How are models constructed?

Modeling tool

(MELTS, PhasePlot, SUPCRT, EQ3/EQ6, THERMOCALC, PERPLE_X)

Internally consistent Thermochemical data/model collections

Solution theory (minerals, melts, gases)

custom software infrastructure

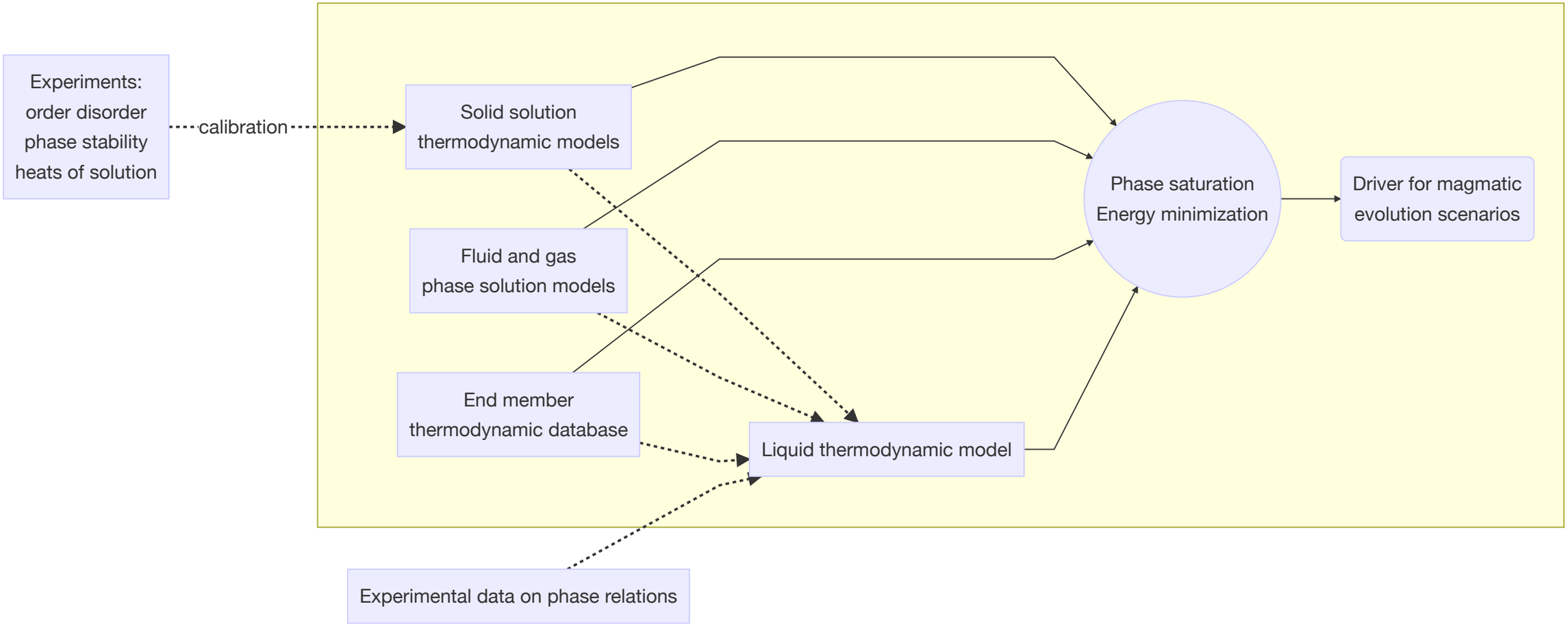
Calorimetric data V(T, P) data

Phase equilibrium experimental data

LEPR **L**ibrary of **E**xperimental **P**hase **R**elations

Mineral volumetric properties, structural properties, phase equilibria

MELTS, pMELTS, rhyolite-MELTS, alphaMELTS, MELTS for Excel, etc.



