Implementation of a Level set method in COMSOL

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1 Introduction

A big section of fluid problems involve moving interfaces, such as oil mixing with water, wave formation due to wind-water interaction, Kevin-Helmholtz instabilities and many more. There are many important parameters to be considered when studying interfaces between two fluids, e.g. big density gradients, surface tension and changing topology.

In order to solve these complex systems a number of numerical techniques has been developed, known as level set methods. Level set methods are computational techniques for tracking moving interfaces. These techniques are able to handle the computational heavy task of resolving the motion of a fluid interface. One of the level set formulations will be considered at in this lab.

2 Theory

Consider a closed curve $\mathbf{l}(t)$ moving in two dimensions. A velocity field $\mathbf{u}$ transports the interface. The domains consisting of the two different fluids can be expressed using the Heaviside function

$$H(\mathbf{r}) \equiv \begin{cases} 0, & \mathbf{r} < 0, \\ 1, & \mathbf{r} > 0, \end{cases}$$

where $\mathbf{r}$ is the signed distance from the closed curve $\mathbf{l}(t)$, which is positive below and negative above the interface.

With this the Level-set function can be defined simply as

$$\phi(\mathbf{r}) \equiv H(\mathbf{r})$$

which will be the function we use to separate the domains between the fluids. The evolution of this function is governed by the convection equation,

$$\phi_t + \mathbf{u} \cdot \nabla \phi = 0, \tag{1}$$

where the incompressibility condition $\nabla \cdot \mathbf{u} = 0$ is applied. The similarities between this equation and the heat equation is very important to the COMSOL implementation later. [2]

By this definition a global density and viscosity can easily be defined

$$\begin{aligned}\rho(\mathbf{r}) &= \rho_g + (\rho_l - \rho_g)\phi(\mathbf{r}),\\ \mu(\mathbf{r}) &= \mu_g + (\mu_l - \mu_g)\phi(\mathbf{r}),\end{aligned} \tag{2}$$

where ρ_g, μ_g, ρ_l and μ_l is the density and viscosity for the gas (top fluid) and liquid (bottom fluid), respectively.

It is necessary to define the normal vector and curvature of the interface for other laters use. These quantities can easily be obtained from the level set function

$$\mathbf{n}_l = \frac{\nabla\phi}{|\nabla\phi|}$$

and

$$\kappa = -\nabla\cdot\mathbf{n}_l = -\nabla\cdot\frac{\nabla\phi}{|\nabla\phi|},$$

where $\mathbf{n}_l$ and κ is the normal vector of the level set function and the curvature, respectively.

A problem in the numerical solution is that the thickness of the interface is not constant and will broaden with time. To solve this problem, an extra term is added to the end of the convection equation 1

$$\phi_t + \nabla\cdot(\mathbf{u}\phi) = \epsilon\nabla^2\phi - \nabla\cdot(\phi(1-\phi)\mathbf{n}_l), \tag{3}$$

where ϵ is a small number dependent on the simulation. A full derivation of this extra term will not be covered here, but can be found on articles online. [2]

Equation 3 is coupled with Navier-Stokes equation through the level set function and the velocity field. In COMSOL Navier-Stokes equation is written as

$$\rho\mathbf{u}_t + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot\Big[-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)\Big] + \mathbf{F}. \tag{4}$$

The other forces $\mathbf{F}$ will be due to gravitation and surface tension. The surface tension term can be written as

$$\gamma\kappa\delta(\mathbf{r}-\mathbf{r}_l)\mathbf{n}_l,$$

where γ is the surface tension coefficient. The Dirac delta function can be simplified as

$$\delta(\mathbf{r}-\mathbf{r}_l) \approx |\nabla\phi|, \quad \mathbf{r}_l \in \mathbf{l}(t).$$

This simplification makes sense when we understand that the gradient of the level set function is zero for every point away from the interface. As we reach the interface the gradient increases to a maximum value in the middle of the interface. Using this approximation the surface tension term can be simplified as

$$\gamma\Big(-\nabla\cdot\frac{\nabla\phi}{|\nabla\phi|}\Big)|\nabla\phi|\frac{\nabla\phi}{|\nabla\phi|} = -\gamma\Big(\nabla\cdot\frac{\nabla\phi}{|\nabla\phi|}\Big)\nabla\phi.$$

We will not consider surface tension in our implementation as it is not necessary for the case we are studying.

