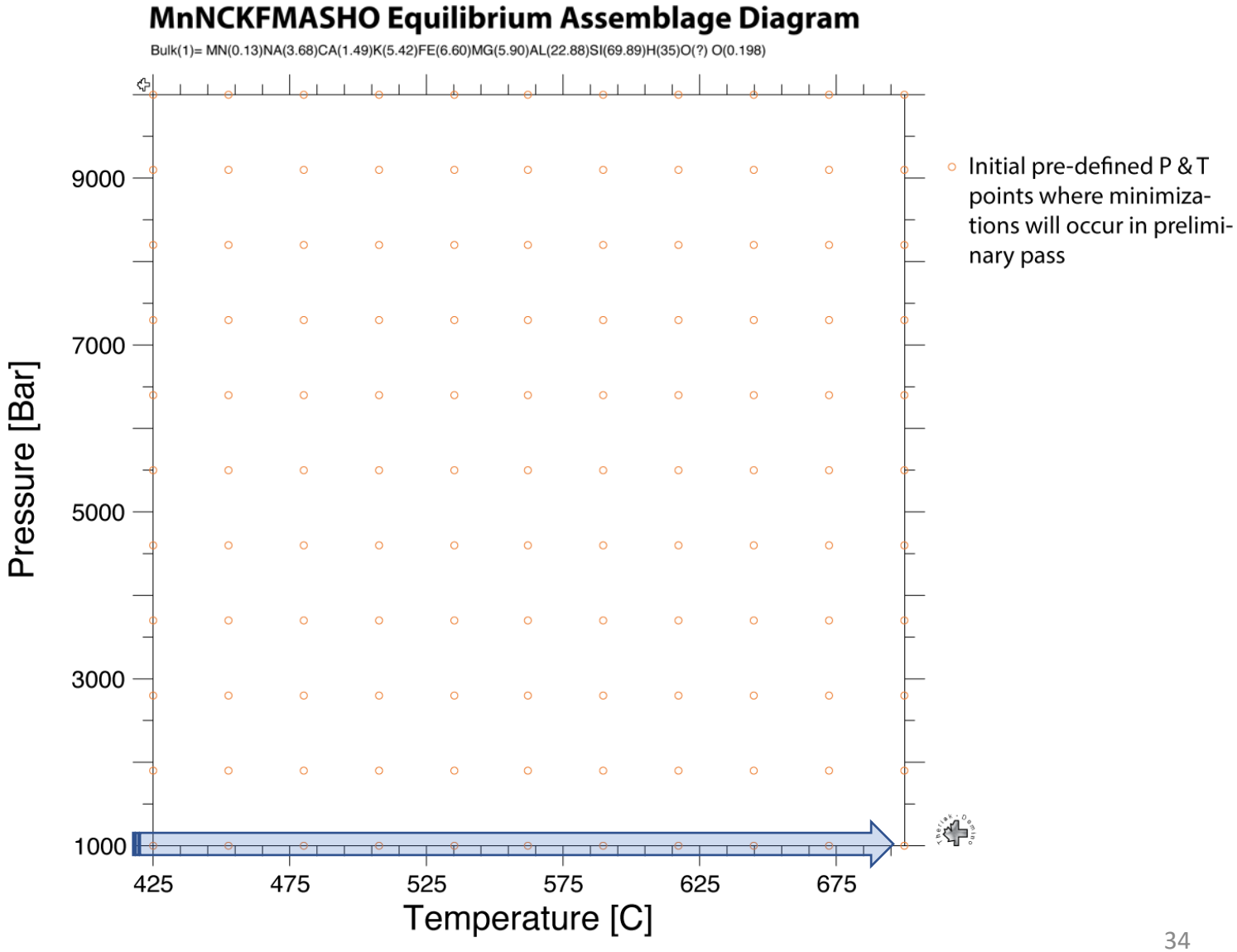
- Details provided in de Capitani & Petrakakis (2010, Am. Min.)
- Searches for assemblage changes over the diagram
- Constrains the location of each assemblage boundary, but does not calculate the boundary directly
- Involves several levels of refinement to build up a complete diagram
- User can control the density of initial grid points; defaults to 10 intervals (11 points) in X and Y directions



Program Domino - Methodology

Initial Pass

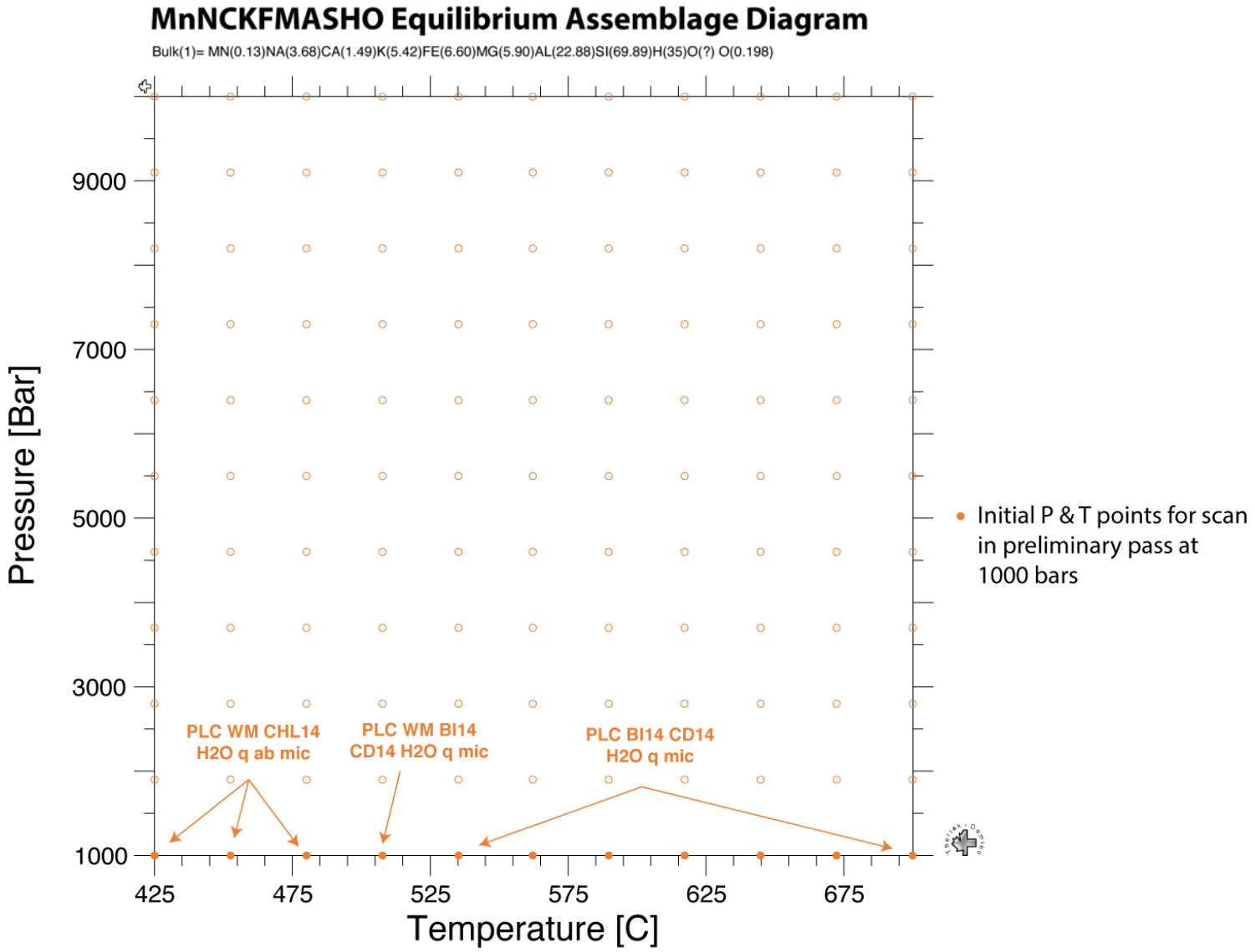
- Calculates Equilibrium assemblage at a series of equally spaced points in X direction, starting at base of diagram



Program Domino - Methodology

Initial Pass

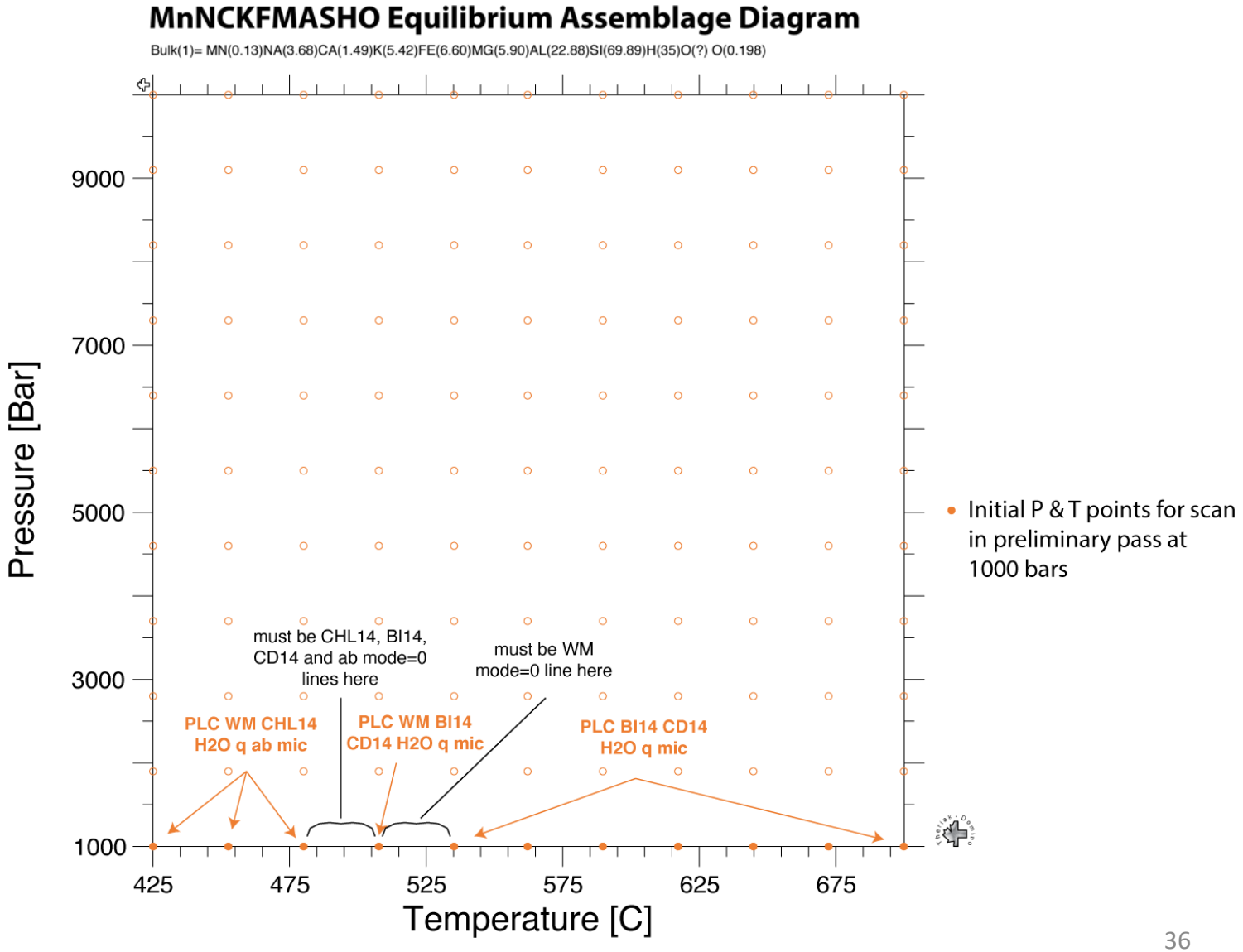
- Calculates Equilibrium assemblage at a series of equally spaced points in X direction, starting at base of diagram
- Records the assemblage at each point and identifies adjacent points with different assemblages



