Summer Fellowship Report

On

Simulation of Water Droplet Impact on Hydrophilic and Hydrophobic surfaces

Submitted by

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Under the guidance of

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Abstract

This case study aims to numerically simulate the behavior of a water droplet falling onto a hydrophobic and hydrophilic surface from an arbitrary height of 5 cm. Volume of Fraction method (VOF) is employed to handle multi-phase interaction between water and air. Adaptive Mesh refinement is being used to get better accurate behavior of water Droplets after impact. The hydrophilic and hydrophobic behavior is governed by the contact angle of the surface.

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Chapter 1

Introduction

Hydrophilic and Hydrophobic surface are widely used in food industries, air-crafts, automobiles, etc. Impact of a water droplet on these surfaces will produce different behaviors. This behavior is studied and simulated using OpenFOAM. Multi-phase model is employed to handle the water and air interface. Since water droplets on impact will separate into very small droplets, adaptive mesh refinement is employed to refine the mesh during simulation to capture small droplets. The fluid domain is meshed and appropriate solver is chosen along with boundary and initial conditions and after the simulation is done, results are obtained and studied.

1.1 OpenFOAM

OpenFOAM (for "Open-source Field Operation And Manipulation") is a C++ toolbox for the development of customized numerical solvers, and pre/post-processing utilities for the solution of continuum mechanics problems, most prominently including computational fluid dynamics. OpenFOAM is freely available and open source, licensed under the GNU General Public Licence. The licence is designed to offer freedom, in particular it encourages users of the software to make modifications or developments.

1.2 Multiphase Model

Multiphase model, employed for this case study is Volume of Fluid (VoF) Model. In computational fluid dynamics, the volume of fluid (VOF) method is a free-surface modelling technique, i.e. a numerical technique for tracking and locating the free surface or fluidfluid interface. It employs a VoF equation along with continuity and momentum which solves for the volume fraction of the fluid. From the volume fraction, density is calculated.

The continuity equation for incompressible flow is as follows

$$\nabla.U = 0$$

The momentum equation for incompressible flow is as follows

$$\frac{\partial \rho U}{\partial t} + \nabla.(\rho U U) = -\nabla p + \nabla.\rho\nu[2S] + F$$

where U is the effective velocity, ρ is the density, p is the pressure, ν is the kinematic viscosity, $[S]$ is the stress tensor and F is the combined sources term. The average values are calculated from the volume fraction α

The Volume of fluid equation is as follows

$$\frac{\partial \alpha}{\partial t} + \nabla.(\alpha U) + \nabla.[U_r \alpha(1-\alpha)] = 0$$

where α is volume fraction of fluid. U_r is the compression velocity which is given by $U_r = U_l - U_g$ and U is the effective velocity obtained by weighted average $U = \alpha U_l + (1-\alpha)U_g$ where the subscripts l and g denotes liquid and gaseous phase respectively. The weighted average values of density ρ and kinematic viscosity ν is calculated from the equations below.

$$\rho = \rho_l \alpha + \rho_g(1-\alpha)$$

$$\nu = \nu_l \alpha + \nu_g(1-\alpha)$$

The calculated weighted average values of density and kinematic viscosity are substituted in momentum equation and continuity equation to solve for the field variables.

Chapter 2

Case Setup

2.1 Geometry and Mesh

The Geometry of the fluid domain is a simple cube of side length 0.1m. The bottom side of the cube is named as walls, the surface for which hydrophilic or hydrophobic boundary condition will be given, all other sides atmosphere. The mesh is generated using blockMesh utility of OpenFOAM, with local cell size 0.005m with simple grading on all sides. The mesh is coarse initially but will be refined during simulation according to the volume fraction of water.

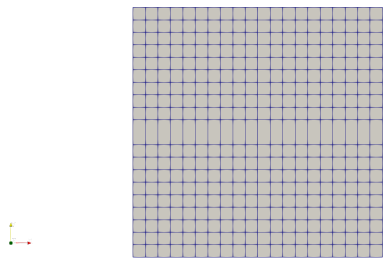

Figure 2.1: Initial Mesh

2.2 Boundary conditions

The boundary conditions employed for the computational domain is given in table 2.1. The alpha water boundary condition for the walls govern the hydrophilic and hydrophobic nature of the surface. For hydrophilic theta0 is 45^o and for hydrophobic theta0 is 135^o.
The water droplet is given as an initial condition using setFields. Region used to set water level is as follows

```
sphereToCell
   {
   origin (0.0 0.0 0.0);
   radius 0.01;
   centre (0.05 0.05 0.05);
   fieldValues ( volScalarFieldValue alpha.water 1 ;
   }
```

2.3 Adaptive Mesh Refinement

In numerical analysis, adaptive mesh refinement (AMR) is a method of adapting the accuracy of a solution within certain sensitive regions of simulation, dynamically and during the time the solution is being calculated, refining the mesh. Adaptive Mesh Refinement is implemented in OpenFOAM in dynamicMeshDict in constant directory.

