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Efficient ab-initio thermodynamic calculations at high pressure and temperature HUGH WILSON, CSIRO Materials Science & Engineering — Prediction of solubility properties and phase diagrams under conditions of high temperature and pressure requires the computation of the Gibbs free energies of materials, a property not directly accessible from molecular dynamics trajectories. Two-step coupling constant integration methods have previously achieved success in the computation of free energies of fluid, solid, and superionic phases of materials by connecting the ab-initio system of interest to a non-interacting reference system via a series of thermodynamic integration steps. These methods, however, require a series of time-consuming and computationally awkward integrations over molecular dynamics trajectories, limiting the utility of the method. Here we propose and demonstrate a method for more efficiently carrying out the same thermodynamic integration without the need for separate molecular dynamics runs, and show how it may be used to carry out the integration up to an order of magnitude more efficiently, in a massively parallel manner, and without the need for code modification. Applications of thermodynamic integration including core solubility in Jupiter and Saturn, and superionic-to-superionic phase transitions in Uranus and Neptune, will be discussed.

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