Phases and components included:

Solid solutions

- olivine Mg-Fe^{2+}-Co-Ni-Ca-Mn
- garnet Mg-Fe^{2+}-Ca
- melilite Mg-Al-Fe^{2+}-Na
- opx Ca-Mg-Fe^{2+}-Al-Fe^{3+}-Na
- cpx (pig) Ca-Mg-Fe^{2+}-Al-Fe^{3+}-Na
- cummingtonite Mg-Fe^{2+}
- amphibole Ca-Mg-Fe2+
- hornblende (pargasite-hastingsite)
- biotite Mg-Fe^{2+}
- feldspar Na-Ca-K
- nepheline Na-Ca-K-[]
- kalsilite Na-Ca-K-[]
- leucite Na-K-H_2O
- spinel Mg-Fe^{2+}-Cr^{3+}-Al-Fe^{3+}-Ti
- rhm oxide Mg-Fe^{2+}-Cr^{3+}-Al-Fe^{3+}-Ti
- ortho oxide Mg-Fe^{2+}-Fe^{3+}
- Fe-Ni alloy (solid and liquid)

Stoichiometric phases

- titanite
- aegirine
- aenigmatite
- muscovite
- quartz
- tridymite
- cristobalite
- corundum
- sillimanite
- rutile
- perovskite
- whitlockite
- apatite
- water
- periclase

Liquid: SiO_2-TiO_2-Al_2O_3-Fe_2O_3-Cr_2O_3-FeO-MnO-MgO-NiO-CoO-CaO-Na_2O-K_2O-P_2O_5-H_2O-(CO_2)

