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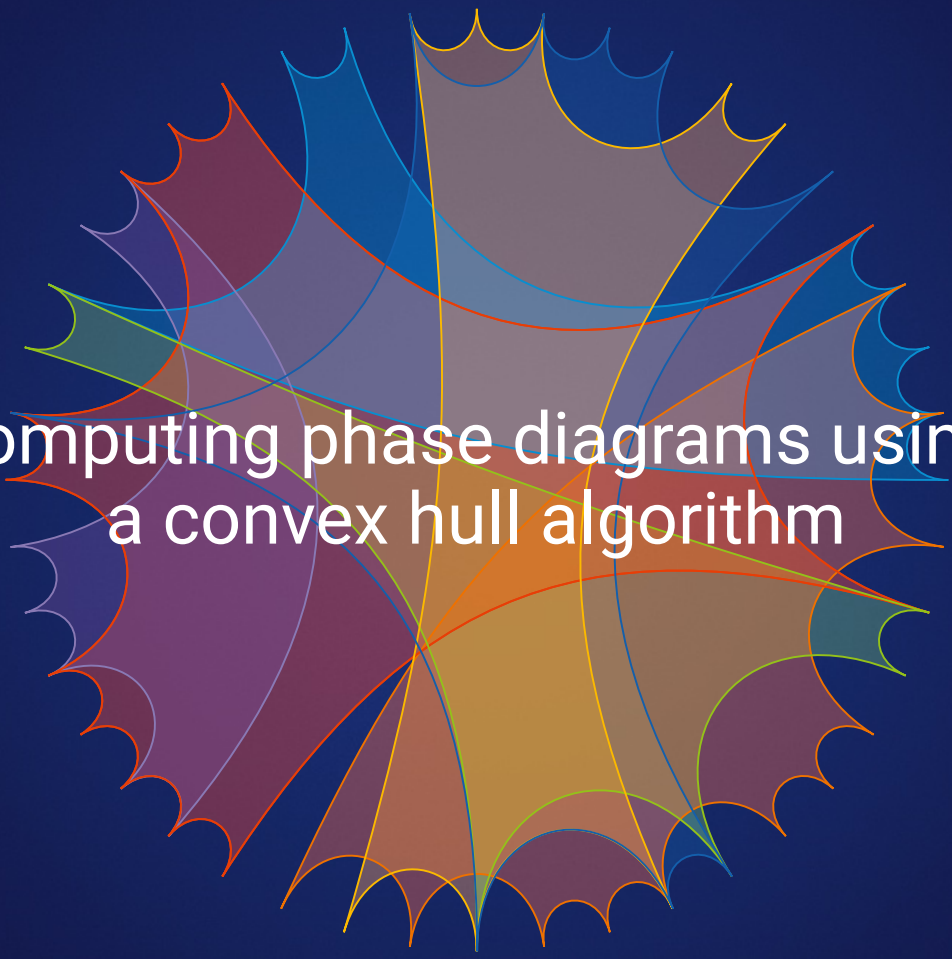

Computing phase diagrams using a convex hull algorithm

June 05, 2026, 1:30 PM, Phil 12 GHs

COFFEE & SNACKS IN ROOM 106

ZOOM: Meeting ID: 935 6549 3662, Code: 928036

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ABSTRACT

Phase diagrams are ubiquitous in physics. Usually they are plotted as a function of ambient conditions, for instance as a function of T (temperature) and P (pressure). In geophysics (rocks and magmas) it is also important to make phase diagrams as a function of composition, typically denoted by X_i. For typical compositions found in Nature, at a given T and P, multiple phases usually co-exist in equilibrium with each other. The compositional phase diagrams can become complex, and computing these diagrams them using the textbook mathematical methods can be cumbersome. However, there is a very simple, but mostly overlooked, computational approach based on the convex hull of a set of phase points, to compute these diagrams efficiently and elegantly. The results from the method not only give the phases at all points in the diagram, but more importantly, they give the geometry and topology of the diagram. This allows the user to gain deep insight in the reason why certain phases are stable and others are not. In this talk I will explain the problem and the method, and I will show example results.

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