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[7-C-01] Error Estimation for Adaptive Mesh Refinement in Droplet Simulations

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Error Estimation for Adaptive Mesh Refinement in Droplet Simulations

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Abstract: We present a one-dimensional shear force driven droplet formation model with a flux-based error estimation. The presented model is derived using asymptotic expansion and a front-tracking method to simulate the droplet interface. The model is then discretized using the Galerkin finite element method in the mixed form. However, the jumps in the solution gradients are discontinuous and can grow faster due to the highly convective pinch-off process. This leads to an erroneous droplet interface and incorrect curvature. Therefore, the mesh must be sufficiently refined to capture the interface accurately. The mixed form of the governing equation naturally provides smooth interface gradients that can be used to compute the error estimate. The computed error estimate is then used to drive the adaptive mesh algorithm.

Keywords: A posteriori error estimation, Adaptive mesh refinement, Mixed-finite element method, Droplet formation.

1 Introduction

The formation of droplets and bubbles is a mature field in physics. These surface tension driven phenomena have been deeply explored using interface tracking and interface capturing approaches. For applications with a symmetrical structure of droplet formation, a one-dimensional model with the interface tracking approach is advantageous in terms of computational costs [1]. We consider a one-dimensional model for shear-induced droplets that estimates droplet sizes for an environment with co-flowing fluids [2]. This one-dimensional model is discretized using the Galerkin finite element approach in the mixed form.

The instability leading to the pinch-off point requires a finer mesh in the region of high curvature. As the interface evolves with the progression of numerical simulation, the mesh must be adaptively refined to control discretization errors, especially in the singularity regions. Therefore, a robust error estimation method is essential in designing an adaptive mesh refinement algorithm for our one-dimensional model. The field of a posterior error estimation has been under continuous and rigorous refinement since the 1908s [3]. The recent advancements in the field of error estimation methods provide some robust strategies, as shown in [4].

In the following sections, we describe the one-dimensional droplet pinch-off model and explain the need for an error estimator. Then, we explore the flux-based error estimation approach and show that the mixed form naturally provides a smooth flux to get the error bounds. Finally, the results present the usefulness of the error estimate in adaptive mesh refinement.

2 Problem Statement

Consider a fluid column slowly flowing with the constant velocity u^d out of a nozzle with the radius h_{in}. The *continuous* (or outer) fluid is co-flowing with the *dispersed* (or inner) fluid column but with a higher velocity u^c. Fig. (1) shows the schematic describing this co-flowing fluids scenario. The superscripts d and c represent dispersed phase and continuous phase fluids, respectively.

The first one-dimensional model using front tracking was proposed by Eggers and Dupont [5] for the droplet pinch-off in a quiescent background under the gravitational force. We start with the Navier-Stokes equations in the cylindrical coordinates. The pinch-off process happens in finite time due to the surface tension forces trying to minimize the surface energy by contracting the interface in the radial direction. The radial contraction is faster than the axial elongation, which allows the solution variables

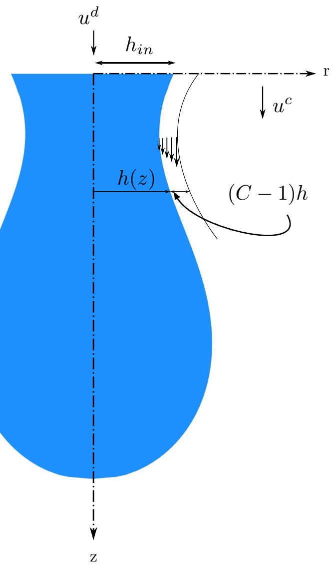


Figure 1: Schematic of a droplet formation in a co-flowing fluid.

to expand asymptotically in r. Finally, the normal forces are balanced by the surface tension forces, which are used to simplify the equation into a one-dimensional model.

In a similar fashion, we consider the droplet pinch-off in another co-flowing fluid under the gravitational and shear forces. We consider the co-flowing fluids with a preserved symmetry around the angular direction. This provides the basis for the one-dimensional approach. The continuous fluid affects the droplet morphology by applying shear force on the interface between two fluids. This shear force effect can be approximated with the asymptotically derived force balance on the interface, leading to the derivation of the one-dimensional governing equations. The full derivation can be found in [6].