Program Domino - Methodology

Initial Pass

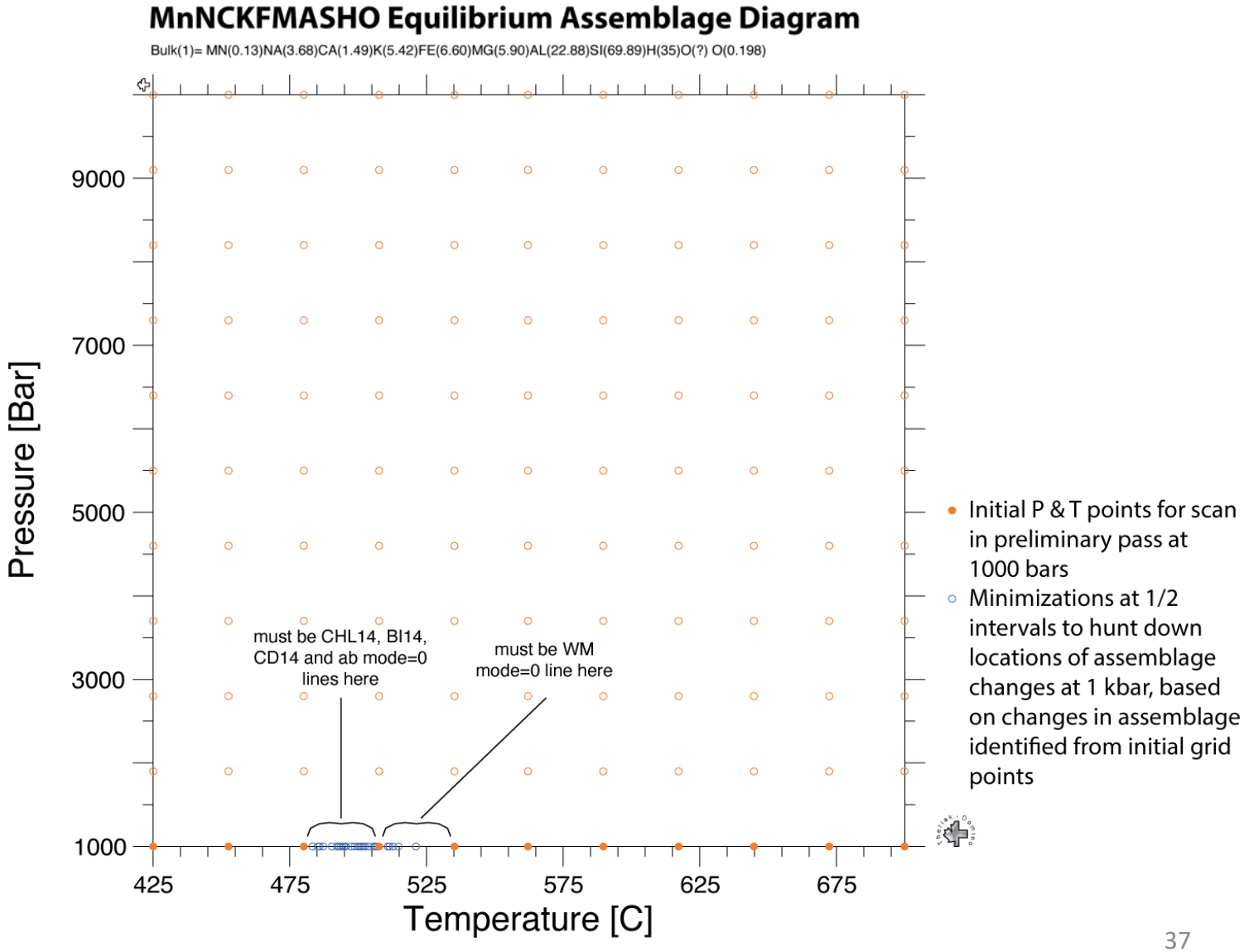
- Calculates Equilibrium assemblage at a series of equally spaced points in X direction, starting at base of diagram
- Records the assemblage at each point and identifies adjacent points with different assemblages



Program Domino - Methodology

Initial Pass

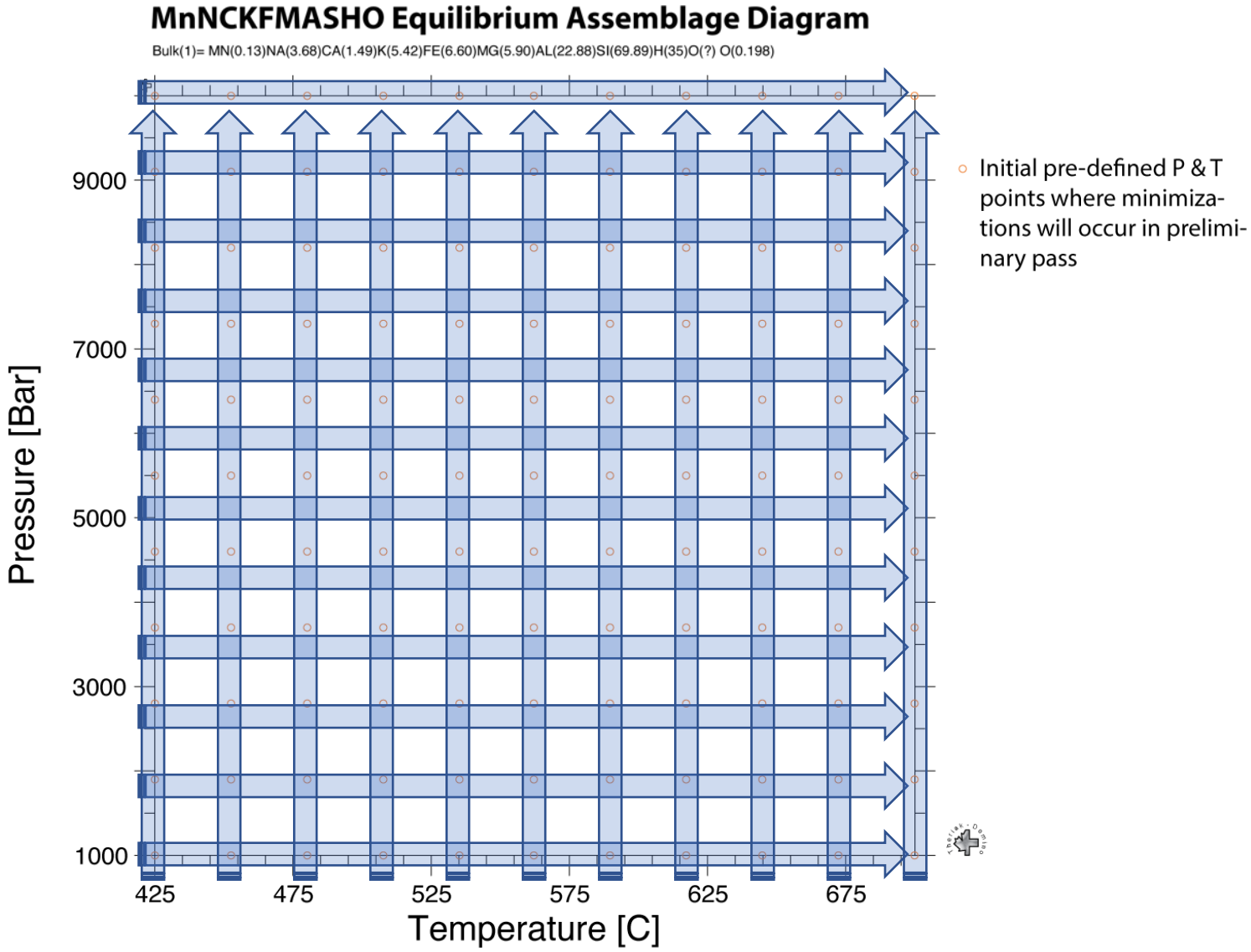
- Calculates Equilibrium assemblage at a series of equally spaced points in X direction, starting at base of diagram
- Records the assemblage at each point and identifies adjacent points with different assemblages
- Goes back to intervals with assemblage changes and does more minimizations at interval halves, repeating until it has located assemblage change boundaries to within some pre-defined x-precision



Program Domino - Methodology

Initial Pass

- Calculates Equilibrium assemblage at a series of equally spaced points in X direction, starting at base of diagram
- Records the assemblage at each point and identifies adjacent points with different assemblages
- Goes back to intervals with assemblage changes and does more minimizations at interval halves, repeating until it has located assemblage change boundaries to within some pre-defined x-precision
- Iterates above procedure at progressively higher Y values
- Then does the same procedure at intervals along the the X axis



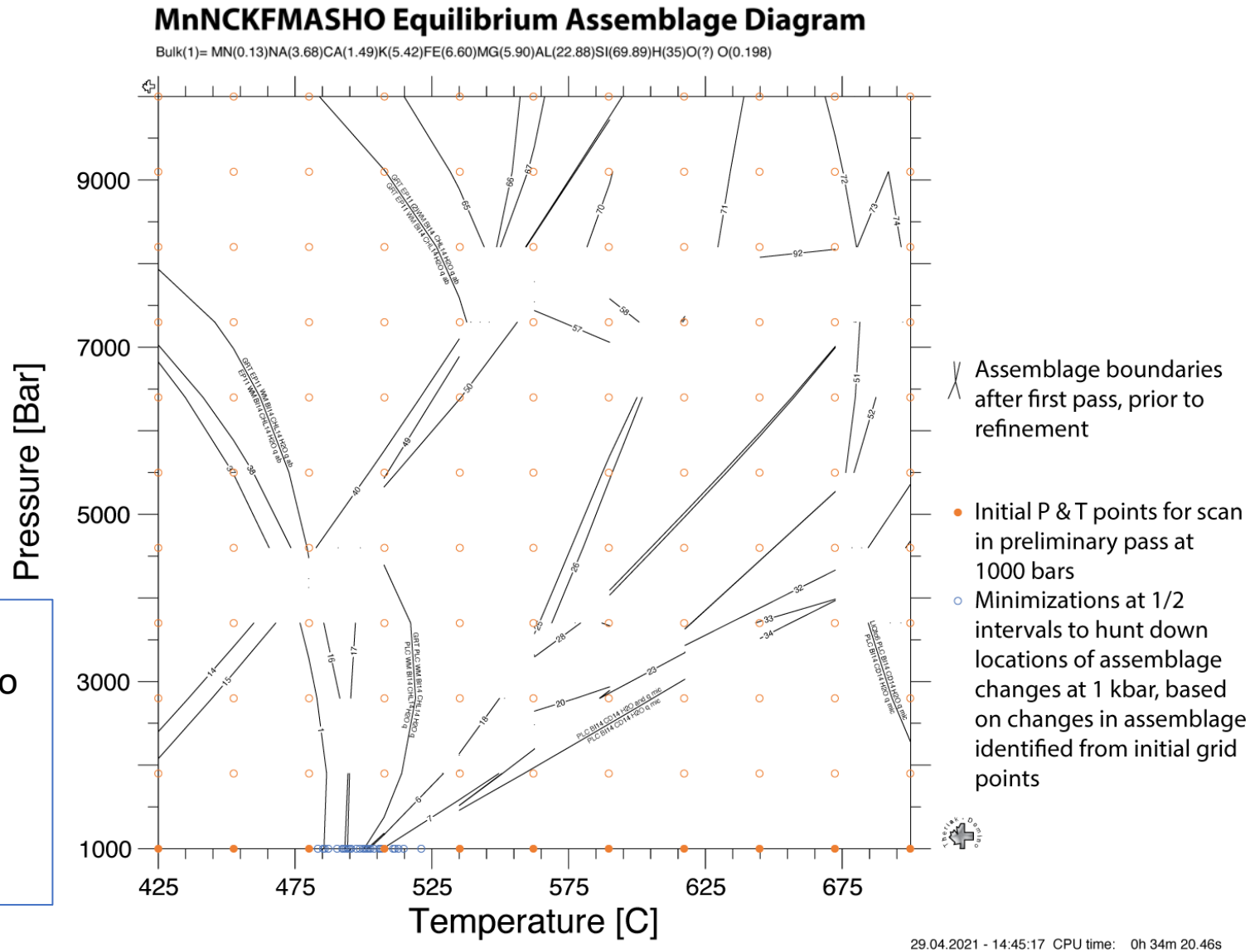
Program Domino - Methodology

Initial Pass

- Can plot the diagram at the end of initial pass (guzzler & explot)
- Domino starts several levels of refinement
- Identifies where lines have an “openend” or have large changes in angle (“bump”), and does more minimizations in those specific areas to complete boundaries