Mass transfer calculations

Gibbs free energy

minimization of G(T, P) **yields** ***m, X, V, etc.***

Helmholtz free energy ***(A = G - PV)***

minimization of A(T, V) **yields** ***m, X, P, etc.***

Enthalpy ***(H = G - TS)***

minimization of H(S, P) **yields** ***m, X, T, etc.***

Internal energy ***(E = G - PV+TS)***

minimization of E(S, V) **yields** ***m, X, T, P, etc.***

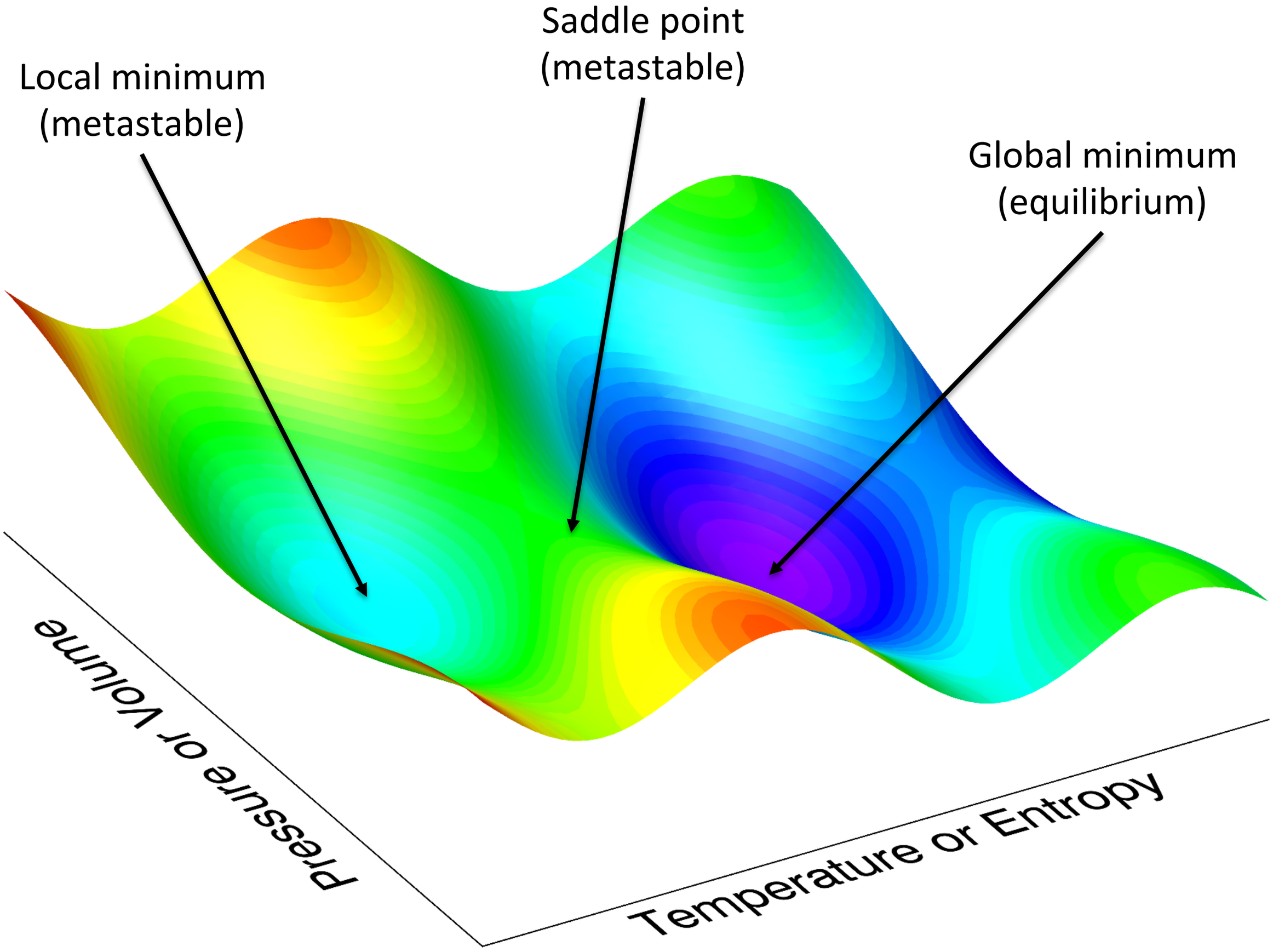
Entropy ***(S = G/T - H/T)***

maximizing of S(H, P) **yields** ***m, X, T, etc.***

