Modeling droplet breakup effects with diffuse interface methods in ALE-AMR code with application in modeling NDCX-II experiments

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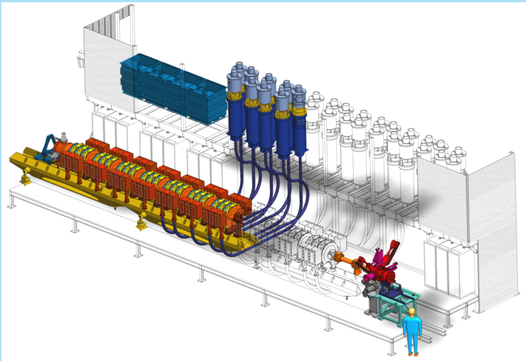
Introduction

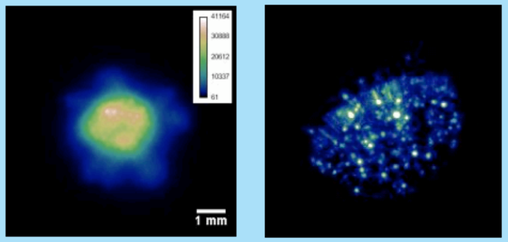
We implement a single-fluid diffuse interface model in the ALE-AMR hydrodynamics code to simulate surface tension effects. We show simulations and compare them to other surface tension models. We benchmark this code against analytic models that incorporate surface tension (showing agreement with Laplace's equation describing the pressure difference between the interior and exterior of a droplet, for example). We also show how this simulation can be used for modeling the NDCX-II ion beam heated target experiments planned to begin in 2012.

Application

Our goal is to accurately simulate the droplet breakup for NDCX-II experiment, for example, predict the correct size distribution and velocity profile for the droplets.



The NDCX-II experiment at LBL will study warm dense matter created by ion heating. Surface tension model is necessary for a correct simulation.



Left: Gated camera image of a carbon target heated by NDCX-I beam. Right: Shower of hot platinum debris fragments(droplets) after the beam pulse.

Model

We base our model on the single fluid diffuse interface model described in [1].

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \vec{V}) \tag{1}$$

$$\rho\left(\frac{\partial \vec{V}}{\partial t} + \vec{V} \cdot \nabla \vec{V}\right) = -\nabla p + \nabla \cdot \sigma_1 + \nabla \cdot \sigma_2 \tag{2}$$

Here σ_1 represents the viscous stress tensor:

$$\sigma_1 = \mu(\nabla \vec{V} + (\nabla \vec{V})^T - \frac{2}{3}\nabla \cdot \vec{V} I). \tag{3}$$

In addition, we have a new tensor term

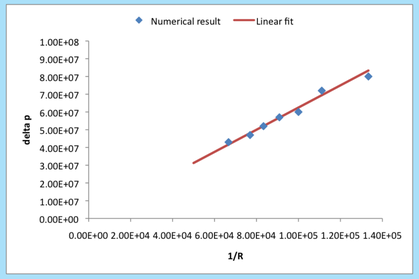
$$\sigma_2 = K((\frac{1}{2}|\nabla \rho|^2 + \rho \Delta \rho) I - \nabla \rho \otimes \nabla \rho). \tag{4}$$

This is the Korteweg stress tensor, which represents surface tension force.

We added a section of code in ALE-AMR that calculates σ_2 and add it to the original stress tensor. The differential operators are approximated by finite difference methods similar to [3].

Benchmark-Laplacian equation

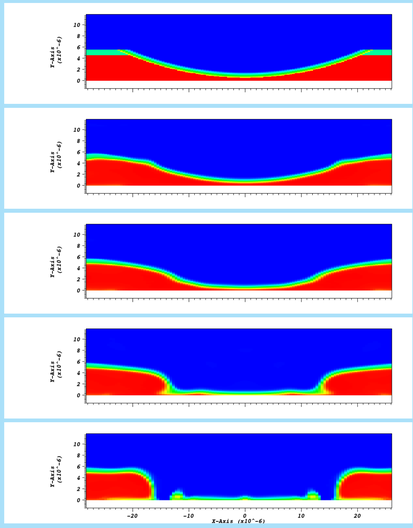
To benchmark the result against the Laplacian equation, we use a droplet below critical temperature, surrounded by vapor of the same material, temperature, and pressure. Then we run the simulation until it reaches equilibrium and record the difference of pressure around the interface.



Benchmark against the Laplacian equation. The x-axis is 1/R, where R is the radius of droplet, and the y-axis is the pressure difference. Red line is the least square fit for the results.

Benchmark-Rayleigh instability

Another classical result of surface tension model is the Plateau-Rayleigh instability. It involves a thin tube of liquid with initial perturbation that will be enlarged due to surface tension effect, and then cause droplet breakup. To simulate this effect, we utilize the 2D axisymmetry module in the ALE-AMR code to reduce comptational complexity, with the symmetrical axis being the central axis of the thin tube. The initial tube was set to be long enough to prevent boundary effects, but we only focus on the center of the tube that has initial perturbation.



Sample of a Rayleigh instability simulation

Surface tension coefficient

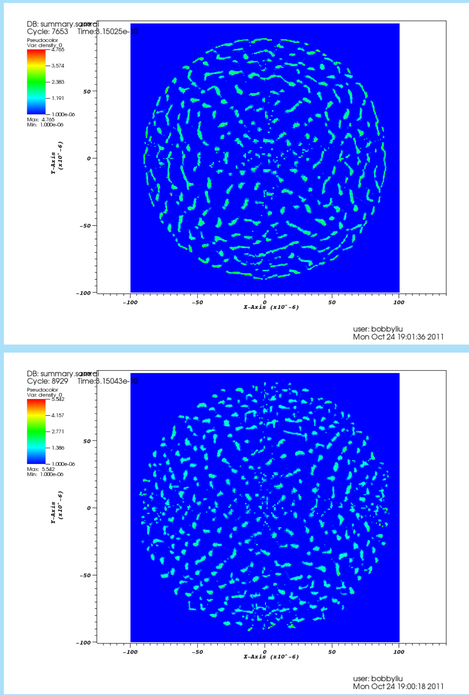
Equivalent surface tension coefficient

$$\alpha = K \int_{-}^{+} (\frac{d\rho}{dz})^2 dz, \tag{5}$$

where z is the normal direction of the interface and the integration is done across the interface [1]. If we write interfacial width as ϵ, then $\alpha \sim K\frac{\delta\rho^2}{\epsilon}$.

Droplet breakup simulation

As for a preliminary simulation of the actual application, we show a result of the droplet breakup simulation using ALE-AMR's void insertion for droplet breakup simulation. The result involves a heated droplet as initial condition. Since the pressure is larger than the surrounding area, it expands before finally breaking up. As we can see, the surface tension model provide a better breakup result than the simulation without it.



Sample of a droplet breakup result without(up) or with(down) surface tension.

References

[1] Nadiga, B. T. and Zaleski, S. Investigations of a Two-Phase Fluid Model In *Contributions to Mineralogy and Petrology 1995*

[2] Denniston, C. and Yeomans, J. M. Diffuse interface simulation of Marangoni convection In *Physical Chemistry Chemical Physics 1999*

[3] Sukumar, N. Voronoi cell finite difference method for the diffusion operator on arbitrary unstructured grids In *International Journal for Numerical Methods in Engineering 2003*