

Visual Analysis of Interface Deformation in Multiphase Flow

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Introduction

This project aims at investigating droplet-related phenomena, especially the influence of forces acting on the surface. To this end, we visualize interface deformation using two quantities: interface stretching and interface bending. This allows the visual analysis of droplet behavior and interface-related forces, such as the surface tension force and forces induced by Marangoni convection. For the latter, we show an application case for debugging and aiding the implementation of the Marangoni term in the solver *Free Surface 3D* (FS3D) [1]. Furthermore, we demonstrate the usefulness of our approach for prediction of droplet breakup.

The simulation data used in this context was generated by the solver FS3D and consists of a *volume of fluid* (VOF) [2] field and a velocity field, stored on a rectilinear grid. For interface reconstruction, *piecewise linear interface calculation* (PLIC) [3] was used. This is the same method as in FS3D and therefore yields results closest to the simulation concerning the surface and the topology of the fluid phases.

Interface Stretching

As a measure for interface stretching, the metric tensor is used, which represents the first fundamental form from differential geometry, defined for the deformation rate of the fluid surface. This technique was already introduced by Obermaier et al. [4]. Note that, while we are speaking of interface stretching, we acknowledge the fact that there cannot be an actual stretching because on a molecular view, this means that whenever the interface is *stretching*, molecules are just moving from the inside of the fluid to the interface. However, we use this expression as it conveys the idea as easily and graphically as possible.

To calculate the deformation gradient tensor \mathbf{F} for a single time step, we can solve the equation

$$\Delta \mathbf{x}' = \Delta \mathbf{x} + \Delta \mathbf{d} = (\mathbf{I} + \mathbf{J}_u \Delta t) \Delta \mathbf{x} = \mathbf{F} \Delta \mathbf{x}, \quad (1)$$

with displacement $\Delta \mathbf{x}$, the change of displacement $\Delta \mathbf{d}$, the identity matrix \mathbf{I} , the Jacobian matrix \mathbf{J}_u of the velocity field \mathbf{u} , and the time step Δt . Using two orthonormal vectors on the PLIC interface and generating the matrix $\mathbf{N} = (\mathbf{e}_r, \mathbf{e}_s)$, we get the metric tensor defined on the PLIC plane spanned by $\langle \mathbf{e}_r, \mathbf{e}_s \rangle$ as

$$\mathbf{I}_f = (\mathbf{F}\mathbf{N})^T (\mathbf{F}\mathbf{N}) \quad (2)$$

From this, the eigenvectors and corresponding eigenvalues can be calculated. While the square roots of the eigenvalues $\sigma_i = \sqrt{\lambda_i}$ directly give the stretching factors, thus $\sigma_i > 1$ indicating stretching and $\sigma_i < 1$ indicating contraction, the eigenvectors $\boldsymbol{\epsilon}_i$ have to be transformed back to 3D space by multiplying with the matrix of the PLIC vectors, hence $\boldsymbol{\epsilon}_i' = \mathbf{N}\boldsymbol{\epsilon}_i$. They represent the stretching direction.

Interface Bending

As interface bending, we understand the change of curvature at an interface position \mathbf{x} from one time step to the next. For its calculation, we now use the shape tensor. This tensor can be calculated from the paraboloid difference of two paraboloids fitted to the interface using least squares, one for the original interface positions, and one for their convected counterparts, as shown in figure 1. The idea to calculate the interface curvature from paraboloid-fitting was discussed by Popinet [5] and is part of the method used in the solver FS3D for the calculation of the interface curvature and the

surface tension force. The convection is computed by using a modified, local velocity field, where for the neighborhood around a position \mathbf{x}_c , the velocity is set to

$$\tilde{\mathbf{u}}(\mathbf{x}_i) = \mathbf{u}(\mathbf{x}_i) - \mathbf{u}(\mathbf{x}_c) - \boldsymbol{\omega} \times \mathbf{x}_i. \quad (3)$$