All of the above as open systems

Korzhinskii potential ***(L = G - n_{O2} μ_{O2})***

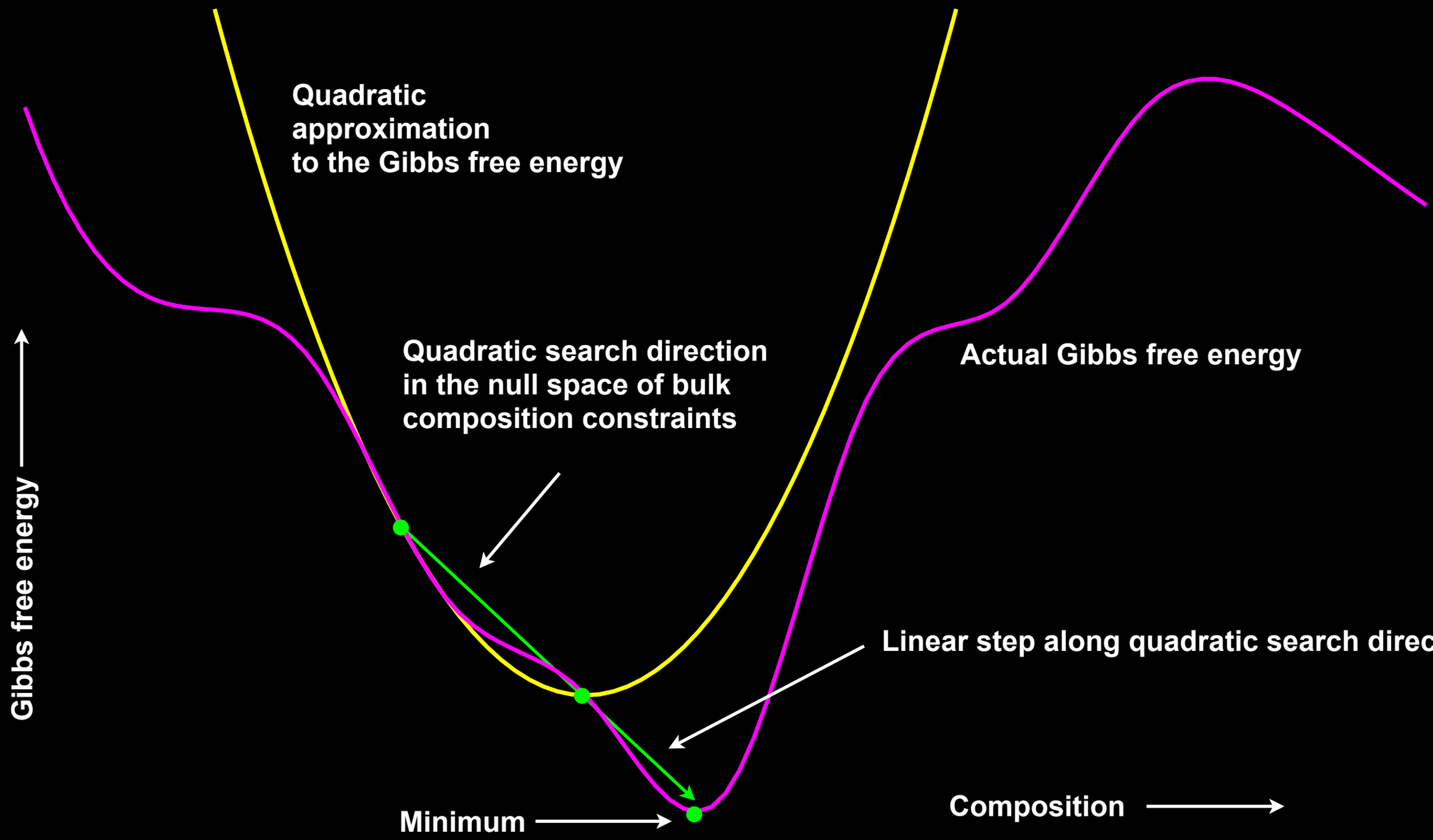
	polythermal isobaric	polythermal isochoric
State 1	$G(T_1,P)$	$A(T_1,V)$
	m_1, X_1, V_1	m_1, X_1, P_1
State 2	$G(T_2,P)$	$A(T_2,V)$
	m_2, X_2, V_2	m_2, X_2, P_2
State 3	$G(T_3,P)$	$A(T_3,V)$
	m_3, X_3, V_3	m_3, X_3, P_3


Local minimum
(metastable)
Saddle point
(metastable)
Global minimum
(equilibrium)
Pressure or Volume
Temperature or Entropy