Domino closely ‘brackets’ the locations of lines on the diagram by doing G minimizations very close to assemblage changes along the grid

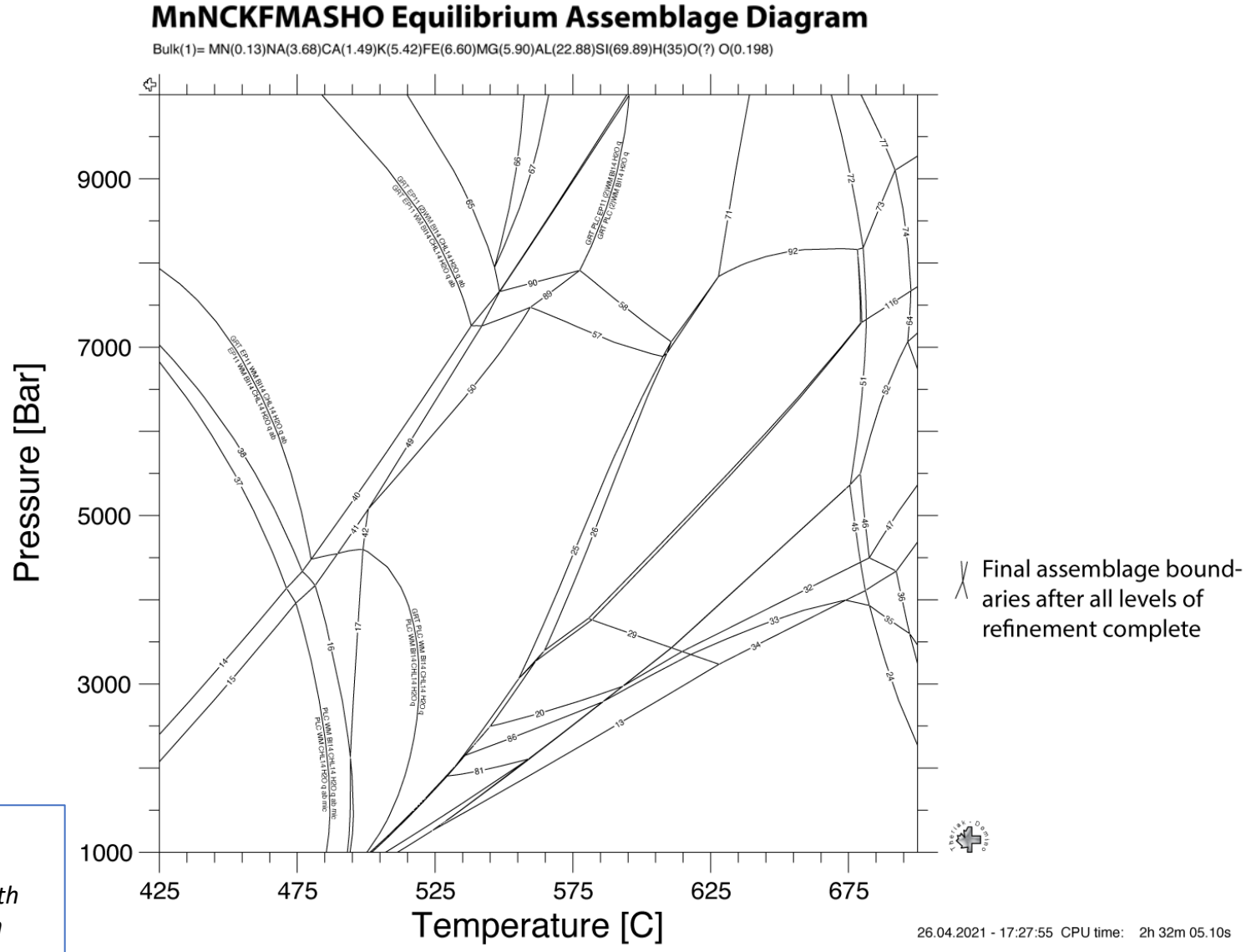
THERMOCALC solves a set of non-linear equilibria to calculate the locations of lines



Program Domino – Raw Output

Final Diagram

- Example of raw undrafted diagram (except title and legend at right)
- User can control the size of labels and types of labels
- Postscript and SVG graphics output produced by bundled programs guzzler & explot
- Polygon fills are not produced by bundled programs, so fills need constructed manually



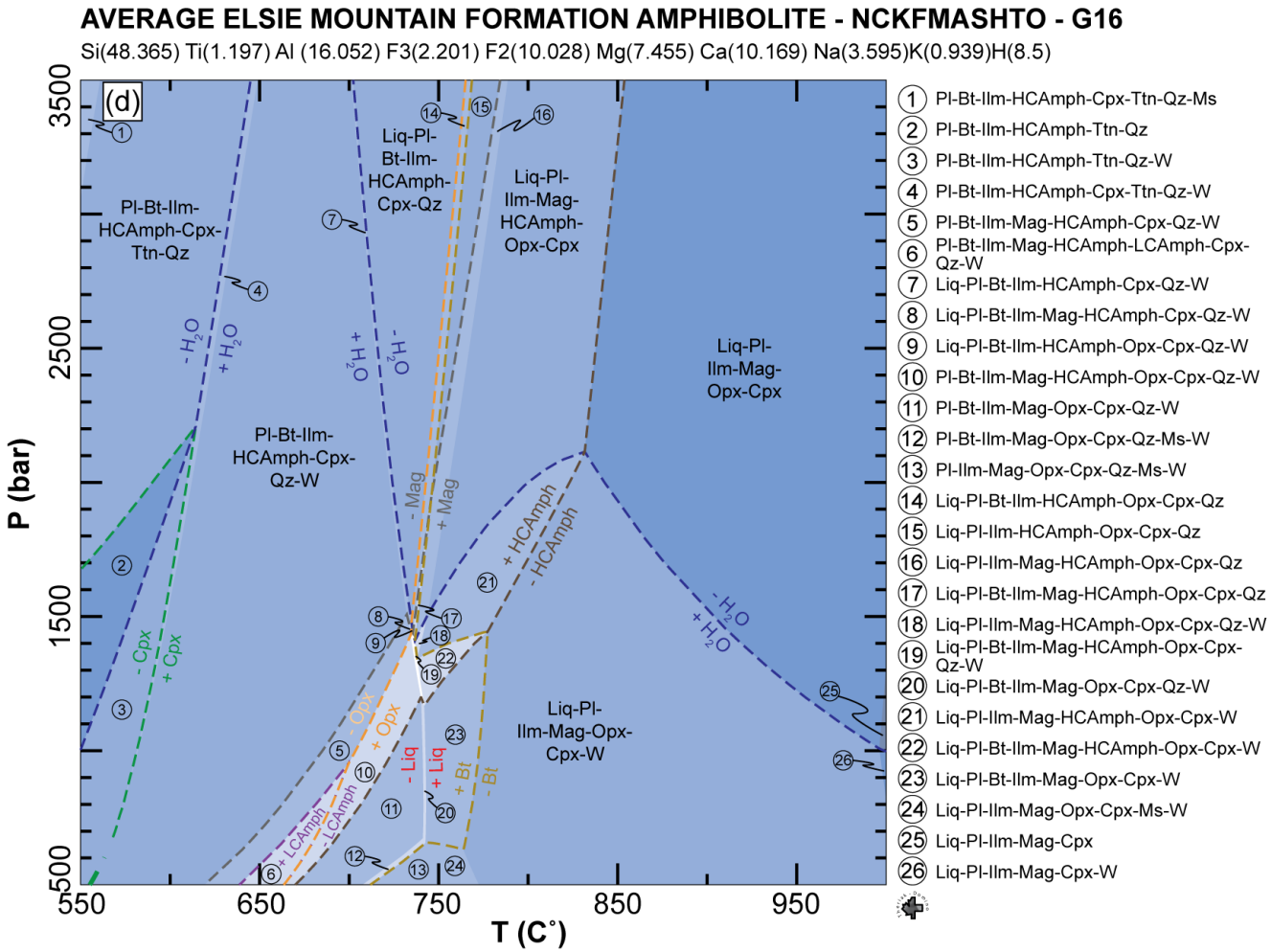
Note: Considering pure microcline for low-T Kfs stability has resulted in destabilizing ternary Kfs (using san member) at low-P/high-T. Dealing with such issues may require calculating the diagram twice.

Average Waterville Fm. Biotite Zone composition used in Tinkham *et al*. (2001)

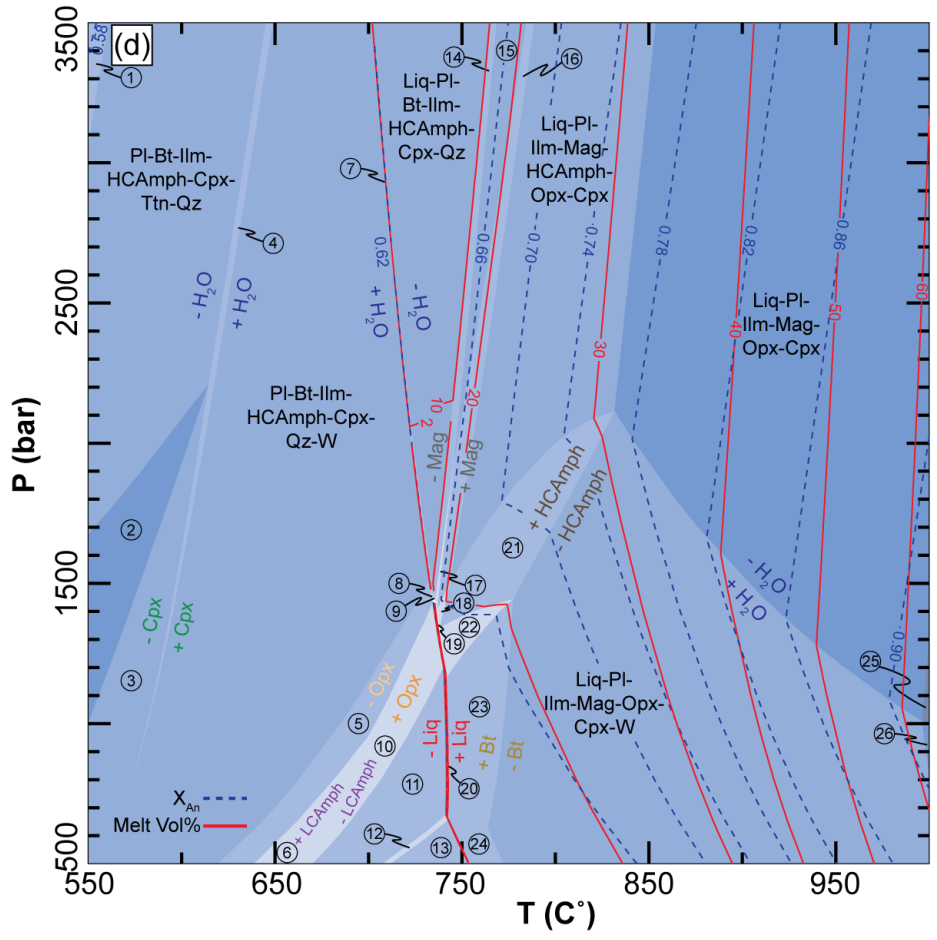
Program Domino - Contours

Manually drafted Domino output

Contours of melt vol % and X_{An}



After Jørgensen et al. (2019)

