Implicit surface tension model for stimulation of interfacial flows

Vinh The Nguyen

University of Massachusetts Dartmouth

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About my project

Project Advisor

- Dr. Mehdi Raessi
- Department of Mechanical Engineering

Project Objective

- To study implicit modeling of surface tension.
- To generate faster and better model that produce no spurious currents and has larger time step restriction.
Introduction

- What is interfacial flow?

- What are the applications?
Interfacial flows, important in many applications

Combustion  Naval hydrodynamics  Spray coating

Spray cooling  Casting

Courtesy of Edwards
Modeling of interfacial flow

- To accurately model the interfacial flow is challenging because:
  - The discontinuity of fluid properties (such as density).
  - The interfacial boundary condition (surface tension).
Currently there are two main interfacial flow models

- **Explicit:**
  Precise but has high computational cost due to small time step restriction.

- **Implicit:**
  Lower computational cost than explicit due to higher time-step restriction.
  Drawbacks: appearing of nonphysical velocities (spurious current)
  
  **Common flow solver:** Continuum surface force (CSF)
Method used

CSF method

- The implicit model studied in this project is based on Continuum Surface Force method
- This method was first proposed by Brackbill et al. 1991

Drawbacks:

- This method generates unphysical velocities (spurious currents)
- The spurious current is caused by:
- Imbalance of the surface tension and pressure gradient.
- Error in computing the curvature. (this project)
Implicit modeling

Nguyen

The pressure drop across the interface:

\[ \Delta p = p_2 - p_1 = \sigma k \]  \hspace{1cm} (1)

\( \sigma \) is the surface tension coefficient
\( k \) is the mean curvature

\[ k = \frac{1}{R_I} + \frac{1}{R_{II}} \]  \hspace{1cm} (2)

\( \delta \) is the delta function represent interface (Raessi et al. 2008)

\[ \vec{F} = (\sigma \kappa \hat{n} + \nabla_s \sigma) \delta \]
My task

Tasks:
- Study the CSF model
- Study the stability of the model (CFL condition) as time-step increases using different curvature solving method: Level set (LS) and Advecting Normal
- Compare the results with exact curvature.

Challenges:
- To get used to the code and understand what’s the function of each parts requires lots of trials errors.
- To manipulate it to do what I want also requires lots of trials and errors.
• The Courant-Friedrichs-Lewy condition (CFL condition) is a necessary condition for convergence while solving partial differential equations numerically.

\[
CFL = \frac{u \Delta t}{\Delta x} \leq C
\]  

(3)

\(C = 1\)
In the LS method, the interface is represented by a smooth function \( \phi \) — called the LS function; for a domain \( \Omega \), \( \phi \) is defined [15] as a signed distance to the boundary (interface) \( \partial \Omega \)

\[
|\phi(\mathbf{x})| = \min(|\mathbf{x} - \mathbf{x}_i|) \quad \text{for all } \mathbf{x}_i \in \partial \Omega
\]

implying that \( \phi(\mathbf{x}) = 0 \) on \( \partial \Omega \). Choosing \( \phi \) to be positive inside \( \Omega \), we then have

\[
\phi(\mathbf{x}) = \begin{cases} 
> 0, & \mathbf{x} \in \Omega \\
0, & \mathbf{x} \in \partial \Omega \\
< 0, & \mathbf{x} \not\in \Omega
\end{cases}
\]

For the 2D interface depicted in Fig. 1a, the discretized LS function, defined at the center of each cell, is shown in Fig. 1c.

The unit normal vector and curvature at any point on the interface are calculated from \( \phi \) by

\[
\hat{n} = \frac{\nabla \phi}{|\nabla \phi|}
\]

and

\[
\kappa = -\nabla \cdot \left( \frac{\nabla \phi}{|\nabla \phi|} \right)
\]

(Raessi et al. 2007)
For a 2D interface between two fluids, depicted in Fig. 1a, the discretized VOF function representing fluid 1 is shown in Fig. 1b. As can be seen, the volume fractions vary sharply from zero to one across the interface. This discontinuous behavior makes it difficult to accurately evaluate the first and second derivatives of \( f \), which leads to inaccurate interface normals and curvatures. Smoothing the \( f \) field prior to evaluating \( f \) improves the values [12]. We assess the accuracy of \( \mathbf{n} \) and \( \mathbf{j} \) calculated from \( f \) in Section 2.3. But first, we briefly present the LS method, which is known to yield more accurate normals and curvatures.

