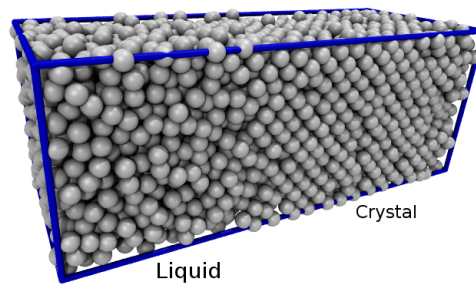


COMPUTING SOLID-LIQUID GIBBS FREE ENERGY DIFFERENCES BY INTERFACE PINNING

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Computing phase diagrams of model systems is an essential part of computational condensed matter physics. I will discuss the interface pinning (IP) method [1-3] for calculating the Gibbs free energy difference between a solid and a liquid. This is done in a single equilibrium simulation by adding an auxiliary harmonic field to the Hamiltonian that biases the system towards two-phase configurations: $\mathcal{H}(\mathbf{R}, \dot{\mathbf{R}}) = \mathcal{H}_0(\mathbf{R}, \dot{\mathbf{R}}) + \frac{\kappa}{2}[Q(\mathbf{R}) - \bar{Q}]^2$, where $Q(\mathbf{R})$ is a crystallinity order-parameter. The Gibbs free energy difference between the phases is simply determined from the average force $-\kappa[\langle Q \rangle - \bar{Q}]$ that the applied field exerts on the system. The coexistence line can be computed efficiently when the IP method is combined with the Newton-Raphson root finding algorithm. Crystal growth rates can be extracted using the Fluctuation-Dissipation theorem [4]. Advantages and drawbacks of the IP method are discussed, and I will present results for the atomistic Lennard-Jones (LJ) model and *ab initio* computations of the period three elements Na, Mg, Al and Si. Please visit http://urp.dk/interface_pinning.htm for details.



The arrangement of LJ particles in an IP-computation.

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