The momentum and the interface equations are given as follows.

$$\frac{\partial u^d}{\partial t} + u^d \frac{\partial u^d}{\partial z} + \frac{\gamma}{\rho}\frac{\partial \mathcal{K}}{\partial z} - \frac{6\nu^d}{h}\frac{\partial u^d}{\partial z}\frac{\partial h}{\partial z}\left(1 + \frac{\mu^c}{\mu^d}\right) - 3\nu^d \frac{\partial^2 u^d}{\partial z^2}\left(1 + \frac{2}{3}\frac{\mu^c}{\mu^d}\right)$$
$$+ \frac{2}{\rho^d}\frac{dp^c}{dz} + \frac{1}{2\rho^d \ln(C)}\frac{dp^c}{dz} - \left(1 - \frac{\rho^c}{\rho^d}\right) g = 0 \quad (1)$$

$$\frac{\partial h}{\partial t} + u^d \frac{\partial h}{\partial z} + \frac{h}{2}\frac{\partial u^d}{\partial z} = 0 \quad (2)$$

Here, parameters γ, ρ, ν, μ, and p represent surface tension coefficient, density, kinematic viscosity, dynamics viscosity, and pressure, respectively. The superscript represents dispersed or continuous phase fluid. $\mathcal{K}$ is the curvature defined by

$$\mathcal{K} = \left[\frac{1}{h\left(1 + \frac{\partial h}{\partial z}^2\right)^{1/2}} - \frac{\frac{\partial^2 h}{\partial z^2}}{\left(1 + \frac{\partial h}{\partial z}^2\right)^{3/2}} \right] \quad (3)$$

The quantity $(C-1)h$ defines the thickness of the shear layer in the continuous phase flow, which defines how much force is experienced by the dispersed phase droplet. The parameter C is a free parameter that can be defined using curve-fitted monotonic functions on the numerical and experimental data [2].

The system of governing equations given by Eqs. (1-2) are then discretized using a Galerkin finite element method using a mixed method [2]. The mixed finite element weak form is given by

$$\int_\Omega q \left[\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial z} - \frac{6\nu}{h}\frac{\partial h}{\partial z}\frac{\partial u}{\partial z}\left(1+\frac{\mu^c}{\mu^d}\right) + \frac{\gamma}{\rho}\left\{ -\frac{s\frac{\partial s}{\partial z}}{h\left(1+s^2\right)^{3/2}} - \frac{s}{h^2\left(1+s^2\right)^{1/2}} \right\} + \frac{1}{2\rho^d \ln(C)}\frac{dp^c}{dz} - \left(1-\frac{\rho^c}{\rho^d}\right) g \right] d\Omega + \int_\Omega \nabla q \left[3\nu\left(1+\frac{2}{3}\frac{\mu^c}{\mu^d}\right)\frac{\partial u}{\partial z} + \frac{\gamma}{\rho}\frac{\frac{\partial s}{\partial z}}{\left(1+s^2\right)^{3/2}} \right] d\Omega - \int_\Gamma q \left[3\nu\left(1+\frac{2}{3}\frac{\mu^c}{\mu^d}\right)\frac{\partial u}{\partial z} + \frac{\gamma}{\rho}\frac{\frac{\partial s}{\partial z}}{\left(1+s^2\right)^{3/2}} \right] d\Gamma = 0 \tag{4}$$

$$\int_\Omega v\left[\frac{\partial h}{\partial t} + u\frac{\partial h}{\partial z} + \frac{h}{2}\frac{\partial u}{\partial z}\right] d\Omega = 0 \tag{5}$$

$$\int_\Omega w\left[s - \frac{\partial h}{\partial z}\right] d\Omega = 0 \tag{6}$$

where, s is the introduced variable for the mixed form that approximates the derivative of the interface distance, that is $\partial h/\partial z$.

The Eqs. (4-6) are solved using $C^0(\Omega)$ elements. The solution algorithm involves moving mesh and calculating the droplet length in a self-consistent way. The algorithm is explained in [1].