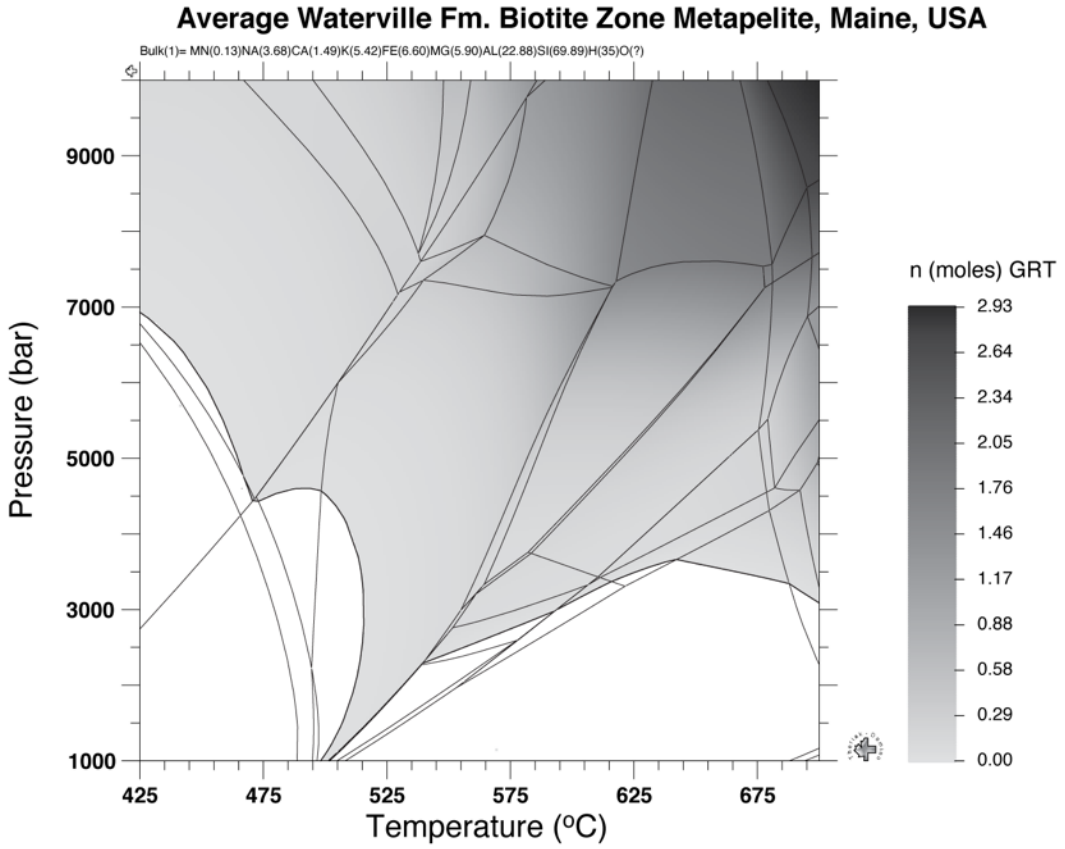


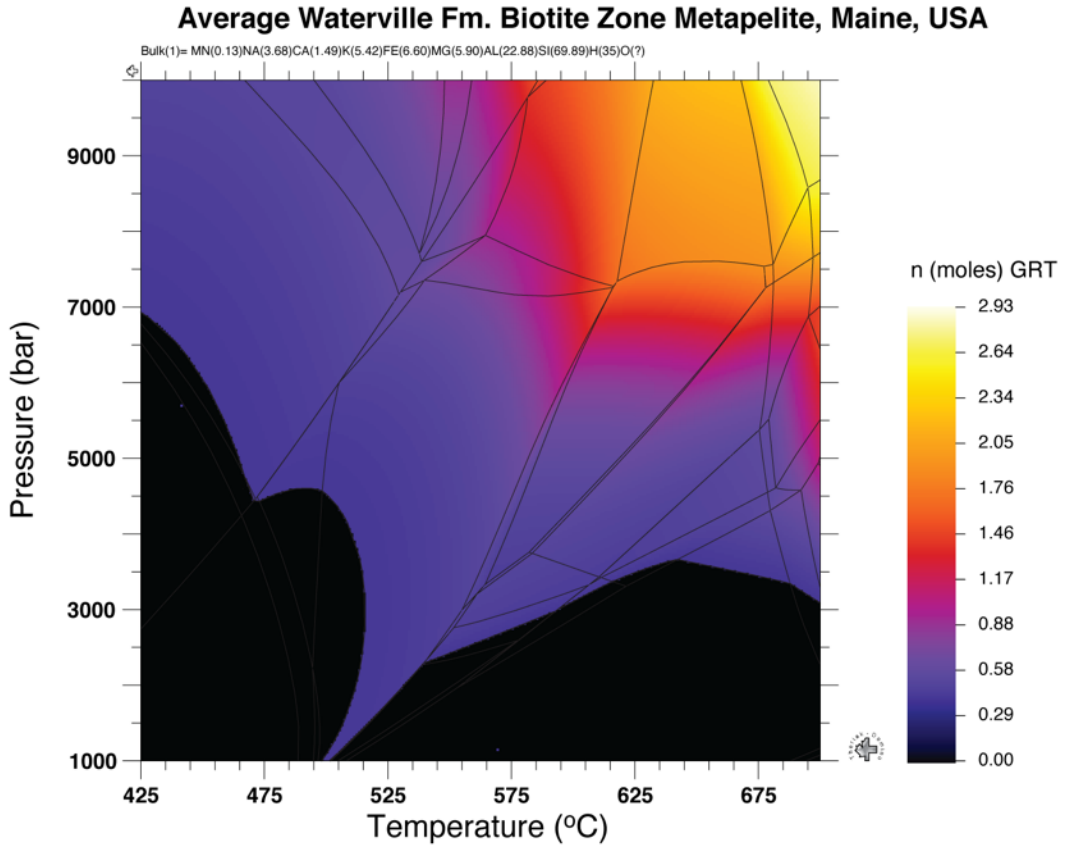
After Jørgensen et al. (2019)

Program Domino – pixel maps

- Can produce ‘pixel maps’ of system and phase properties
- Minimizations at an array of X-Y points (up to 250 pts in X and Y)
- Produces grayscale pgm and ps images
- Can plot gradients along X or Y of any property

- Output on left was generated from program makemap
- Can easily convert to color with 3rd-party software (ImageJ, Mathematica, Matlab, etc.)





Domino – pixel maps

- For this MnNCKFMASH calculation, 263 different files saved that can be mapped
- Maps produced by bundled program makemap
- A complexity in the way phases are identified sometimes requires user to combine output from more than one file to produce a complete map

System properties

U, G, H, S, V, V_solids, TS, PV
%H2O in solids
weight of solids
density of solids

Phase properties

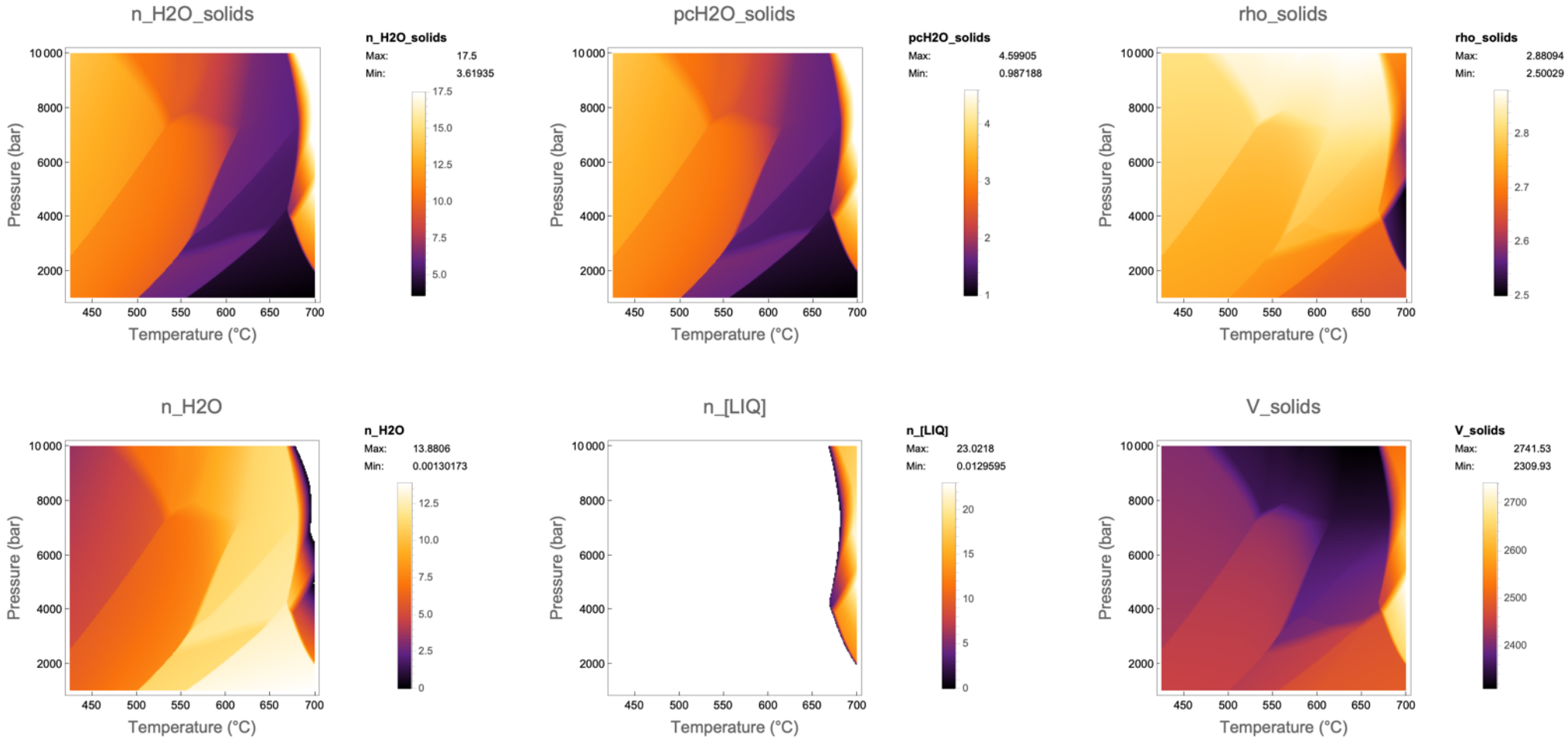
Al pfu Si pfu Mg#
moles of phase
moles & weight of H2O in phase
density of phase
proportion (x_) of end members

