

Abstract Submitted
for the 4CF15 Meeting of
The American Physical Society

A Convex Hull Algorithm for Finding New Superalloys¹ JACOB HANSEN, CHANDRAMOULI NYSHADHAM, GUS HART, Brigham Young University — In computational materials science identifying new stable phases is a primary strategy for developing new materials. Constitutional phase diagrams can be calculated from first-principles to narrow the scope of experimental searches. In complicated materials, those that contain more than two components, identifying these phases from many calculations is a convex hull finding problem. We have developed a framework that implements the qhull code[1] and automatically generates convex hulls for ternary intermetallic systems. Using this framework we examined 2224 systems in which we identified 75 new superalloys that have not been reported in experimental literature. Discovering new superalloys such as these has potential to revolutionize materials of the 21st century. [1]www.qhull.org

¹ONR (MURI N00014-13-1-0635)

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Date submitted: 11 Sep 2015

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