### 2.2. Level set method

In the LS method, the interface is represented by a smooth function \( \phi \) called the LS function; for a domain \( \mathcal{X} \), \( \phi(\mathbf{x}) \) is defined [15] as a signed distance to the boundary (interface) \( \partial \mathcal{X} \):

\[
\phi(\mathbf{x}) = \text{min} \left( \frac{\langle C_0(\mathbf{x}) \rangle}{||C_1(\mathbf{x})||} \right)
\]

For all \( \mathbf{x} \in \mathcal{X} \) \((\neq 0)\):

\[
\phi(\mathbf{x}) = 0 \quad \text{on} \quad \partial \mathcal{X}.
\]

Choosing \( \phi \) to be positive inside \( \mathcal{X} \), we then have:

\[
\phi(\mathbf{x}) > 0 \quad \text{in} \quad \mathcal{X};
\]

\[
\phi(\mathbf{x}) < 0 \quad \text{outside} \quad \mathcal{X};
\]

\[
\phi(\mathbf{x}) = 0 \quad \text{on} \quad \partial \mathcal{X}.
\]

For the 2D interface depicted in Fig. 1a, the discretized LS function, defined at the center of each cell, is shown in Fig. 1c. The unit normal vector and curvature at any point on the interface are calculated from \( \phi \) by

\[
\mathbf{n} = \frac{\partial \phi}{\partial \mathbf{r}}
\]

and

\[
\mathbf{j} = \frac{\partial^2 \phi}{\partial \mathbf{r} \partial \mathbf{r}}
\]

Since \( \phi \) is smooth and continuous across the interface (see Fig. 1c), \( \mathbf{n} \) can be calculated accurately. In the LS method, the motion of the interface is defined by the following advection equation:

\[
\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0
\]

When \( \phi \) is advected, the \( \phi = 0 \) contour moves at the correct interface velocity; however, contours of \( \phi \neq 0 \) do not necessarily remain distance functions. This can result in an irregular \( \phi \) field that in turn leads to problems (Raessi et al. 2007).
As reviewed earlier, the evolution of the LS function is governed by Eq. (10)

$$\frac{\partial \phi}{\partial t} + \vec{u} \cdot \nabla \phi = 0$$

Defining $\vec{N} = \nabla \phi$ as the vector normal to the contours of $\phi$, the above equation can be rewritten as

$$\frac{\partial \phi}{\partial t} + \vec{u} \cdot \vec{N} = 0$$

Taking the gradient of Eq. (14), we obtain

$$\frac{\partial \vec{N}}{\partial t} + \nabla (\vec{u} \cdot \vec{N}) = 0$$

Eq. (15) is the advection equation for normals. In 2D Cartesian coordinates, Eq. (15) results in the following equations:

$$\frac{\partial N_x}{\partial t} + \frac{\partial}{\partial x} (uN_x + vN_y) = 0$$

(16)

and

$$\frac{\partial N_y}{\partial t} + \frac{\partial}{\partial y} (uN_x + vN_y) = 0$$

(17)

(Raessi et al. 2007)
Case study: Static drop

- Static water drop in zero gravity.
- $\rho_1 = \rho_2 = 10^3 \text{Kg/m}^3$
- $\mu_1 = \mu_2 = 0.05$
- $g = 0$
- Surface tension time-step restriction $\Delta t_{ST} = 0.03$

(Raessi et al. 2008)
What I did

- Code
  - Export CFL to screen
  - Export CFL vs Time as txt file
  - Observe the grow of CFL over time and to stop when CFL > 1
  - Plot CFL vs. Time using Matlab
Results - Level Set method vs. Exact Curvature