~/Docs/PEQ-2021/AWBZ/PT-MnNCKFMASH-ds62a-275pix — -zsh

~/Docs/PEQ-2021/AWBZ/PT-MnNCKFMASH-ds62a-275pix — -zsh ~/Docs/PEQ-2021/AWBZ/PT-MnNCKFMASHO-ds62a — -zsh

```
Y-axis : Pressure [Bar]      1000.00000    10000.00000

functions available for mapping:

[b]: b-rich solution    n: mass [mol]    wt: weight    x: mole fraction

   1: Al_pfu_[abh]          2: Al_pfu_[ames]         3: Al_pfu_[anC]          4: Al_pfu_[annm]         5: Al_pfu_[clin]
   6: Al_pfu_[daph]         7: Al_pfu_[east]         8: Al_pfu_[fm]           9: Al_pfu_[fs]          10: Al_pfu_[h2oL]
  11: Al_pfu_[mu]          12: Al_pfu_[pa]          13: Al_pfu_[phl]         14: G_system             15: G_tot
  16: H_tot                17: Mg#_[alm]            18: Mg#_[ames]           19: Mg#_[annm]           20: Mg#_[clin]
  21: Mg#_[daph]           22: Mg#_[east]           23: Mg#_[fcrd]           24: Mg#_[fm]             25: Mg#_[fs]
  26: Mg#_[fst]            27: Mg#_[gr]             28: Mg#_[h2oL]           29: Mg#_[hcrd]           30: Mg#_[mu]
  31: Mg#_[pa]             32: Mg#_[phl]            33: Mg#_[spss]           34: PV-_tot              35: S_tot
  36: Si_pfu_[abh]         37: Si_pfu_[ames]        38: Si_pfu_[anC]         39: Si_pfu_[annm]        40: Si_pfu_[clin]
  41: Si_pfu_[daph]        42: Si_pfu_[east]        43: Si_pfu_[fm]          44: Si_pfu_[fs]          45: Si_pfu_[h2oL]
  46: Si_pfu_[mu]          47: Si_pfu_[pa]          48: Si_pfu_[phl]         49: TS_tot               50: U_tot
  51: V_solids             52: V_tot                53: assemblage           54: n_H2O                55: n_H2O_H2O
  56: n_H2O_[ames]         57: n_H2O_[annm]         58: n_H2O_[clin]         59: n_H2O_[daph]         60: n_H2O_[east]
  61: n_H2O_[fcrd]         62: n_H2O_[fst]          63: n_H2O_[h2oL]         64: n_H2O_[hcrd]         65: n_H2O_[mu]
  66: n_H2O_[pa]           67: n_H2O_[phl]          68: n_H2O_solids         69: n_H2O_zo             70: n_[GRT]
  71: n_[abh]              72: n_[alm]              73: n_[ames]             74: n_[anC]              75: n_[annm]
  76: n_[clin]             77: n_[daph]             78: n_[east]             79: n_[fcrd]             80: n_[fm]
  81: n_[fs]               82: n_[fst]              83: n_[gr]               84: n_[h2oL]             85: n_[hcrd]
  86: n_[mu]               87: n_[pa]               88: n_[phl]              89: n_[spss]             90: n_ab
  91: n_and                92: n_ky                 93: n_mic                94: n_q                  95: n_sill
  96: n_zo                 97: pcH2O_solids         98: rho_H2O              99: rho_[abh]           100: rho_[alm]
 101: rho_[ames]          102: rho_[anC]           103: rho_[annm]          104: rho_[clin]          105: rho_[daph]
 106: rho_[east]          107: rho_[fcrd]          108: rho_[fm]            109: rho_[fs]            110: rho_[fst]
 111: rho_[gr]            112: rho_[h2oL]          113: rho_[hcrd]          114: rho_[mu]            115: rho_[pa]
 116: rho_[phl]           117: rho_[spss]          118: rho_ab              119: rho_and             120: rho_ky
 121: rho_mic             122: rho_q               123: rho_sill            124: rho_solids          125: rho_zo
 126: vol_H2O             127: vol_[abh]           128: vol_[alm]           129: vol_[ames]          130: vol_[anC]
 131: vol_[annm]          132: vol_[clin]          133: vol_[daph]          134: vol_[east]          135: vol_[fcrd]
 136: vol_[fm]            137: vol_[fs]            138: vol_[fst]           139: vol_[gr]            140: vol_[h2oL]
 141: vol_[hcrd]          142: vol_[mu]            143: vol_[pa]            144: vol_[phl]           145: vol_[spss]
 146: vol_ab              147: vol_and             148: vol_ky              149: vol_mic             150: vol_q
 151: vol_sill            152: vol_zo              153: wt_H2O_H2O          154: wt_H2O_[ames]       155: wt_H2O_[annm]
 156: wt_H2O_[clin]       157: wt_H2O_[daph]       158: wt_H2O_[east]       159: wt_H2O_[fcrd]       160: wt_H2O_[fst]
 161: wt_H2O_[h2oL]       162: wt_H2O_[hcrd]       163: wt_H2O_[mu]         164: wt_H2O_[pa]         165: wt_H2O_[phl]
 166: wt_H2O_solids       167: wt_H2O_zo           168: x_abL_[h2oL]        169: x_abh_[abh]         170: x_abh_[anC]
 171: x_afchl_[ames]      172: x_afchl_[clin]      173: x_afchl_[daph]      174: x_alm_[alm]         175: x_alm_[gr]
 176: x_alm_[spss]        177: x_ames_[ames]       178: x_ames_[clin]       179: x_ames_[daph]       180: x_anC_[abh]
 181: x_anC_[anC]         182: x_anL_[h2oL]        183: x_annm_[annm]       184: x_annm_[east]       185: x_annm_[phl]
 186: x_cel_[mu]          187: x_cel_[pa]          188: x_clin_[ames]       189: x_clin_[clin]       190: x_clin_[daph]
 191: x_crd_[fcrd]        192: x_crd_[hcrd]        193: x_daph_[ames]       194: x_daph_[clin]       195: x_daph_[daph]
 196: x_east_[annm]       197: x_east_[east]       198: x_east_[phl]        199: x_en_[fm]           200: x_en_[fs]
 201: x_fa2L_[h2oL]       202: x_fcel_[mu]         203: x_fcel_[pa]         204: x_fcrd_[fcrd]       205: x_fcrd_[hcrd]
 206: x_fm_[fm]           207: x_fm_[fs]           208: x_fo2L_[h2oL]       209: x_fs_[fm]           210: x_fs_[fs]
 211: x_fst_[fst]         212: x_gr_[alm]          213: x_gr_[gr]           214: x_gr_[spss]         215: x_h2oL_[h2oL]
 216: x_hcrd_[fcrd]       217: x_hcrd_[hcrd]       218: x_kspL_[h2oL]       219: x_mat_[mu]          220: x_mat_[pa]
 221: x_mgts_[fm]         222: x_mgts_[fs]         223: x_mmbi_[annm]       224: x_mmbi_[east]       225: x_mmbi_[phl]
 226: x_mmchl_[ames]      227: x_mmchl_[clin]      228: x_mmchl_[daph]      229: x_mncd_[fcrd]       230: x_mncd_[hcrd]
 231: x_mnopx_[fm]        232: x_mnopx_[fs]        233: x_mnstm_[fst]       234: x_mstm_[fst]        235: x_mu_[mu]
 236: x_mu_[pa]           237: x_obi_[annm]        238: x_obi_[east]        239: x_obi_[phl]         240: x_ochl1_[ames]
 241: x_ochl1_[clin]      242: x_ochl1_[daph]      243: x_ochl4_[ames]      244: x_ochl4_[clin]      245: x_ochl4_[daph]
 246: x_odi_[fm]          247: x_odi_[fs]          248: x_pa_[mu]           249: x_pa_[pa]           250: x_phl_[annm]
 251: x_phl_[east]        252: x_phl_[phl]         253: x_py_[alm]          254: x_py_[gr]           255: x_py_[spss]
 256: x_q4L_[h2oL]        257: x_san_[abh]         258: x_san_[anC]         259: x_slL_[h2oL]        260: x_spss_[GRT]
 261: x_spss_[alm]        262: x_spss_[gr]         263: x_spss_[spss]
```

AWBZ: H2O, melt, density and volume maps



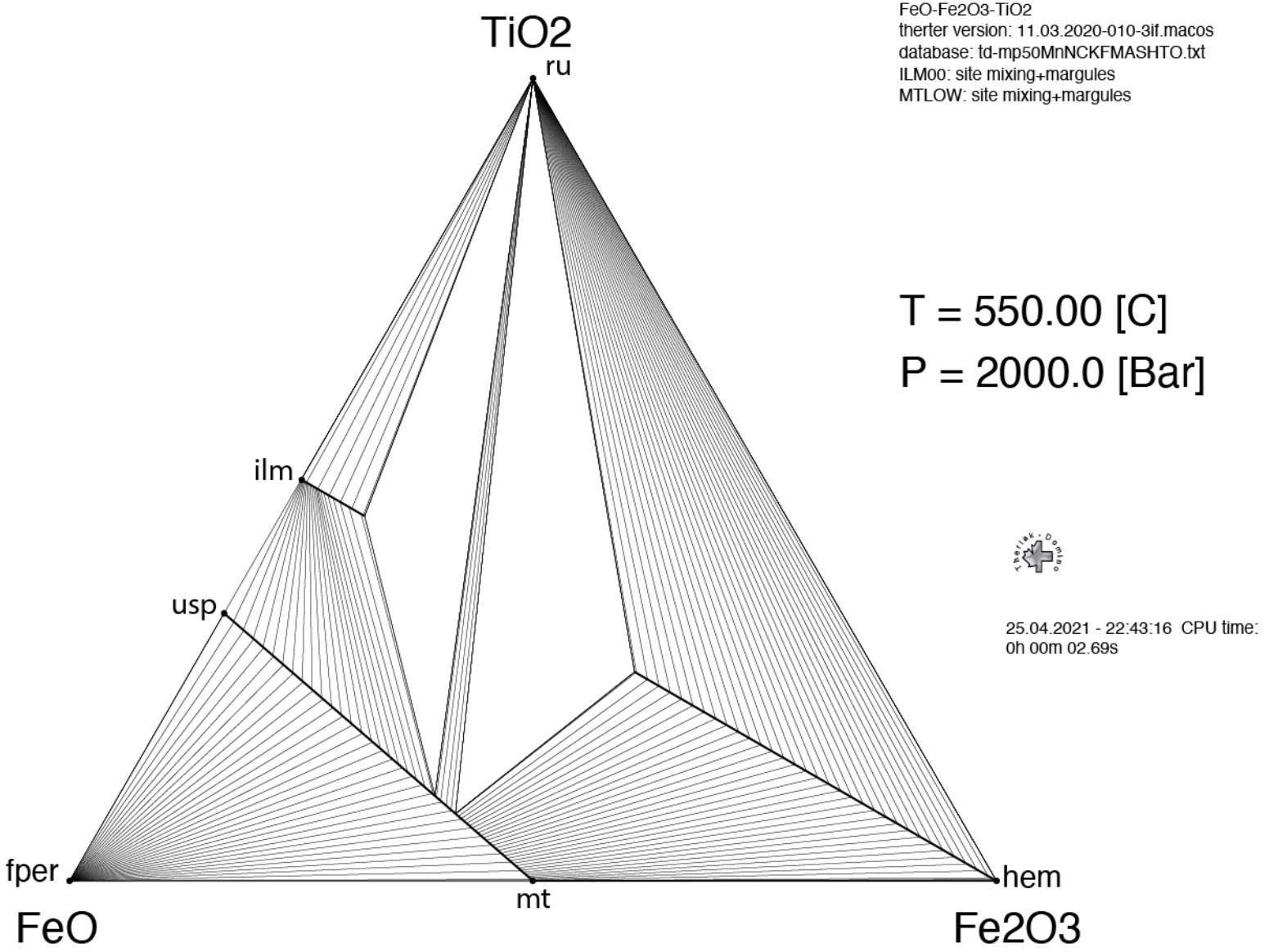
A simple script in Mathematica was used to automatically convert all domino pixmap output files to color maps

Programs Therter and Therbin

Calculates ternary phase diagram at a fixed P & T

- Phases lie within the plane of the diagram
- Tie-lines connect coexisting phases
- Good for simple systems & visualizing miscibility gaps

Program Therbin is the same, just plots a binary system instead of ternary



THERIAK-DOMINO – add-on, extension, integration

Geochemistry Geophysics Geosystems G3

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THERIAK_D: An add-on to implement equilibrium computations in geodynamic models

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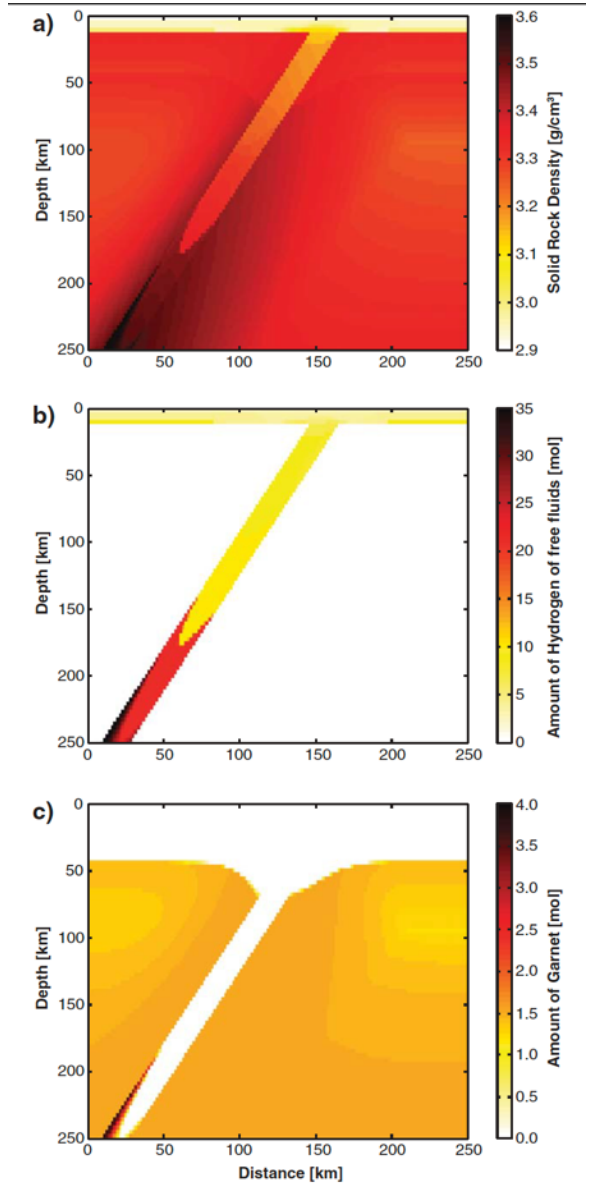
Duesterhoeft & de Capitani (2013) give examples of how to call Theriak from other program, and how to link directly to Theriak subroutines

Other examples:
Theria_G (Fred Gaidies)
Bingo-Antidote (Duesterhoeft & Lanari, 2020)



Duesterhoeft & de Capitani (2013)

Usage Pitfalls & Pointers

Three most common user issues I've noticed

1. Using solution models with ferric iron members when the bulk system composition is ferric free
    - This can result in failed calculations or diagrams with many short squiqqly lines!
    - The program tries to make a ferric member stable because there is no explicit ferric- or ferrous-iron system component, only an FE system component; look in the output for pure elements in your assemblage, which is often a sign that this problem is occurring
    - Can be resolved by 'commenting out' all ferric-bearing members (put an ! in front of all ferric phase components in the site composition lines to comment them, or comment all ferric phase component entries (! or *** MuNERAL DATA ***)
    - Alternatively, can resolve this by adding a small amount of extra oxygen to stabilize a small amount of ferric iron components (see point 2 on how to add extra oxygen)

Usage Pitfalls & Pointers

Three most common user issues I've noticed

2. Entering bulk system compositions

System composition is input as molar elements, not as oxides, and not as weight percent.

