

1107-49-441

Maria Emelianenko* (memelian@gmu.edu), **Igor Griva** and **Jeff Snider**. *Optimization challenges in phase diagram calculation.*

Phase diagrams are used as blueprints for materials design and discovery. Extensive effort in the materials community is dedicated to calculating phase diagrams for multicomponent systems of technological importance. The process amounts to minimizing Gibbs free energy subject to linear and nonlinear constraints and in the presence of multiple local minima, which presents challenges when it comes to identifying globally stable equilibria. Complex interaction between the constraints warrants extra care when designing a reliable computational methodology. This talk will survey existing strategies and compare their results to the optimal solutions delivered by a novel set-based constrained minimization algorithm. Pitfalls and advantages of each method will be discussed. (Received January 20, 2015)