The dynamicMeshDict is as follows,

```
   dynamicFvMesh dynamicRefineFvMesh;
   dynamicRefineFvMeshCoeffs {
         refineInterval 1;
         field alpha.water;
         lowerRefineLevel 0.1;
         upperRefineLevel 0.9;
         unrefineLevel 0.005;
         nBufferLayers 1;
         maxRefinement 3;
         maxCells 1000000;
         dumpLevel true;
         correctFluxes ((phi none) (nHatf none) (rhoPhi none) (ghf none));
   }
```

Boundary	**U**	**p_rgh**	**alpha.water**
atmosphere	type inletOutlet; value (0 0 0);	type fixedValue; value uniform 0;	type inletOutlet; value uniform 0;
walls	type noSlip;	type fixedFluxPressure; Value uniform 0;	type constantAlphaContactAngle; theta0 45; limit gradient; value uniform 0;

Table 2.1: Boundary Conditions for Hydrophilic Surface

Sl.No.	Description	Value
1	Kinematic viscosity of water	1e-06 m^2/s
2	Density of water	1000 kg/m^3
3	Surface Tension	0.072 N/m
4	Kinematic viscosity of air	1.48e-05 m^2/s
5	Density of air	1 kg/m^3

Table 2.2: Properties of Fluids

2.4 Solver and Simulation control

interFoam solver is used for this simulation. The official definition for this solver is as follows:

Solver for 2 incompressible, isothermal immiscible fluids using a VOF (Volume of Fluid) phase-fraction interface capturing approach. The VOF model can model two or more immiscible fluids by solving a single set of momentum equations and tracking the volume fraction of each of fluids throughout the domain. Typical applications include the prediction of jet breakup, the motion of large bubbles in a liquid, the motion of liquid after a dam break, and the steady or transient tracking of any liquid-gas interface. Simulation control values are given in controlDict in system folder of the case folder. The time step is adjustable with respect to courant number as well alpha courant number.

The transport properties for case is setup in transportProperties file in constant directory in which the value of density and kinematic viscosity for both air and water are given as well as surface tension value is also given.

The important control values as given in controlDict is as follows

startTime 0;
endTime 1;
deltaT 0.000001;
writeControl adjustableRunTime;
writeInterval 0.005;
maxCo 1;
maxAlphaCo 1;
maxDeltaT 0.001;

Chapter 3

Result and analysis

3.1 Mesh Refinement

The mesh is refined at each time interval based on the volume fraction of water (alpha.water) field value where the values are above 0.9 and less than 0.1, upto a level of 3. The refining of mesh during simulation of hydrophilic surface can be seen in the figure 3.1. The same can be seen for hydrophobic surface also.

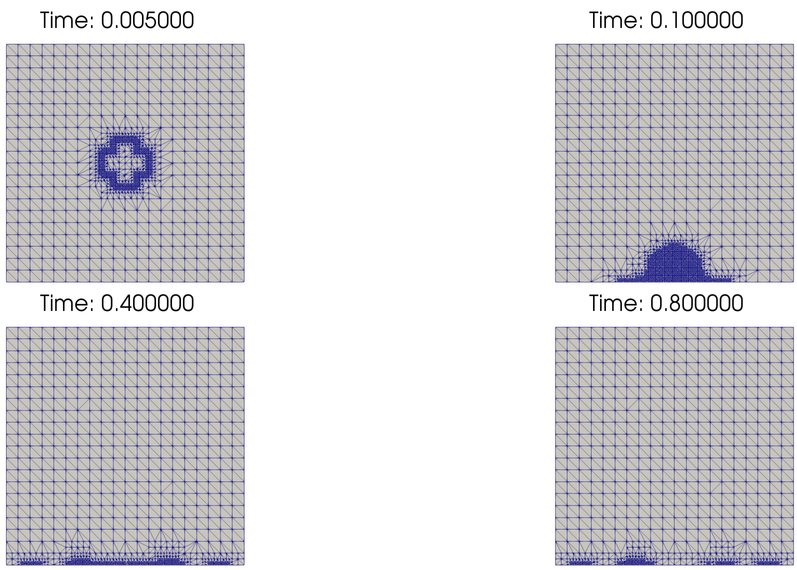

Figure 3.1: Mesh Refinement at different time steps

3.2 Volume Fraction of Water

The result of field alpha, which is the volume fraction of water, will show us the behavior of water droplet impacting on both the hydrophilic and hydrophobic surface.

