Modeling droplet breakup effects with applications in the warm dense matter NDCX experiment

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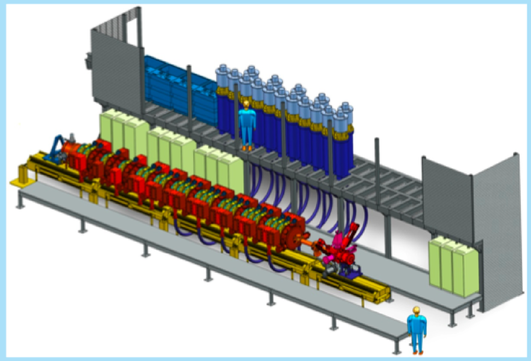
Introduction

We combine a single-fluid diffuse interface model with the ALE-AMR code to simulate surface tension effects. We show the result of a test case, and compare it to the result without surface tension. The model describes droplet formation nicely.

Application



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

Model

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

$$\frac{d\rho}{dt} = \nabla \cdot (\rho \vec{V}) \tag{1}$$

$$\rho(\frac{d\vec{V}}{dt} + \vec{V} \cdot \nabla \vec{V}) = -\nabla p + \nabla \cdot \sigma_1 + \nabla \cdot \sigma_2 \tag{2}$$

Here σ_1 represents the viscous stress tensor:

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

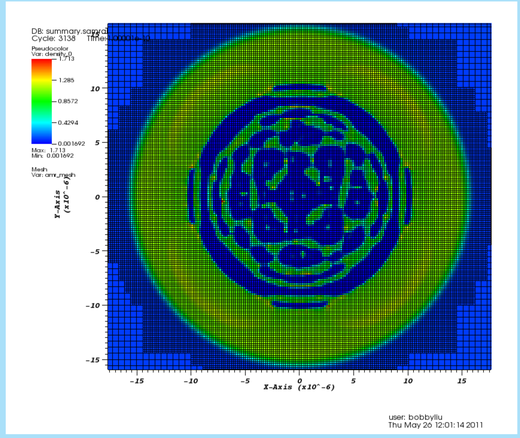
In addition, we have a new tensor term

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

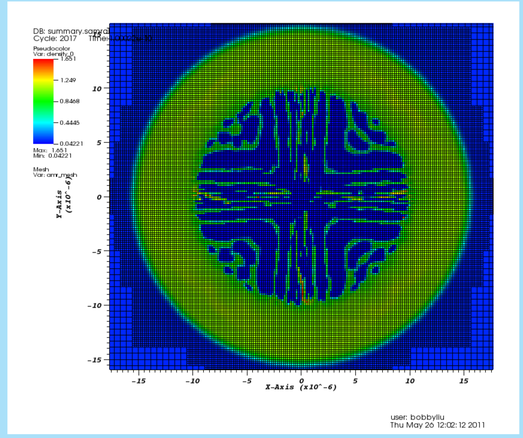
This is the Korteweg stress tensor, which represents surface tension force.

Numerical Simulation

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].
We use two different scenarios to show the results for this model. The first one involves an expanding Aluminum drop over critical temperature surrounded by Aluminum gas under critical temperature. It resembles the development of a droplet after being heated by ion beam in the NDCX-II experiment. Both results show material breakup due to physical instability of spinodal region, but the surface tension model clearly forms droplets while the other one does not.

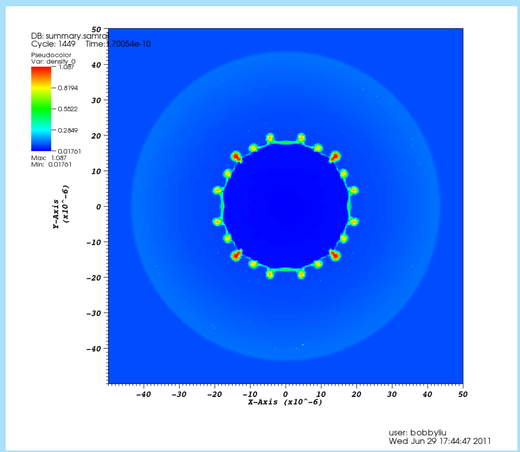


a) Droplet Breakup with Surface Tension

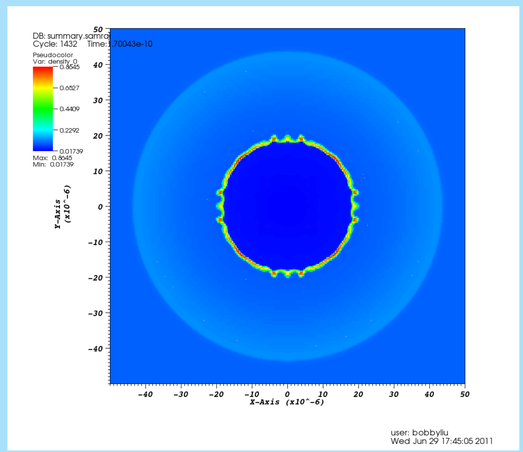


b) Droplet Breakup without Surface Tension

The second scenerio involves an Aluminum shell with a very high temperatured Aluminum vapor inside. It resembles the development of an Aluminum capsule after the inside is heated up via fast ignition.



a) Pressure Driven Expansion with Surface Tension



b) Pressure Driven Expansion without Surface Tension

Properties of the model

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 $\alpha \sim K\frac{\delta\rho^2}{\epsilon}$.
This surface tension coefficient depends on temperature. Temperature changes the density and pressure of the two phases, thus affect the surface tension. For example, for Van der Waals fluid $\alpha \sim (T_c - T)^{3/2}$, where T_c is the critical temperature.[2]

Advantages and disadvantages

Advantage:
1. It is easy to be adapted into the current full-scale fluid simulation. The only change necessary is an additional term to the stress tensor.
2. This model does not require explicit physical state of the two phases. It will be more convenient for running the same code over different materials and more importantly, when temperature changes.

Disadvantage:
1. Since we only have one parameter K, we cannot adjust ϵ and α individually. We can only derive from scaling properties that $\epsilon \sim K^{1/2}$ and $\alpha \sim K^{1/2}$.
2. It is difficult to calculate surface tension directly from input parameter. Although all diffuse interface models suffer from this problem.

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*