3 Implementation

Following is a step-by-step implementation of the level set formulation in Comsol using two physics modules; laminar flow and heat transfer in fluids. We will also use a mathematics module called Wall Distance.

3.1 Initial system and definitions

1. Choose a 2-dimensional system.

2. We need two comsol physics interfaces in order to describe the fluid- and interface motion. For fluid motion we pick the laminar flow interface. Under "Fluid Flow -> Single-Phase Flow" choose "Laminar Flow (spf)" and add it to your system. In order to implement the interface equations to our system we use the Heat Transfer module. Pick "Heat Transfer in Fluids (ht)" under "Heat Transfer" and add it to your system. It is logical also to rename the Heat Transfer dependent variable to "phi".

3. In order to define the initial phi we also need a mathematical module called "Wall Distance", found under "Mathematics -> Wall Distance (wd)". This module calculates the distance to a boundary at all points.

4. The study should be time dependent.

5. First we have to add the global parameters. These are the width and height of the container (47.9 and 29.7 centimeters), density and viscosity for the two fluids ($\rho = 1000\text{kg/m}^3$ for the heavier fluid and $\rho = 800\text{kg/m}^3$ for the lighter fluid. The viscosity can be equal for the two fluids. $\mu = 10^{-3}$Pas is reasonable) and two points which define the y-coordinates of the edges of the initial water surface. See figure 1.

6. A few component variables has to be added under "Definitions" in "Component 1". These are the global definitions of viscosity (mu_global) and density (rho_global) dependent on phi (see equation 2). It is easier later if the magnitude of the gradient of phi is defined as a variable. In order to avoid division by zero the gradient is expressed as magGradPhi = sqrt((phix+eps)^2+(phiy+eps)^2), where eps is Comsol's predefined variable for the smallest machine number.

7. Under component definitions a step function has to be added which will represent the smooth water-water interface. Right click on definitions under component 1 and choose "Step" under "Functions". Set the function name to "iniphi". The step function should go from 1 to 0. The size of the transition zone is dependent on the mesh and our system, but a good value in this case is 0.01.

3.2 Building the geometry

8. The geometry is quite simple for this simulation. Add a rectangle with the y-zero level to be at the top of the rectangle and the x zero level to be in the middle of rectangle. This rectangle will be our fluid container.

9. Three polygons have to be added which will be our interface line and boundary lines for the fine mesh in the center of the container. See figure 1. The interface line will be drawn between two points at each end of the container. That is, at x equal W/2 and -W/2. The y-coordinates at each point should be defined in the parameters.

10. The other two polygons should be some distance above and under the interface line. These polygons will determine the space where we will have a finer mesh in our tank. See figure 1.