- I would enter the composition of magnetite in one of these 2 equivalent ways:

  - FE(3)O(4) * Equivalent to 1 FeO + 2 $FeO_{1.5}$
  - FE(3)O(?) O(1) * Results in 3 FeO + 1 O == 1 FeO + 2 $FeO_{1.5}$

The O(?) tells the program to calculate the O required to form the default set of oxides from the given elements; see database header

3. Program installation/startup problems

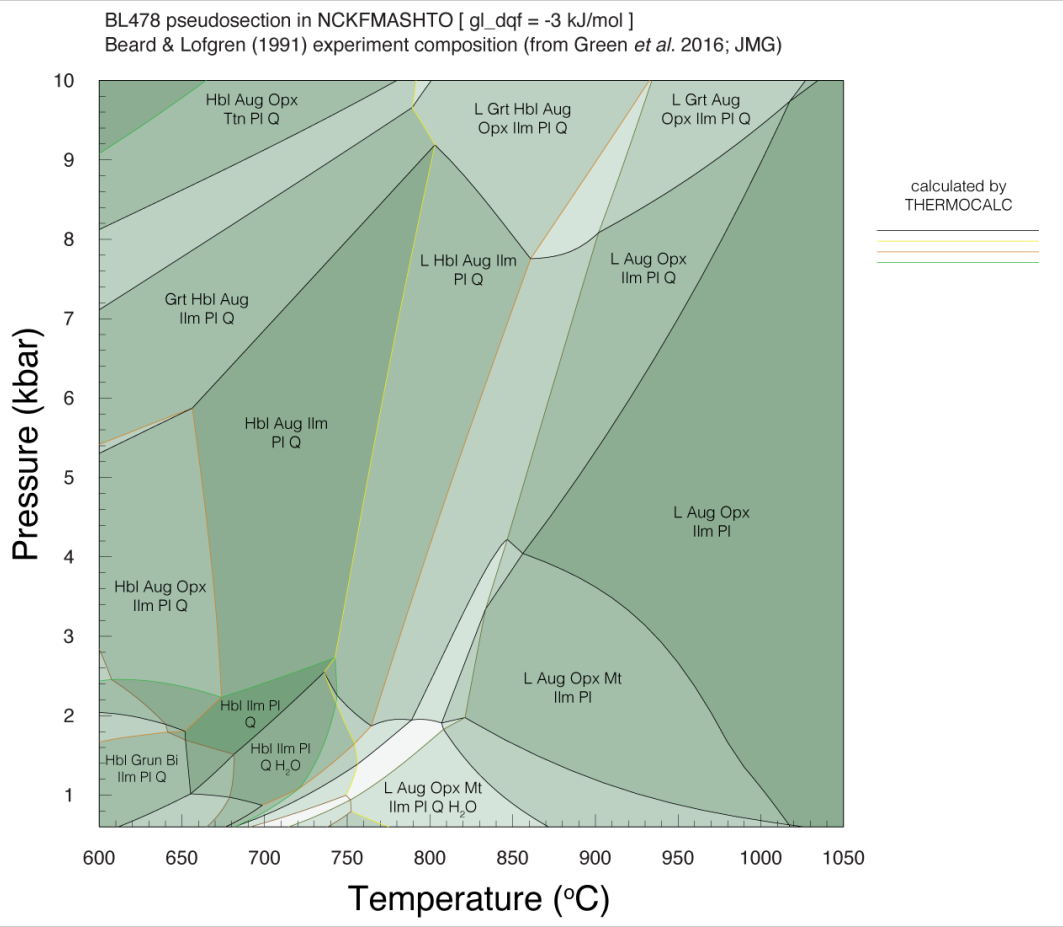
Programs from the official distribution site require additional linked libraries (gcc)

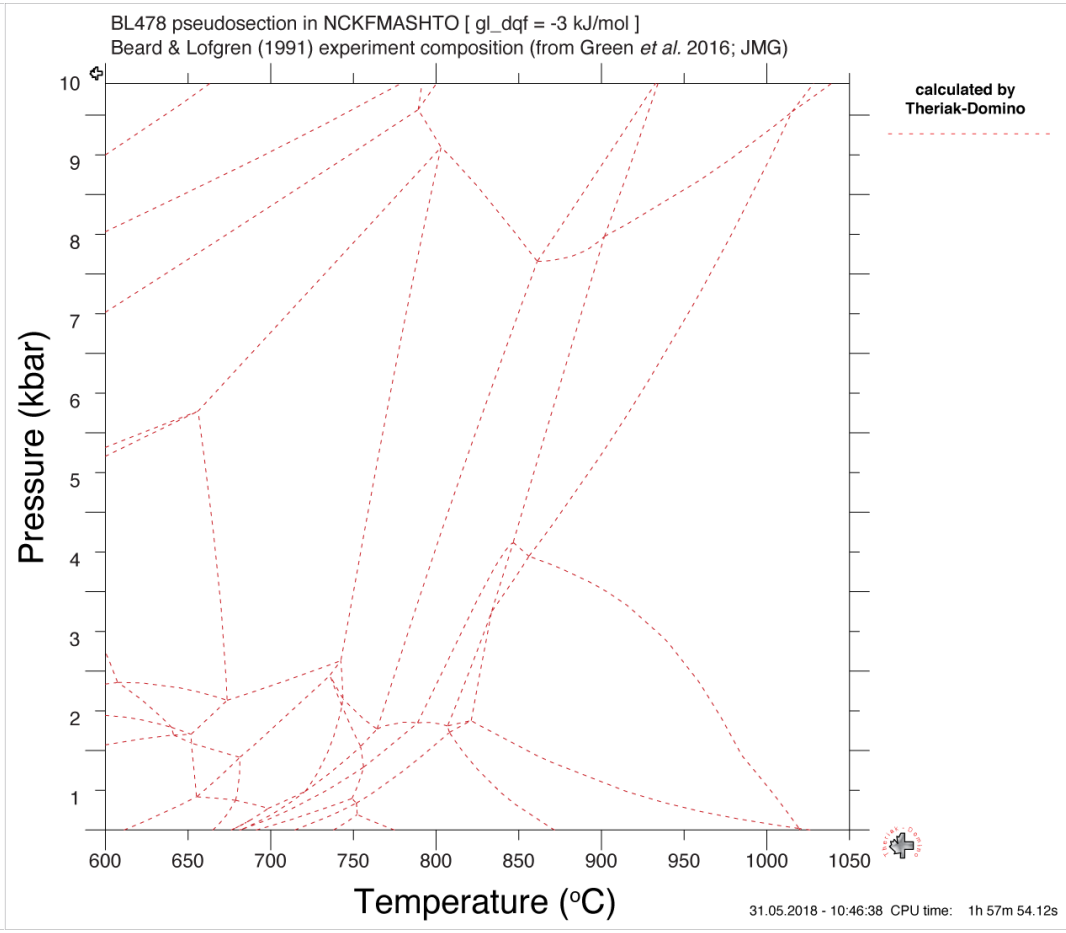
- Install those libraries separately (can be difficult on Windows), or
- Download from alternate sites, where programs are not dependent on additional libraries

Usage Pitfalls & Pointers: more advice

4. Take advantage of the *** SEEDS *** feature in the database
    - SEEDS are equilibrium compositions of phases at a fixed diagram coordinate (P-T, T-X, etc.). The output for seeds are listed in the log file of program Theriak (and on screen) when you specify extra output (put a 1 in front of your bulk system composition)
    - If you are generating a diagram in Domino, run Theriak at the corners and in a few interior points of the diagram; place each SEED that is generated towards the bottom of the database file (I delete old SEEDS that are already present)
    - SEEDS are generally not required, but they can decrease computation time and generally reduce the number of failed minimizations (don't add too many; 6-15 SEEDS entries generally helps)

THERMOCALC and Domino Equilibrium Assemblage Diagrams





You will get the same results IF you use the exactly the same database, solution models, and bulk system composition

Both have their strong and weak points.
Why not use both?

