Data Science Innovations That Streamline Development, Documentation, Reproducibility, and Dissemination of Models in Computational Thermodynamics: An Application of Image Processing Techniques for Rapid Computation, Parameterization and Modeling of Phase Diagrams

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Cyberinfrastructure for Computational Thermodynamics

Research ⟷ Instruction

ThermoFit

Web-based and standalone platform(s) for hypothesis testing, database interrogation, model integration and model development (MELTS, PhasePlot, EQ3/EQ6)

Databases of Materials Properties

"Thermodynamic databases"

Databases of rock/mineral/fluid compositional and physical data

Models in the Cloud

(web services)

Computational thermodynamics deals with geometry:
z = f(x,y),
where for example z can be the Gibbs free energy and consequently x, y are T, P.

A surface of this kind can always be mapped to image format, where x and y are the coordinates of a pixel and z is its intensity.

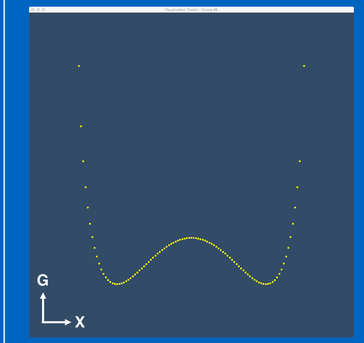
Rapid computation of Phase and Physical Property Diagrams

VTK, Visualization Toolkit (open source at vtk.org)

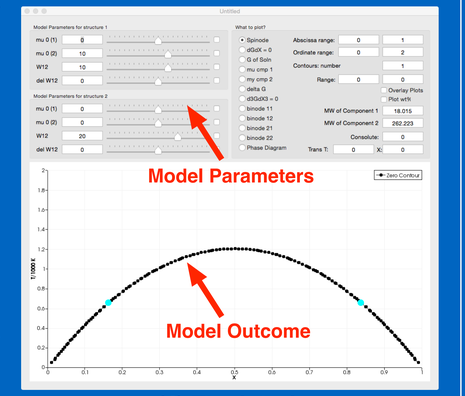
Real time model parameter updates by manipulation of model outcomes

The location of geometrical features of these energy surfaces, like zero contour lines, gradients, minima, maxima, loci of maximal curvature, etc., provide the model outcomes that we seek. The software to calculate these features must be fast and robust. The properties of each pixel can be estimated using massively parallel architecture and the geometrical features can be extracted using image processing software libraries.

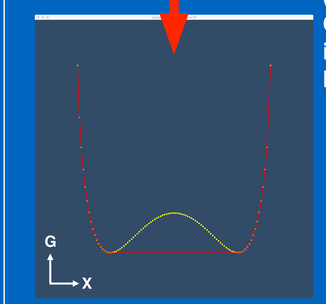
Example: Solvus construction using convex hulls



(1) Construct an image of the Gibbs free energy versus X (composition) with T increasing into the page.

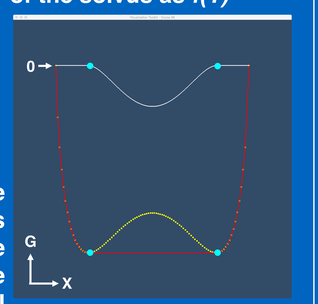


(4) The interior zero contour of the difference curve gives the location of the solvus as *f(T)*

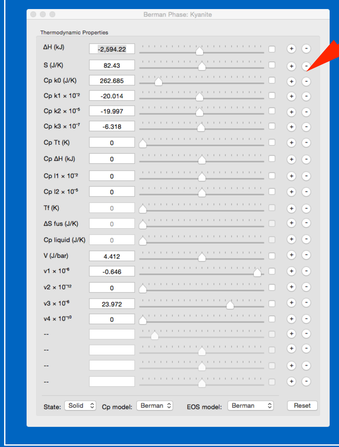


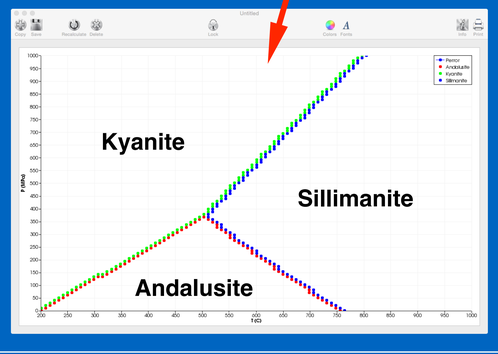
(2) Wrap the Gibbs energy in a convex hull (red curve)

(3) Difference the Gibbs energy curve with the convex hull



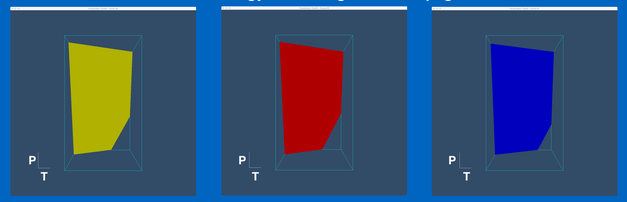
Example: Phase diagram construction using "Boolean union" surface addition and zero contour extraction





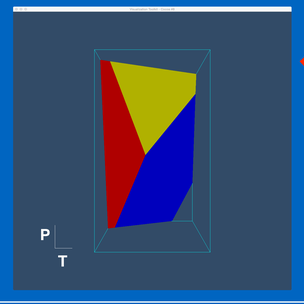
(1) Construct z = G(T,P) "images"

Gibbs energy *increasing* out of the page

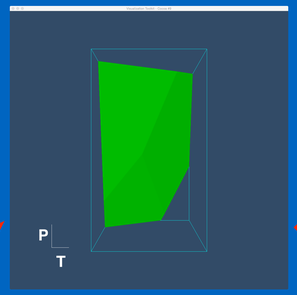


Andalusite | Sillimanite | Kyanite

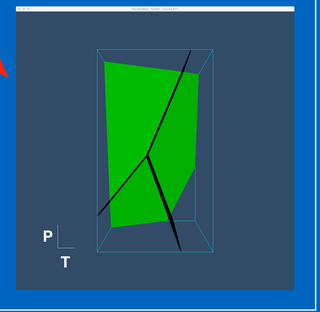
(2) Combine and overlay the images of the Gibbs energies of all three phases



(3) Form a "boolean union" of the three surfaces, which yields the convex hull of the minimum Gibbs energy in T-P space



(4) Subtract the original Gibbs surface for each phase from the convex hull derived in step 3.



(5) Extract the zero contour from the surface given in step 4. This contour defines the P-T phase boundaries.