On the Hydrophilic surface, the droplet seems to be adhering to the surface. This happens due to the value of contact angle being less than 90°. On the hydrophobic surface, the droplet seems to flow without much adherence. This may be due to molecular structure. This behavior can be seen from the contour plot of volume fraction of water as seen in Figure 3.2.

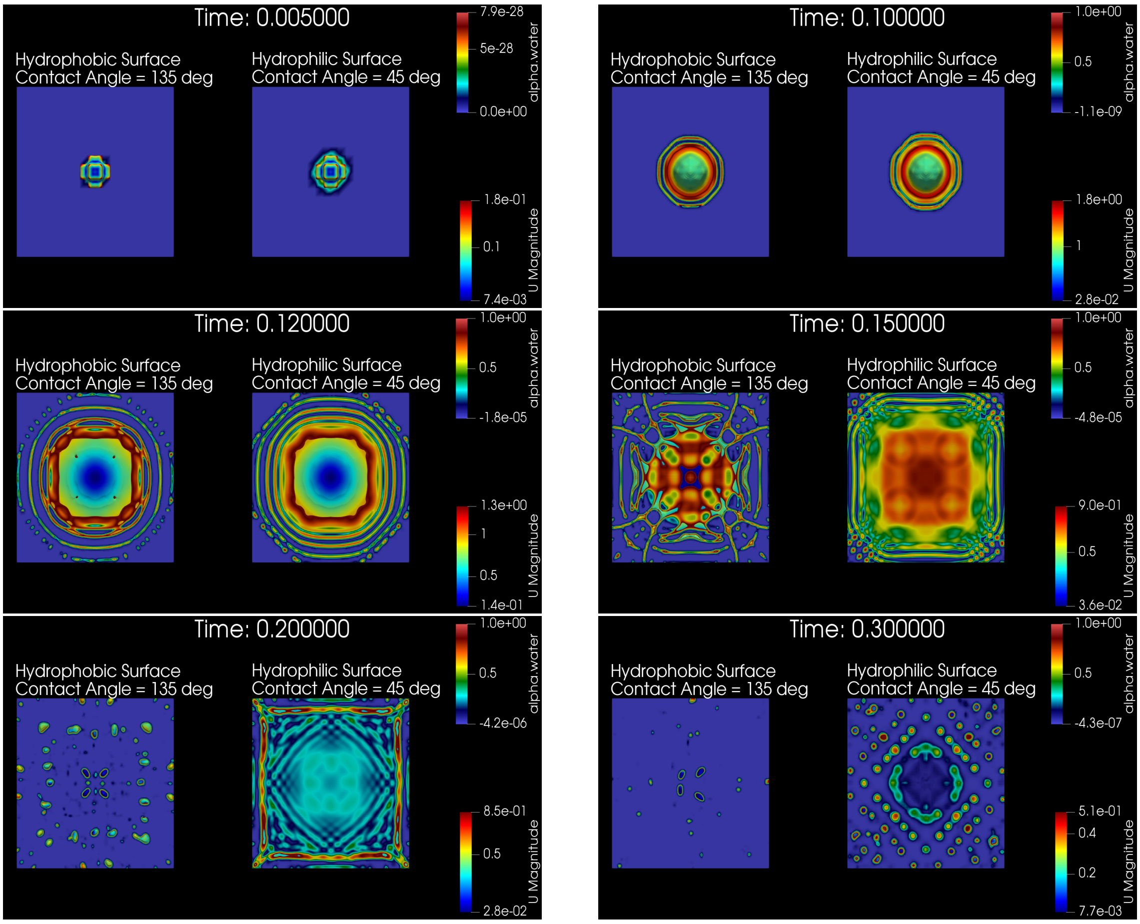

Figure 3.2: alpha field (volume fraction of water) at different time steps

Chapter 4

Conclusion

This project has been done to analyse the behavior of water droplet on hydrophilic and hydrophobic surfaces and the results from the simulation are of expected behavior. This case study explores the capability of OpenFOAM for multiphase modelling combined with adapting mesh refinement.

Reference

- OpenFOAM User Guide
- Tutorial Case for Mesh Refinement by Tobias Holzmann
- OpenFOAM wikipedia page
- interFoam explanation from openfoamwiki.net
- How to post-process multiphase results - openfoamwiki.net
- "Description and utilization of interFoam multiphase solver" by Santiago Mrquez Damin-Final Work-Computational Fluid Dynamics