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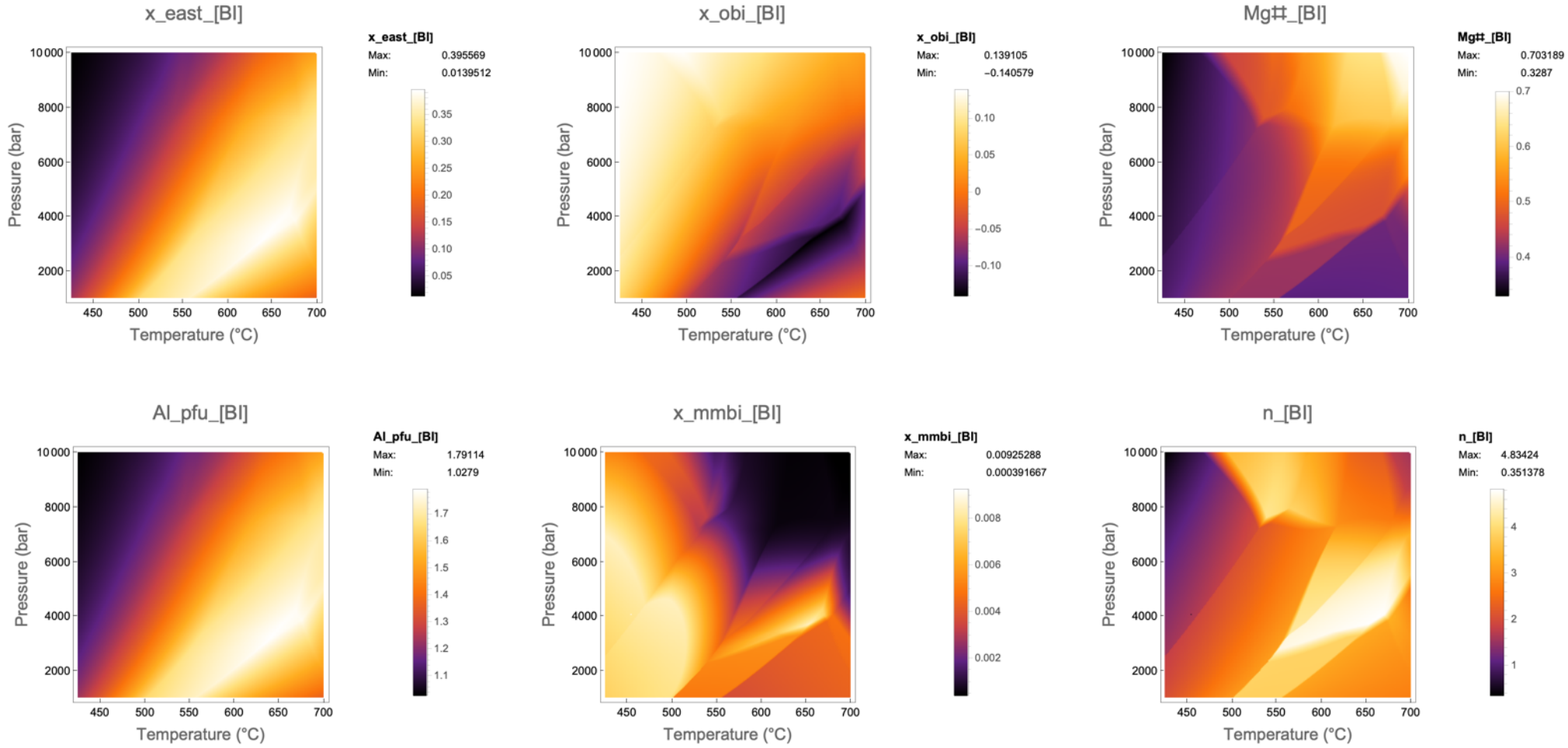
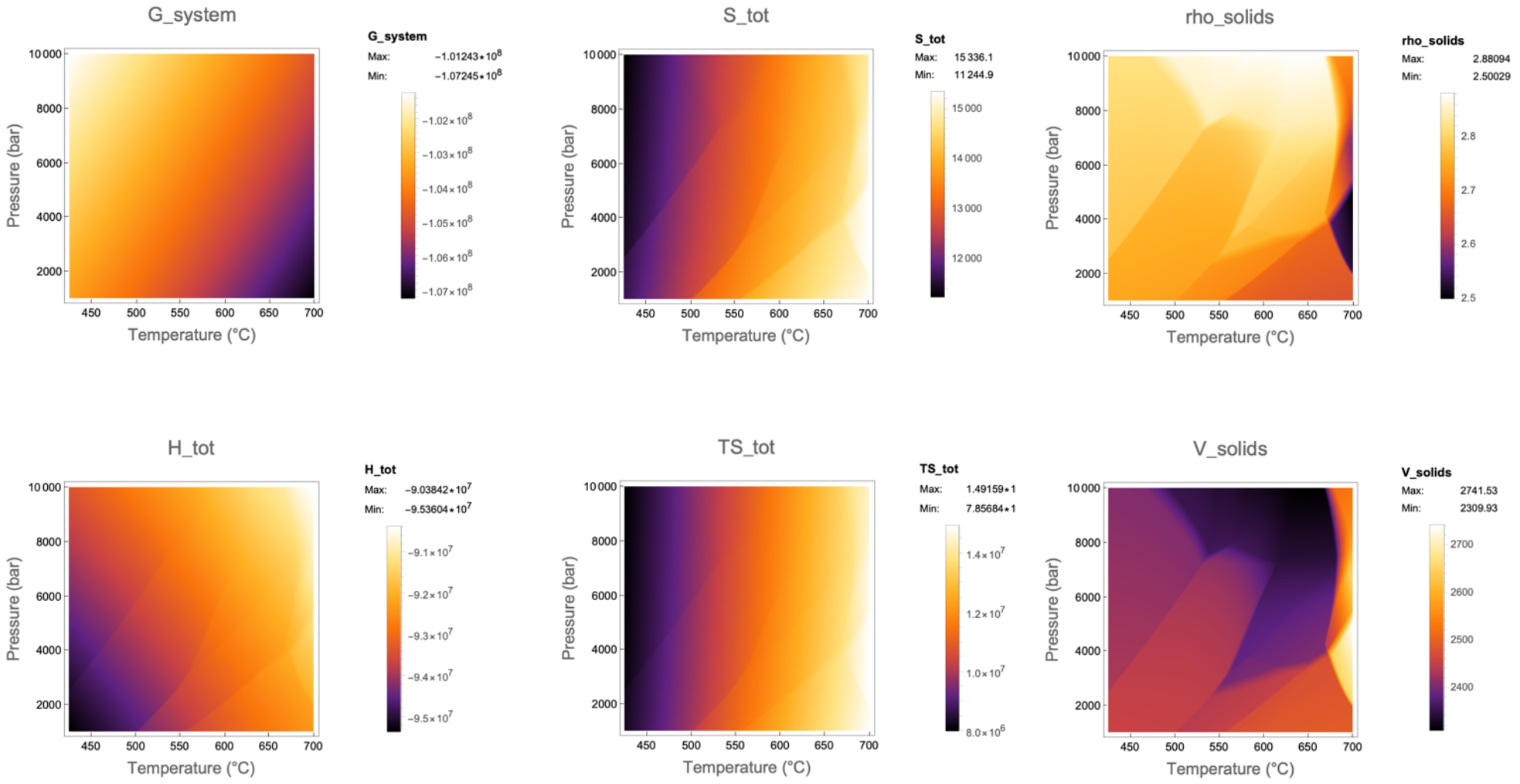
Program Domino – pixel maps

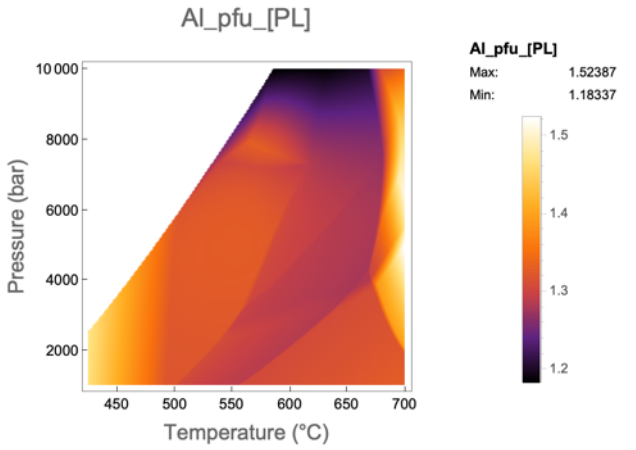
- Biotite composition and abundance maps
- Production automated using simple Mathematica script

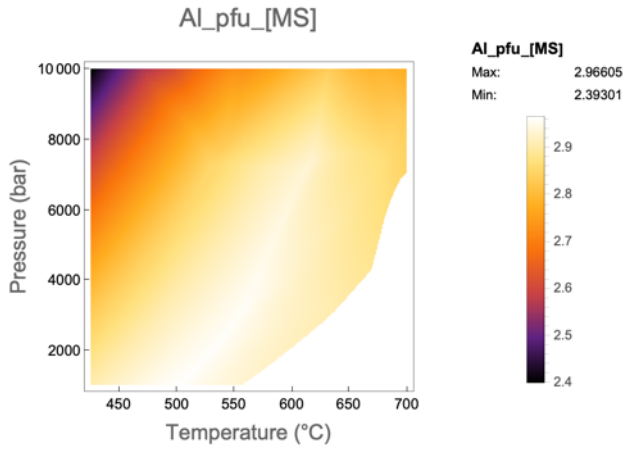


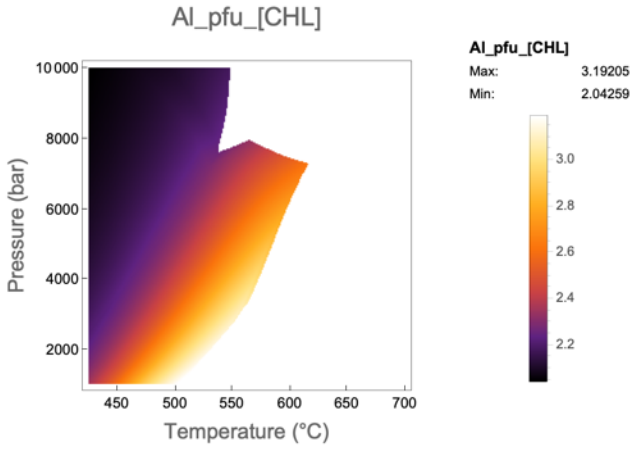
Program Domino pixel maps: AWBZ system properties