Here, the advection velocity is set to the original velocity minus the velocity at the center and a possible rotation of the interface, where $\boldsymbol{\omega}$ is the average angular velocity. This ensures, that both paraboloids share the same origin and orientation. An example of this is shown in figure 1. The set of advected interface points is thus given by

$$\mathbf{x}'_i = \mathbf{x}_i + \Delta t \tilde{\mathbf{u}}(\mathbf{x}_i). \quad (4)$$

The paraboloid difference is then $p_d = p_{adv} - p_{orig} = a_0 r^2 + a_1 s^2 + a_2 r s$ and can be used to define the shape tensor

$$\mathbf{S} = \begin{pmatrix} 2a_0 & a_2 \\ a_2 & 2a_1 \end{pmatrix}. \quad (5)$$

From this, the principal curvatures $\kappa_{1,2}$ and their corresponding directions $\mathbf{k}_{1,2}$ can be calculated. While the directions show again the orientation, the principal curvatures represent the respective curvature change, with $\kappa_i < 0$ indicating an increase in convexity, and $\kappa_i > 0$ an increase in concavity.

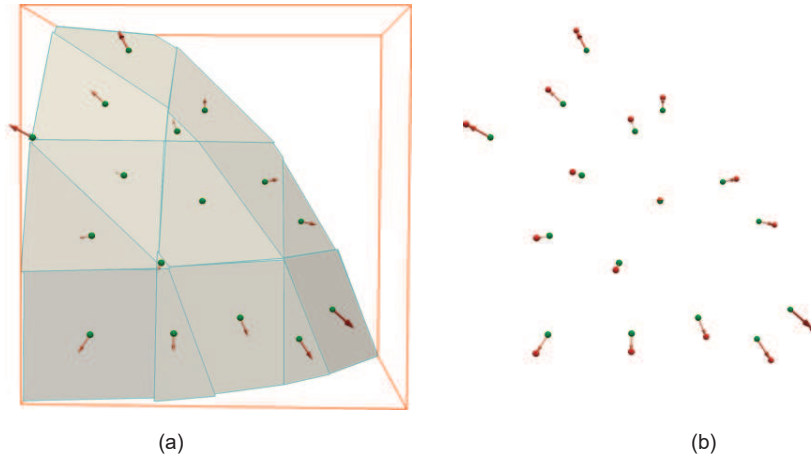


Figure 1. Advection of interface points. In (a) one can see the original interface points and the modified simulation velocity on the PLIC interface. In (b), both the original and the advected points are shown.

Results and Discussion

In this section, we show the usefulness and applicability of our approach using two datasets. On the first one, a dataset from simulating two rain drops colliding in an off-center heads-on collision, we discuss interface stretching. On the other one from a simulation of two coalescing droplets, we demonstrate the application of interface bending. In both cases, we use colored tube glyphs, their orientation visualizing the direction of stretching and bending, respectively, and the color indicating their magnitude.

Colliding rain drops

In figure 2, the visualization of interface stretching is presented. For magnitudes larger than one and indicating stretching we use red, for magnitudes smaller than one and indicating contraction we use blue. For values close to one, the color is gray. As the values can lie between 0 and infinity, logarithmic scaling is applied. In figure 2 (a) and (b) you can see the larger and the smaller eigenvalues and eigenvectors, respectively. Looking at the tunnel-like structures, one can observe that there is an elongation along the tunnel and a contraction perpendicular to that. This indicates that the fluid is moving from the tunnels into the larger formations, while at the same time the tunnels are becoming thinner. From this, one can predict that the tunnels are going to collapse and the formations break up into droplets. This is supported by the topology of the subsequent time steps in figure 2 (c) and (d) which indeed show a droplet breakup.

