Numerical Simulation of Homogeneous Nucleation at Large Driving Forces

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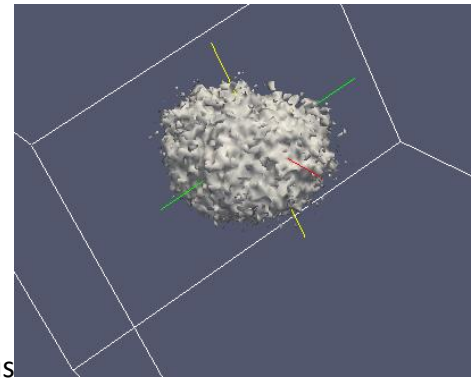
Abstract

The problem of *nucleation*—emergence of a new state of matter (*phase*)—is central to many branches of physics from cosmology to materials physics to biophysics. Although the main reason for the nucleation—some kind of instability of the old phase—is the same in all of these examples, the actual realization may be very different. I consider the case of homogeneous nucleation—no inoculants or defects, where the process is assisted by internal fluctuations. In many physical situations this process proceeds far away from equilibrium that is, at large driving forces—large free energy difference between the old and new phases—when the standard approach of the stationary nucleation rate is not applicable. Examples are crystallization of organic fluids, colloids, low dimensional systems, etc.

I numerically simulate the process in the framework of the stochastic Ginzburg-Landau approach where the internal thermal noise is modeled as an additional stochastic force of specified intensity. To validate the method I calculated the equilibrium properties of the metastable state using the perturbation theory and Feynman diagrams and compared the results with the simulations. I also present theoretical calculations of the *lifetime* (first-passage time)—time needed for the critical nucleus to assemble from the initially homogeneous old phase. I analyze dependence of the lifetime on the driving force, intensity of noise, and volume of the system. Contrary to the traditional view, I find the lifetime to be inversely proportional to the square root of the volume instead of the volume itself. The three-dimensional *critical nuclei* obtained in simulations have large degree of ramification (see Figures below).

3Dnucleus 

2D-projection