Seeding approach to bubble nucleation

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Liquid-to-vapor transition plays a very important role in science and technology, as shown by issues such as degassification of steel, jet printers or volcanism. Homogeneous bubble nucleation occurs from a metastable liquid; i.e., a liquid heated over the coexistence temperature (boiling) or stretched below the coexistence pressure (cavitation). To understand this transition the Classical Nucleation Theory (CNT) is typically used although there are some discrepancies, even for Lennard-Jones fluids, in the numerical results of the nucleation rate, that is, the number of critical bubbles formed per unit time and volume [1, 2].

With the goal of understanding this discrepancy, we perform Molecular Dynamics simulations and we use a novel technique called Seeding that we have implemented in liquid-to-solid transition [3]. We embed an artificial bubble of a certain size in the metastable fluid and then estimate the temperature at which this seed is critical. This information combined with CNT gives results for the interfatial free energy and the nucleation rate. This cheap but approximate technique can easily be used in more complex systems like water, where other expensive calculations have already been done [4].

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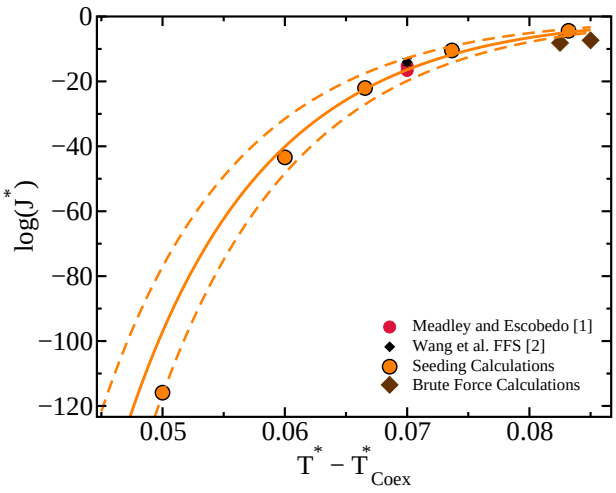

Fig. 1. Nucleation Rate as a function of temperature scaled with the coexistence temperature at constant pressure of $P^* = 0.026$. Seeding calculations are shown in orange: points for data and lines for fit (solid) and error (dashed).