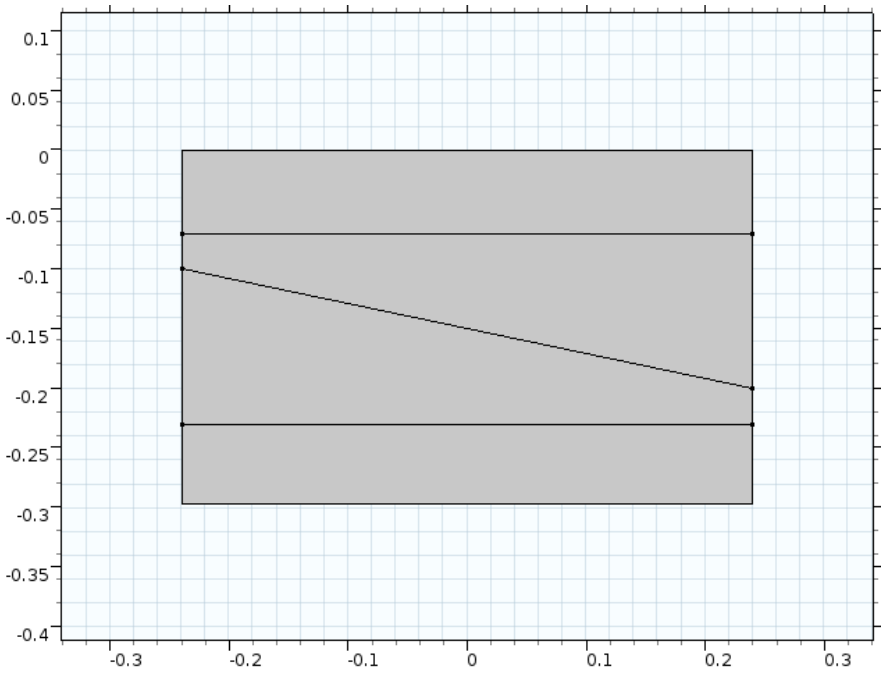

Figure 1 – The container with proper lines drawn in Comsol.

3.3 Settings for the physics

11. Now we consider our physics modules. Make sure the Discretization[1] for Laminar Flow is set to P2+P1.

[1] If you can't find discretization, press the eye-icon under "Model Builder" and cross in everything.

12. In "Fluid Properties 1" we add our global viscosity and density variables defined earlier.

13. Under "Initial Values 1" we want to start with a hydrastatic pressure. This gives an initial pressure as -g_const*rho_global*y, where g_const is the gravitational constant already defined in COMSOL.

14. Two more terms have to be added to our system. One is gravitation, which we get by adding a "Volume Force" to our laminar flow module. The gravitational force should be -g_const*rho_global in the y-direction.

15. For stabilization purposes, we add a "Pressure Point Constraint" found under "Points", which should act on one of the upper points of the container, where the pressure is zero.

16. In the Wall Distance module Not much has to be done, we only need to define what boundary we calculate the distance from. Add a boundary "Wall" to this module and choose the initial interface drawn in the geometry. The dependent variable from Wall Distance is the reciprocal distance from the boundary at all points, G2.

17. Next we move to the Heat Transfer in Fluids module. The discretization should be "Quadratic".

18. In "Fluid 1" it is important that the velocity field is dependent on the laminar flow module (abbreviated as spf), set the velocity field to "Velocity field (spf)" in the list. The pressure can be set to "User defined". The thermal conductivity constant corresponds to the stabilization term found in equation 3. It should be defined as 0.05*(h/3-phi*(1-phi)/magGradPhi), where h is COMSOL's predefined element size and magGradPhi is the magnitue of the gradient of phi as defined in step 6. In this simulation $\epsilon = h/3$ works pretty good. An overall constant of 0.05 helps with stabilization. Density, heat capacity and ratio of specific heats should all be set to 1.

19. With initial values we want to specify the initial water surface. This means that the step function should go from 1 to 0 across the interface line we added earlier. The initial step function (in this case called iniphi) takes an argument, which should be 0 at the interface. Utilizing the reciprocal distance from the boundary we can define the initial phi as follows: Above the interface in the "gas" domain we want phi to go from 1 to 0. In the "liquid" domain we want phi to go from 0 to 1. Add another "Initial Values" to the Heat Transfer module. In this, choose the "liquid" domain with the "Temperature" set to 1-iniphi(1/G2), where G2 is the reciprocal difference from the wall distance module and iniphi is the step function defined in step 7. This gives us the wanted condition that the initial phi goes from 0 to 1. Correspondingly, by choosing the "gas" domain in the first "Initial Values" we set the "Temperature" to be iniphi(1/G2).

20. For stabilization purposes, two ”Temperature” boundaries can be added at the bottom and top of the container, where the ”temperature” should be 1 at the bottom and 0 at the top.

3.4 Building the mesh

21. The choice of mesh is very important depending on what parameters are chosen for the simulation. Click on Mesh and select the Sequence type to "User-controlled mesh". Right-click on Mesh and select a Size component. In the Size under Geometric Entity Selection you select the domains you want to affect. Under Settings you can as a first test select Predefined to Normal and then select Custom and check all boxes. The parameters at each box should now represent the settings for a Normal mesh. If this guide has been followed a maximum element size of roughly 0.008 and a minimum of $4.5 \cdot 10^{-5}$ seems to work well in most cases. This mesh should be in the space between the two lines drawn earlier. The rest of the mesh can be made larger, coarse or normal by adding a new Size component and selecting the Domains of interest. An example mesh can be seen in figure 2.

