Issues with extension past the singularity formation, pinch-off, and merging

The solution procedure outlined above for the initial set-up with three distinct regions separated by two interfaces extends (with little more algorithmic complications - see below) to arbitrary number of regions and interfaces (separating distinct phases), a situation which will certainly arise past the stage of pinching and/or collision of these two interfaces. The computational procedure that will induce this change is described below.

Topological Changes and Transitions

Theory: I have sketched in Fig. 1 local bifurcation scenarios at the intersection of two interfaces and events in the life of these interfaces immediately preceding and after the bifurcation. Initially, two distinct interfaces separate three different phases labeled 1,2,3 with overall flow direction from phase 1 to phase 3. In Fig. 1, four snapshots in increasing time are shown going from left to right (in the direction of arrow). The first one shows two disjoint non-intersecting interfaces. At a later stage, two interfaces just touch creating a quadruple junction as shown in the second snap. From balance of surface tension forces at the junction (assuming equilibrium), one can easily find that, in general, such a quadruple junction is thermodynamically unstable and will first dissociate into two less unstable (thermodynamically speaking) triple junctions (shown in fourth snap), but my insight is before it does so, it has to go through the scenario shown in the third snap. Actually, from pure thermodynamic consideration, even triple junction in most cases (depending on surface tensions at three interfaces) will be unstable but hydrodyamical considerations may stabilize it through creation of ripples on the interfaces. This problem can be even more interesting in the presence of non-uniform interfacial surface tension forces which, by the way, is also changing due to interfacial flow and interfacial surfactants. Numerical simulation of our problem may be a catalyst for unleasing new bifurcation scenarios since these are really open problems. During the course of this project, it will allow me to delve into these issues. Literature dealing with triple junctions, in general, is very limited. In this connection it is worth citing Upmanyu et.al [6], Miksis et.al. [1], [2], Novica-Cohen [3], Rowlison [4], and Rowlison et.al. [5].

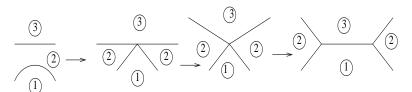


Figure 1: Topological Transitions

Based on these local bifurcation pictures, one can easily envision topological changes of interfaces as they evolve. Fig. 2 and Fig. 3 show only two of the many possibilities. Fig. 2 shows a sequence of likely topological changes. The first shot shows two disjoint non-intersecting interfaces at some instant of evolution. At a later stage, necking of the two

interfaces happens as shown in the second snap giving rise to a quadruple junction which eventually dissociates into two triple junctions giving rise to a topology shown in the third snap in this figure. In Fig. 3, another possibility is shown through five snapshots. The first snap shows the bottom interface is close to a pinch-off. Second snap shows that the interface has developed a geometric singularity where it is about to snap. Third snap shows scenario immediately following this event. Fourth shows the necking of the closed interface encasing fluid 1 and the top interface. The necking point again is a quadruple junction which dissociates into two triple-junctions. Following this dissociation, the interfacial topology will probably look like the one in the fifth shot. During the evolution process, both (Fig. 2 and Fig. 3) and many other topological changes can occur at different times and some of these changes can happen even simultaneously with different segments of the interfaces.

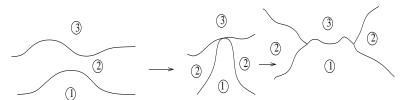


Figure 2: Topological Changes: One Possibility

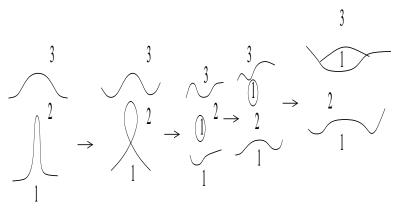


Figure 3: Topological Changes: Second Possibility

Numerical Issues (Handling these transitions numerically):

For numerical purposes, discrete nodes on the interfaces move in space in discrete steps. Consider the snapshot (a) in Fig. 4 where the the interfaces are disjoint and their motion is modeled by the movement of the nodes on these interfaces. These nodes have moved and the interfaces reconstructed from joining these nodes (simple algorithm) have partially crossed each other as shown in snapshot (b). Now, logical situation would be, in the context of our physical problem, to surgically remove the dotted portion of the interface (there is another choice here and I do not have space to go into this). Then onwards, use the new interface shown in snapshot (c) in Fig. 4. However, physics should also be taken into consideration in the surgical process. For example, if the phases 1 and 3 in snapshot (a) were same, then in snapshot (c), the line connecting the two triple junctions is not a true interface and this should be removed as well. Therefore, the algorithm should also take this into consideration even if initially the three phases were distinct because this is a possibility during the evolution

process: please see the last snapshot in Fig. 3 where the phase 1 appears on either side of the phase 2 in part of the flow domain. There are lots of other considerations that will surely arise and I will try to resolve them as much as possible by doing research by interacting, if necessary, with colleagues working in this area some of whom I know professionally very well. In this connection, use of local mesh refinement and adaptivity will be made but only to the point that is physically meaningful. For example, the mean free path of a liquid is about 0.3 micron (it is about 1 micron for gases) which puts a limitation on the grid size that should be used - it should be at least several orders of magnitude higher and not other way round because the fluid equations that we are using break down as we try to capture physics at the level of mean free path.

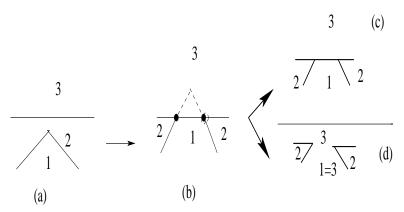


Figure 4: Topological Changes: Numerical Consideration

References

- [1] M. Miksis and J. Keller, Surface tension driven flows, SIAM J. Appl. Maths., 43 (1983), pp. 268–277.
- [2] M. Miksis and J. Vanden-Broeck, *Motion of triple junction*, J. Fluid Mech., 437 (2001), pp. 385–394.
- [3] A. NOVICA-COHEN, Triple junction of cahn-hillard system, Physica D, 137 (2000), pp. 1–24.
- [4] J. Rowlison, Cohesion, Cambridge University Press, Cambridge, UK., 2002.
- [5] J. ROWLISON AND B. WIDOM, Molecular Theory of Capillarity, Claredon Press, 1989.
- [6] M. UPMANYU AND D. SROLOVITZ, Triple junction mobility: A molecular dynamics study, Interface Science, 7 (1999), pp. 307–319.