The flow becomes highly convective as the droplet interface evolves up to a point when it starts forming the neck. The radial contraction of the interface accelerates faster than the elongation, hence rapidly approaching the singularity. This behavior should be captured accurately to get the precise equilibrium droplet profiles. Numerical approaches like finite element methods are bounded by the discretization parameter. Hence, the numerical solution entails the discretization error.

3 Error estimation

When approaching the singularity, the high-curvature regions quickly develop high stresses. An error in the solution can cause the interface to advect in an incorrect direction, providing an incorrect droplet profile. A coarser mesh must be refined to improve the solution in those regions and get an accurate force balance, leading to more accurate droplet profiles. This refinement can be done adaptively by estimating the true error in the solution using a posteriori error estimation approach. The foremost goal is to compute the discretization error in the droplet interface evolution.

Since the solution is approximated with $C^0(\Omega)$ continuity., the gradients of the solutions are discontinuous across the element boundaries. This discontinuity strongly reflects on the curvature, which can produce erroneous equilibrium droplet profiles. We can use a flux-recovery based approach to drive the adaptive mesh refinement. The flux-recovery approach aims to post-process a smooth gradient from the FE solution and determine the error estimator based on the error in the smoothed and non-smoothed gradients.

In the droplet pinch-off model, we get the velocity (u) and the droplet radius (h) as the solution. However, the mixed form approach utilizes the approximation of the gradient $\partial h/\partial z$ as a part of the solution. In other words, the mixed variable s already provides a smooth gradient of h. If the true gradient is $\partial\bar{h}/\partial z$, the quantity s is assumed to retain better accuracy than $\partial h/\partial z$ since the slope (or flux) s is part of the equilibrium equations and coupled with the curvature derivatives in the momentum equations. The true error norm in the gradient can be written as

$$||e|| = \left|\left|\frac{\partial\bar{h}}{\partial z} - \frac{\partial h}{\partial z}\right|\right| \approx \left|\left| s - \frac{\partial h}{\partial z}\right|\right| \tag{7}$$

The quality of the estimate clearly depends on how good the approximation 's' is of the true slope $\partial\bar{h}/\partial z$. Assuming there exists $c \in (0,1)$ such that

$$\left|\left|\frac{\partial\bar{h}}{\partial z} - s\right|\right| \leq c\left|\left|\frac{\partial\bar{h}}{\partial z} - \frac{\partial h}{\partial z}\right|\right| \tag{8}$$

Using the triangle inequalities, the bounds on the true error in terms of the error estimate follow directly that

$$\frac{\eta}{1+c} \leq ||e|| \leq \frac{\eta}{1-c} \tag{9}$$

where $\eta = ||s - \partial h/\partial z||$ is the error estimate of the true error. It is clear that the smaller the c, the better the error estimate.

This approach can also be viewed from the residual based error estimation perspective. A residual based a posteriori error estimation approach directly utilizes the finite element solution. Defining the error in the energy norm, one can also derive upper and lower error bounds for the error in the slope 's' using the element residuals.

Here, the error bounds given in Eq. (9) are used to refine the mesh adaptively. A simple h-refinement can be done cyclically:

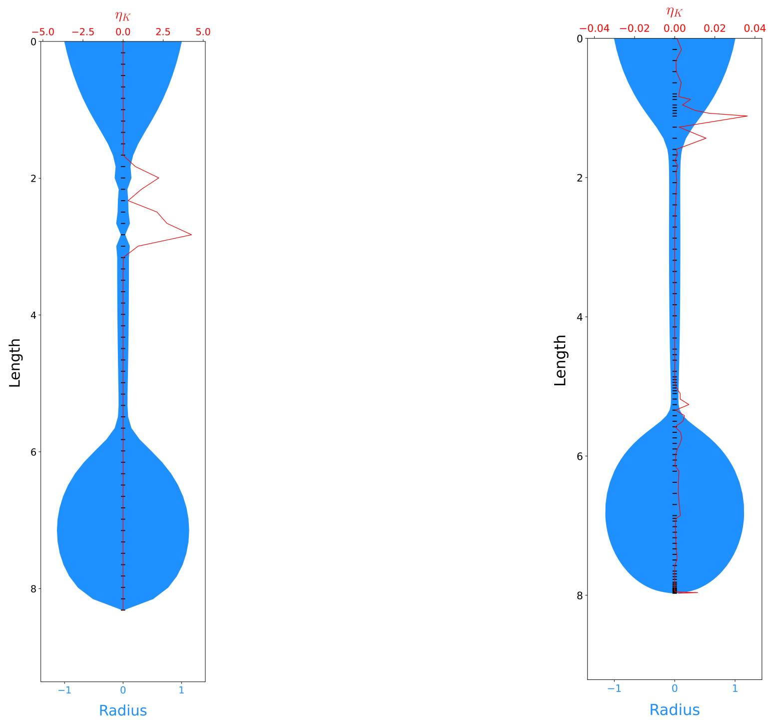
$$\text{solve} \rightarrow \text{estimate error} \rightarrow \text{mark elements} \rightarrow \text{refine}$$

The element are marked using the maximum threshold $\bar{\eta} = \lambda \ \max_{K \in \mathcal{T}_h} \eta_K$, where $\lambda \in [0, 1]$. Here, K represents an element from the triangulation $\mathcal{T}_h$. This simple strategy allows marking elements K such that $\eta_K \geq \bar{\eta}$.

4 Results

The adaptive mesh refinement strategy as explained in the previous section is used for the droplet simulation for a 85% glycerol solution in the background with quiescent air. The material properties are used from [1]. As the simulation progresses, we track the error evolution along with the droplet interface. This provides an insight on how the error progresses as the curvature changes. Fig. (2) shows the evolved error superposed on the droplet profile for both no refinement and adaptive refinement. The evolution profiles are shown at the same time stamp.

Fig. (2a) shows the error plot along the droplet length on a non-refined grid. The top of the neck is a high velocity region where the upstream flow pushes the droplet axially. However, the radial velocity is much faster than this axial push. Hence as explained before, the discontinuous interface slope (or the



(a) Error on the non-refined grid. (b) Error on the adaptively refined grid.

Figure 2: Error plots superposed on the 85% glycerol droplet profile.

gradient) grows quickly. This is clearly visible at the top of the neck where the element-wise error is large. Due to the large error, the droplet interface shows instabilities and hence the simulation diverges. This instability is clearly visible in the droplet profile.

Using the flux-based error estimation explained in the previous section, the mesh is adaptively refined with $\lambda = 0.1$. This means that the elements where the error is larger than 10% of the maximum value are marked and refined. The choice of this criterion is based on the observation in the error evolution for non-refined grid. The element patches with large error are usually the ones where the curvature gradient is large, e.g. the tip of the drop, top of the neck, and pinch-off region.

The error plot on an adaptively refined grid is shown in Fig. (2b). Compared to the non-refined grid, the error plot shows the error reduction by a factor of 100. The curvature at the top of the neck region is now much smoother and the interface instabilities are not present. Also, comparing only the droplet profile, the non-refined version is coarse at the tip. Whereas the refined version of the droplet is much smoother. It is crucial to have more accurate droplet profile to calculate the volume of the pinched-off droplet. The refined version provides more accuracy and stability with only optimally added computational cost.

5 Conclusion

We presented a simple yet effective strategy to compute the error estimate for droplet simulations with front tracking method. The one-dimensional model used for the simulations is accurate for shear induced droplet in a co-flowing environment. The mixed form equations naturally incorporate a smooth flux as a part of the solution, which allows us to use the flux-based error estimation. The comparison of error evolution for 85% glycerol droplet in a quiescent air is presented for non-refined and adaptively refined grid. This comparison shows that the adaptively refined grid provides improved stability and accuracy in capturing the droplet interface. The one-dimensional model has been previously used for conducting uncertainty quantification (UQ) analysis for droplet atomization in a hybrid rocket combustion [7]. The presented error estimate can further enhance the accuracy of the UQ analysis.

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