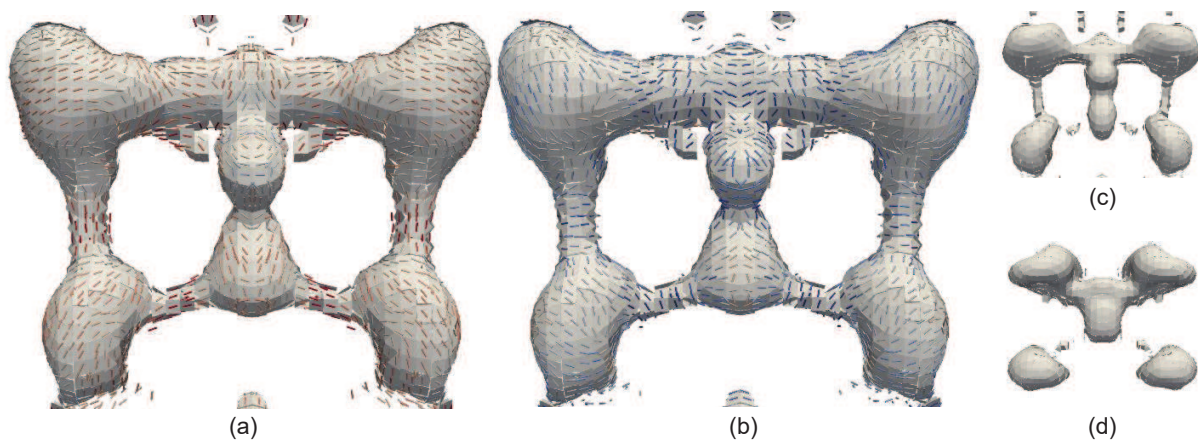


Figure 2. Interface stretching. In (a), the larger eigenvalues and corresponding eigenvectors are shown in red. In (b), analogously, the smaller values are visualized indicating contraction in blue. Subsequent time steps are depicted in (c) and (d).

Coalescing droplets

To show the usefulness of the visualization of interface bending, we apply it to a dataset which was generated in a simulation performed by the FS3D solver considering Marangoni convection in a work-in-progress implementation. The start configuration of the simulation consists of two droplets, one water droplet on the left and one ethanol droplet on the right, at the onset of coalescence. Due to the resulting gradient of the surface tension force, the Marangoni convection induces a force that acts along the surface. This leads to the coating of the left droplet with fluid of the right one. In figure 3, interface bending is visualized with red glyphs for an increase in concavity and blue glyphs for an increase in convexity. Gray glyphs indicate no change for values around zero. One can observe a capillary wave forming at the junction of the two coalescing droplets and moving along the surface to the left. This is an expected phenomenon. Here, our method helps in identifying this wave: in front of the wave we can see an increase in convexity and behind an increase in concavity. Thus, by only looking at a single time step, we can assess the movement of the wave.

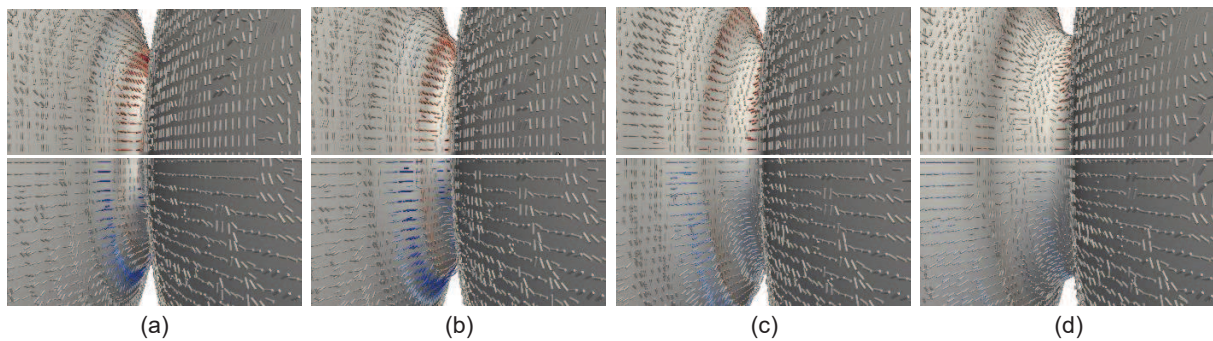


Figure 3. Interface bending. The time steps from (a) to (d) show an increase in concavity in the upper row and an increase in convexity in the bottom row. Because of symmetry, both rows show the same dataset mirrored on the x-axis.

References

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