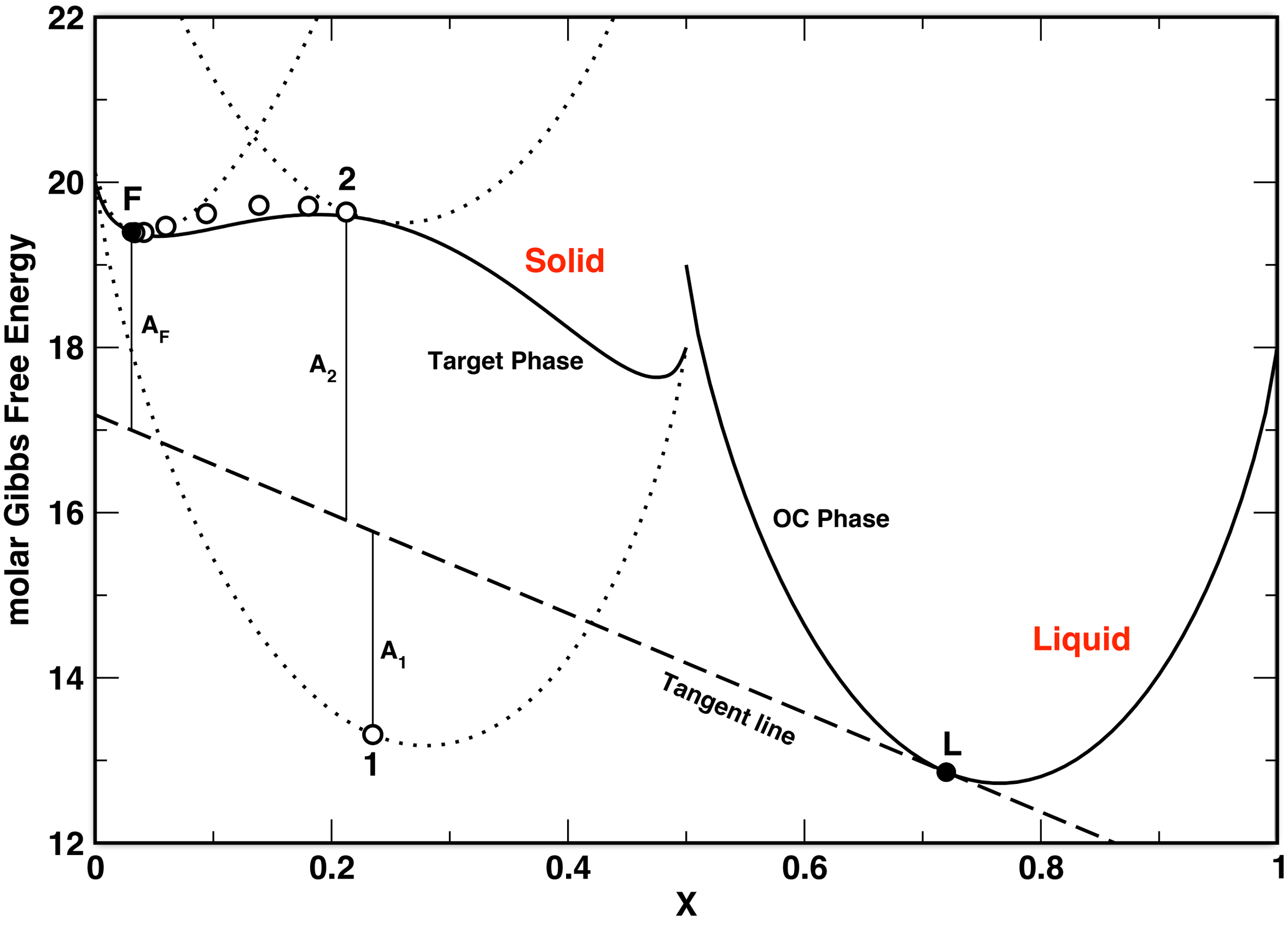
Computational method for solving for the abundances and compositions

Gibbs free energy minimization for T, P grids using a fully second order Newton method

Helmholtz free energy for T, V grids; Enthalpy for S, P grids; Internal Energy for S, V grids



Most time consuming calculation: phase saturation algorithm



MELTS Failures and solutions

- **Calc-alkaline magmas**
  - **Inability to accurately model hornblende-liquid and biotite-liquid phase equilibria. Due to a dearth of applicable experimental data. Not necessarily a problem with formulation of liquid solution theory.**
- **Phase equilibria above ~ 4 GPa and < 30 GPa**
  - **A decade ago, the problem was a dearth of experimental data. That is no longer the case. Now the difficulties are an EOS for the liquid state (solved), a more sophisticated solution model for the liquid (solved) and solution theory for high-pressure phases.**
- **Phase equilibria at pressures > ~ 30 GPa**
  - **Here the problem is lack of experimental data and insufficient understanding of structural transformations that accompany compression of the liquid. But, there is hope!**
- **Sulfur-bearing mixed fluid systems**
  - **Mixed H_2O-CO_2-sulfur bearing systems are the goal. The ability to model redox equilibria involving iron and sulfur is an attainable objective.**
- **Automating calibration and maintenance of models**