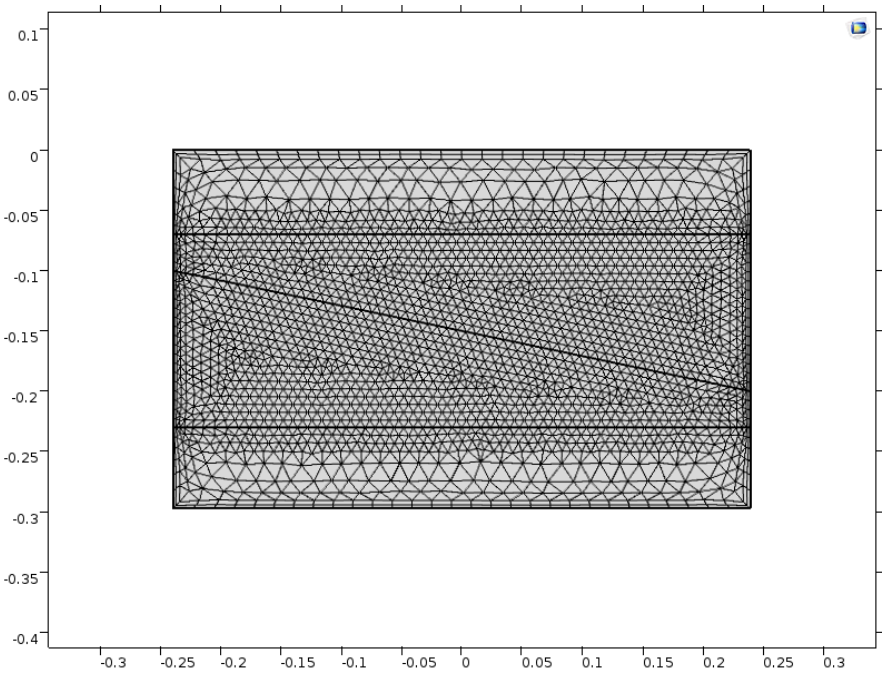

Figure 2 – The container with mesh calculated in Comsol. Note the smaller mesh inside the boundary lines.

3.5 Solving the system

22. Before we solve this system (which you must be very eager to do) we have to first calculate the Wall Distance to get an initial value for phi. Add another stationary study (right-click on the top level of the Model builder tree and select Add Study), and tune the solver to solve only for the wall distance (under the new Study / Step 1). This should produce a plot where the value is increasing further away from the interface.

23. We also need to make some adjustments to the system solver. To begin with, we only solve for the Laminar Flow and Heat Transfer modules. Then, we need to define that we use the solution from the Wall Distance solver. Under "Step 1: Time Dependent" choose "Values of Dependent Variables" and under "Values of variables not solved for" choose "User controlled". Choose "Solution" under method and pick the Wall Distance study under "Study".

24. Finally, we want to solve this system using a segregated solver rather than a fully coupled one. In order to add this, right click "Solver configurations" under the study, and choose "Show default solver". Under this, go to "Solution 1". Right click "Time-dependent Solver 1" and choose "Segregated". Right click "Segregated 1" and add another "Segregated Step". Under these steps we choose what physics to solve for at each step. In the first step, add only the "Pressure" and "Velocity field" from the laminar flow module. In the second step add only the "Temperature" to solve for.

25. It can be interesting to see whilst solving how the system develops in time. To do this, right click your study and choose "Get Initial Value". Then, under "Step 1: Time Dependent" in the settings window under "Results While Solving", choose "Temperature (ht)", which is a surface plot of ϕ.

26. Compute the system for a specified time. 0 to 1 seconds is a good place to start on to make sure that you have implemented the system correctly.

References

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[2] Barnkob, Rune. Andersen Baekbo, Mathias. Two Phase Flow by Level Set Method *A conservative level set method for two phase flow* 1.3: 7.
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