- Level set
  The timestep was increase as: \( \Delta t = 0.5, 2, 4\Delta t_{ST} \)

- Exact curvature
Result: Level set at $dt = 4, 8\Delta t_{ST}$

- **Level set** $dt = 4, 8\Delta t_{ST}$

- **Exact curvature** $dt = 8\Delta t_{ST}$
Result - Level set vs. Exact Curvature for maximum timestep

- **Level set**
  \[ dt = 3.167, 3.2\Delta t_{ST} \]

- **Exact curvature**
  \[ dt = 6.67, 7\Delta t_{ST} \]
Result: Level set vs Advecting Normal

CFL vs. Time for Exact Curvature

CFL @dt=0.095s AN
CFL @dt=0.096s AN
CFL @dt=0.095s LS
CFL @dt=0.096s LS

Student Version of MATLAB
The errors associated with curvatures calculated from the LS function $\phi$, for a circle of radius 0.15 centered at (0.5, 0.5) in a $1 \times 1$ domain, at different mesh resolutions:

<table>
<thead>
<tr>
<th>$\Delta x$</th>
<th>$l_\infty$</th>
<th>Order</th>
<th>$l_1$</th>
<th>Order</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/16</td>
<td>0.5472</td>
<td>1.55</td>
<td>0.2963</td>
<td>1.58</td>
</tr>
<tr>
<td>1/32</td>
<td>0.1875</td>
<td>-1.79</td>
<td>0.0991</td>
<td>-0.51</td>
</tr>
<tr>
<td>1/64</td>
<td>0.6481</td>
<td>0.61</td>
<td>0.1407</td>
<td>-0.11</td>
</tr>
<tr>
<td>1/128</td>
<td><strong>0.4234</strong></td>
<td>-0.43</td>
<td>0.1518</td>
<td>-0.02</td>
</tr>
<tr>
<td>1/256</td>
<td>0.5689</td>
<td>-0.29</td>
<td>0.1537</td>
<td>0.34</td>
</tr>
<tr>
<td>1/512</td>
<td>0.6963</td>
<td>0.11</td>
<td>0.1215</td>
<td>-0.01</td>
</tr>
<tr>
<td>1/1024</td>
<td>0.6453</td>
<td></td>
<td>0.1227</td>
<td></td>
</tr>
</tbody>
</table>

Table 6: The errors associated with curvatures calculated by the $\bar{N}$ method, for a circle of radius 0.15 centered at (0.5, 0.5) in a $1 \times 1$ domain, at different mesh resolutions:

<table>
<thead>
<tr>
<th>$\Delta x$</th>
<th>$l_\infty$</th>
<th>Order</th>
<th>$l_1$</th>
<th>Order</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/16</td>
<td>$3.87 \times 10^{-1}$</td>
<td>1.72</td>
<td>$2.11 \times 10^{-2}$</td>
<td>1.73</td>
</tr>
<tr>
<td>1/32</td>
<td>$1.18 \times 10^{-1}$</td>
<td>2.11</td>
<td>$6.33 \times 10^{-2}$</td>
<td>2.20</td>
</tr>
<tr>
<td>1/64</td>
<td>$2.73 \times 10^{-2}$</td>
<td>2.07</td>
<td>$1.38 \times 10^{-2}$</td>
<td>1.94</td>
</tr>
<tr>
<td>1/128</td>
<td><strong>$6.51 \times 10^{-3}$</strong></td>
<td>1.95</td>
<td><strong>$3.60 \times 10^{-3}$</strong></td>
<td>2.03</td>
</tr>
<tr>
<td>1/256</td>
<td>$1.68 \times 10^{-3}$</td>
<td></td>
<td>$8.83 \times 10^{-4}$</td>
<td></td>
</tr>
</tbody>
</table>
Conclusion

Proved:

- To accurately compute the curvature is crucial and it can increase the stability of the solution for implicit model.
Future Research

- Continue to study the implicit models.
- Starting with the simulation.
References

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