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# Direct Numerical Simulation of Bubble Growth in a Nanocavity

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We use for the first time a Phase-Field (PF) model[1] to simulate the growth process of a single bubble nucleated in a nanocavity. We compare the growth rate and temperature distribution of PF predictions with those from Molecular Dynamics (MD) simulations. The domain is composed of a tethered solid wall (restrained with a spring force), a cavity and a liquid phase that transitions to vapour when the system temperature exceeds the saturation point[2]. The MD simulations consider the NVT ensemble with Lennard-Jones interactions. A Nose-Hoover thermostat is used to control the temperature at the lower boundary and induces the heating process. Fixed boundary conditions are applied at the top and bottom faces of the simulation box, whereas periodic boundary conditions are used in the lateral and spanwise directions. The PF simulations are carried out with the same dimensions as the MD system, but with a much larger time-step. The thermal conductivity and heat capacity of the wall and of the liquid phase are obtained by solving the inverse problem using the MD results before the nucleation event. Once a bubble is formed, a second inverse problem is solved to identify the flow coefficients which govern interface motion and thermal transport of the Lennard-Jones fluid during the initial stages of bubble growth. After the bulk properties have been determined, the PF simulations are carried out completely independently from the MD results. The results show the agreement between the continuum model and the MD data when we match the physical properties in the PF simulations. In a second stage of our research, we intend to use MD data to obtain the statistical properties of the thermal fluctuations in the liquid phase as a function of the local temperature and distance to the wall. This information will be fed into the PF model (in the form of 'noise' with identical statistical properties to the thermal fluctuations added to the liquid density), which will allow us to use a continuum model to study boiling from first principles including the highly complex phenomenon of nucleation.

## REFERENCES

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