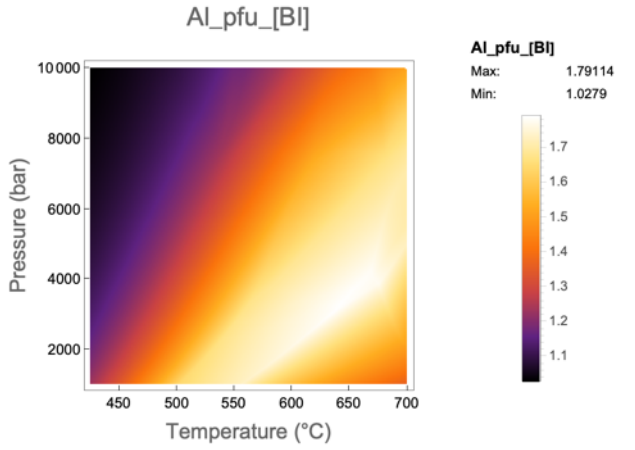


AWBZ: Al pfu maps

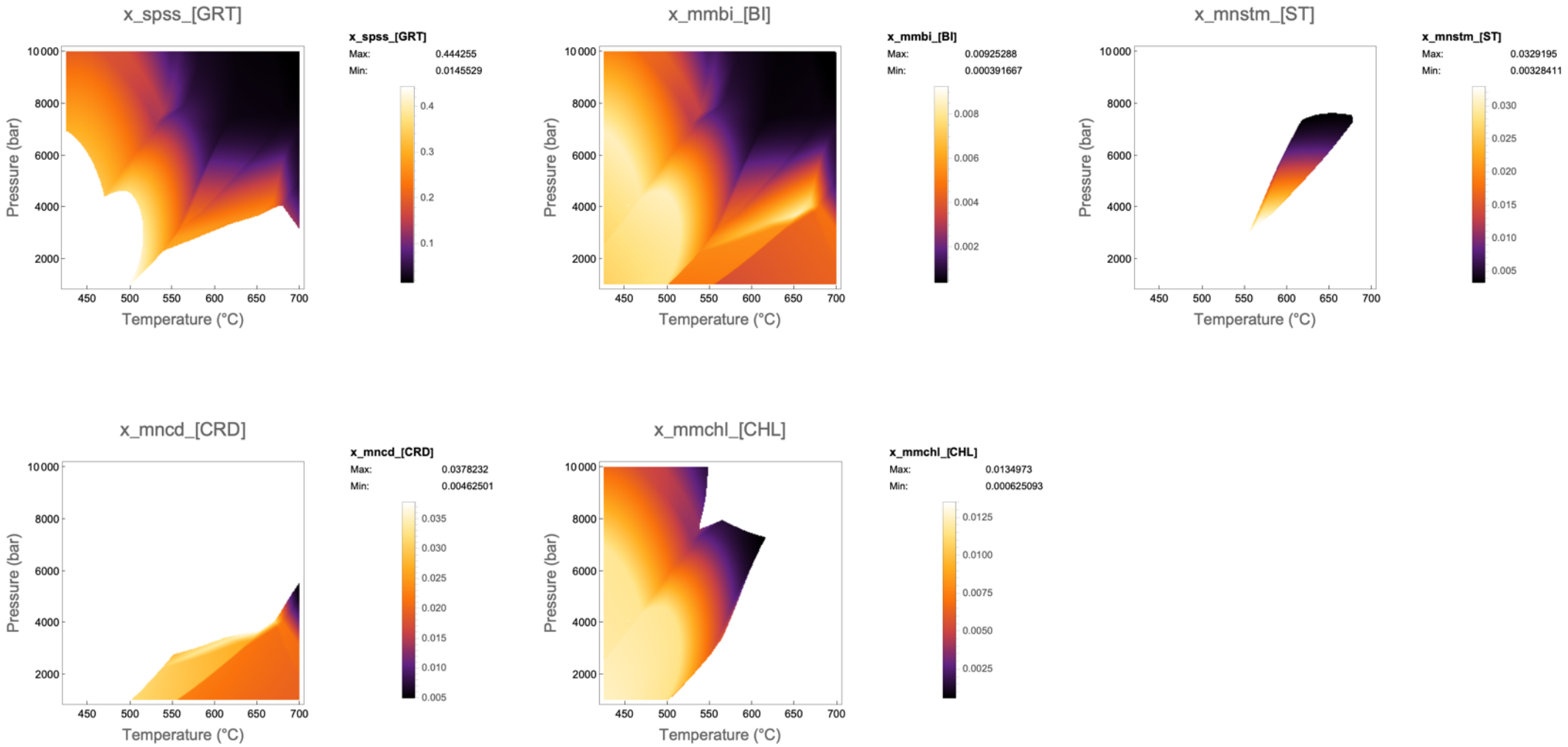




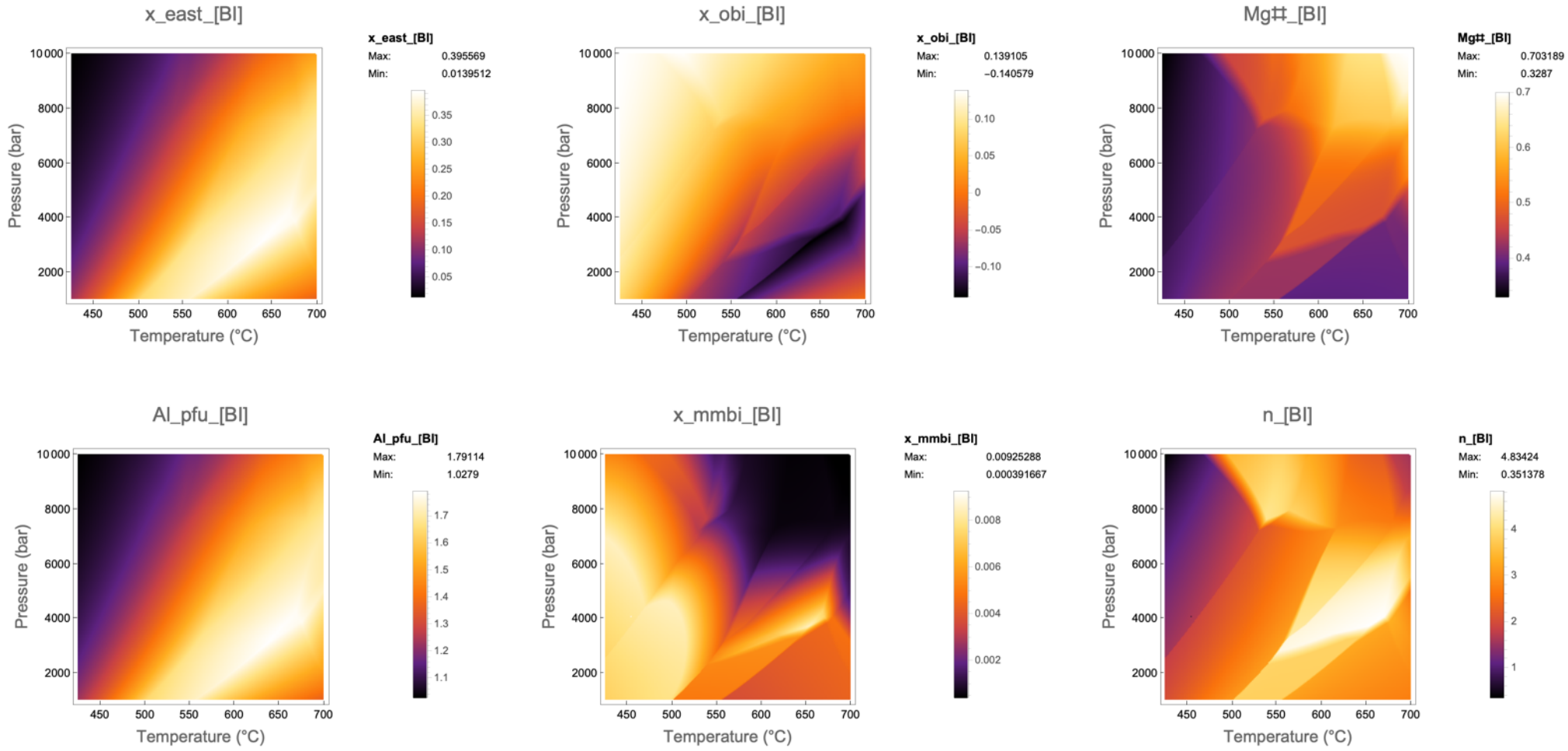




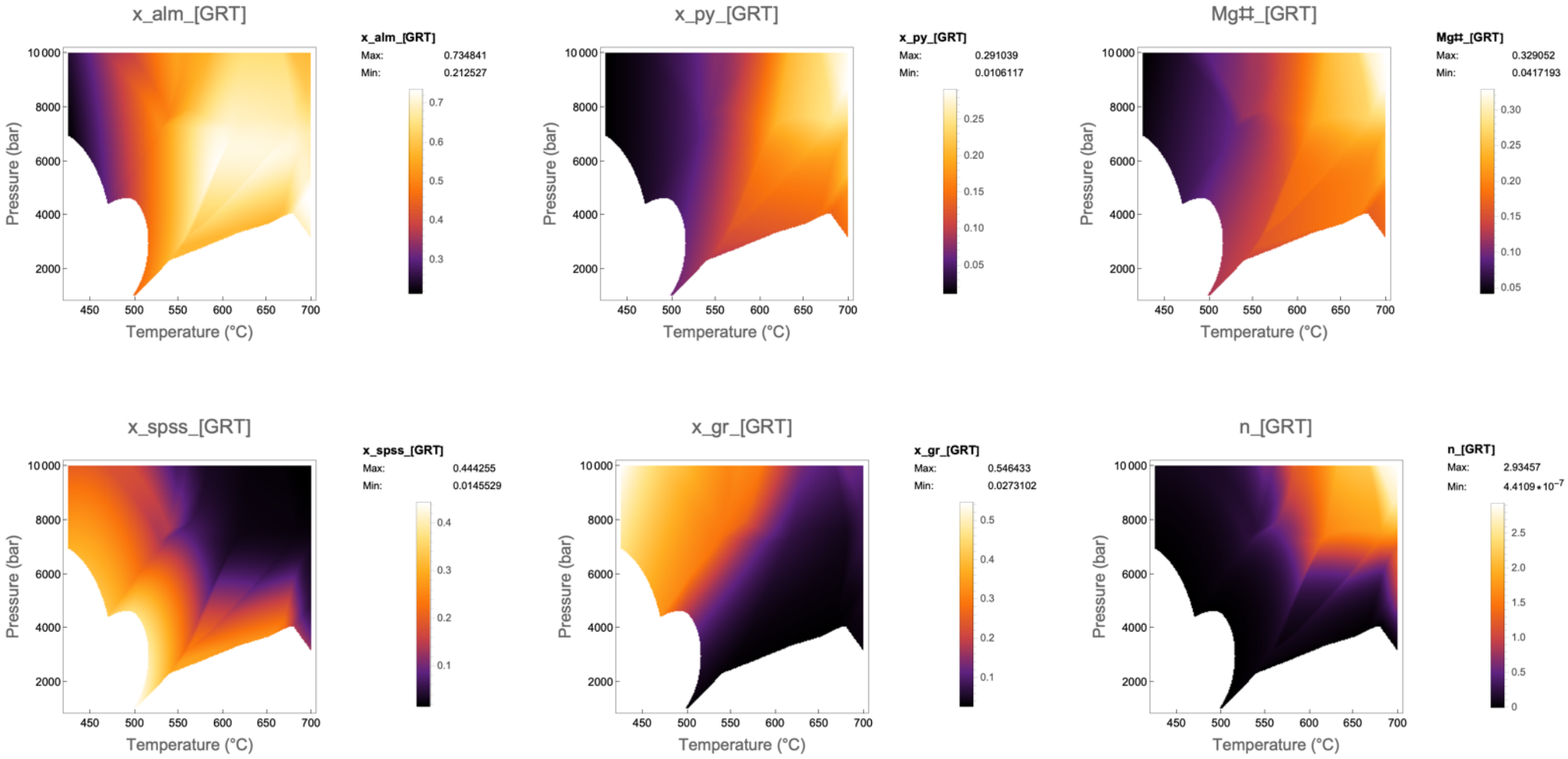
AWBZ: : proportion Mn phase components



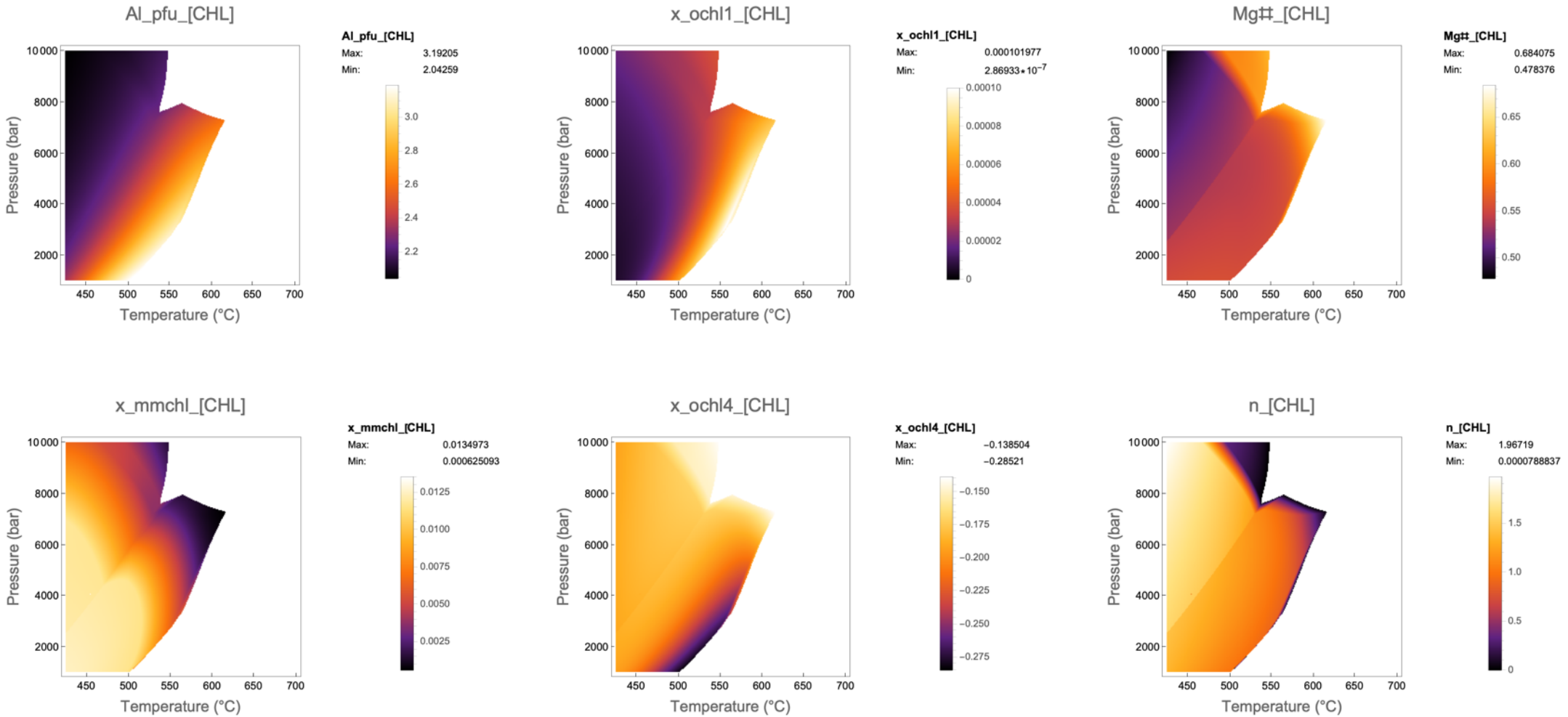
AWBZ: Biotite composition and abundance maps



AWBZ: Garnet composition and abundance maps



AWBZ: Chlorite composition and abundance maps



Holland & Powell (2003) ternary feldspar

Plagioclase binary

- When using THERMOCALC, you can manually change between the PlC and PlI model depending on T and feldspar composition
- The PlI model is more stable than the PlC model when plagioclase compositions indicate you should be using PlC; this is a severe problem for the G minimizers because they always find the phase with the lowest G