Computational Modeling Approaches to Multiscale Design of Icephobic Surfaces

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Motivation

• While sacrificial coatings and mechanical and thermal solutions exist for the problem of ice accretion, a passive, durable icephobic coating is desirable for a breadth of applications.

• To design such a surface, more understanding is needed about the mechanisms of ice formation at a smaller scale i.e. individual droplets.

• The complexity of first-principles approaches and Multiphysics modeling is prohibitive for this problem that is still lacking in experimental observations.
Project Objective

- To aid in the design of surfaces that prevent icing, a model of impact ice formation at the single droplet scale was proposed.
- No existing model simulates simultaneous impact and freezing of a single supercooled water droplet.
- For the 10-week project, a low-fidelity feasibility study was the goal.
Outline

• Motivation
  • No existing model simulates simultaneous impact and freezing of a supercooled water droplet
  • For the 10-week project, a low-fidelity feasibility study was the goal

• Method
  • Built on Open Foam
  • Use of built-in tools
  • Writing python script
System and Software Specifications

• Oracle Virtual Box 4.3.28
• OS: Ubuntu 14.04 ‘trusty’
  • OpenFOAM 4.0 (paraview 5.0.1 included)
  • Enthought Canopy Express 1.7.3.3333 python distribution
• Easily transported contained environment
Model - OpenFOAM

• Mesh built using OpenFOAM application blockMesh
• Custom solver was assembled from two existing solvers
  • interFoam 2-phase incompressible flow solver
  • moveDynamicMesh mesh motion solver
• Built-in Newtonian transport model
Model – Ice Formation

- No support for nucleation-based spontaneous phase transformations in OpenFOAM
- Manipulation of temperature was unsuccessful in yielding a \( v \_\text{transformation} \) that was constant \( \text{wrt} \) distance from wall
- A three-phase (air water ice) method was abandoned in favor of mesh deformation
Model – Ice Formation Mesh Movement

• Ideally, the model would deform the boundary at the wall without moving the internal mesh

• OpenFOAM topology change utilities were not able to allow for this approach

• Internal mesh motion was necessary to prevent mesh failures

• Efforts were taken to minimize or circumvent the effects of this motion on the results where possible
Model – Ice Formation Calculations

• A python script was written to work with the boundary condition timeVaryingMappedFixedValue to define the scalar field pointMotionUx
Model – Ice Formation Calculations

- The fixed normal distance to the top surface of the water at each mesh point in the boundary was calculated.
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• Dry points were excluded
Model – Ice Formation Calculations

- For most mobile points, $x'$ was set to $v_{\text{transf}}$
- If the distance was smaller than $v_{\text{transf}} \times \Delta t$, $x'$ was set to the distance/$\Delta t$
- If the distance was 0 or less, $x'$ was set to 0
Mesh movement effects

- The droplet surface is displaced along with the mesh
- Extracting water surface using the latest mesh causes a runaway ice growth
- To prevent this, the current water region was imposed on the original mesh to calculate the water surface

These regions of 0 motion are found, despite the water surface (shown in white) shown to be more than a cell away from the boundary.
Mesh movement effects

• The diffusivity was set to minimize the shape change of the internal mesh and to prefer entire planes of cells to move together
Mesh Density Limitations

- At higher mesh densities, a glitch interfered with simulations.
- Also visible in this image is a result of simulating with too high cell thickness near the wall.
Results

• Using the viscosity, density, and surface tension of water at -30 Celsius, droplets of diameter 100, 200, and 400 um, impacting a surface at 40 m/s