

# 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

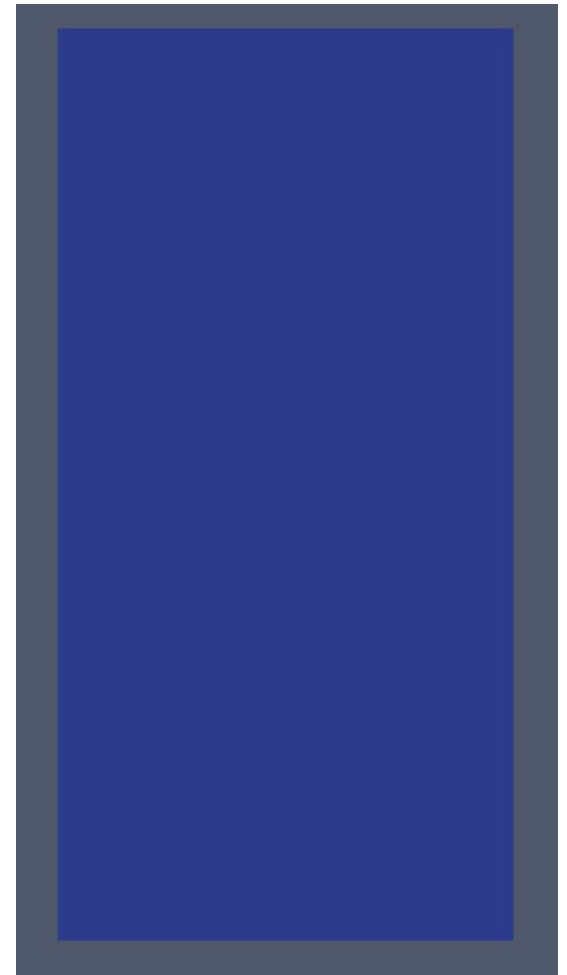
- Oracle Virtual Box 4.3.28
- OS: Ubuntu 14.04 'trusty'
  - OpenFOAM 4.0 (paraview 5.0.1 included)
  - Enthought Canopy Express 1.7.3.3333 python distribution
- Easily transported contained environment

# 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  $v$ \_transformation that was constant wrt distance from wall
- A three-phase (air water ice) method was abandoned in favor of mesh deformation



Blue = Solid

Red = Liquid

# 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

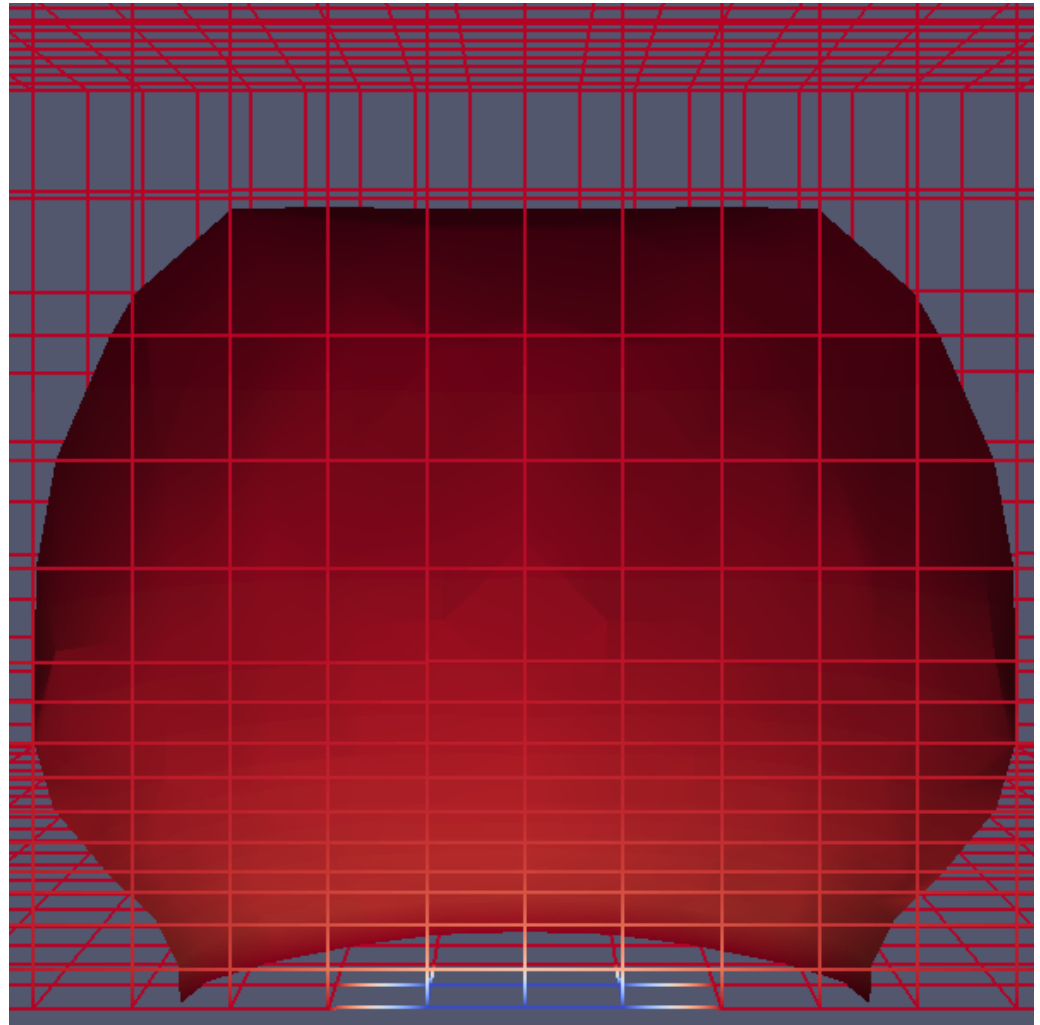


# Model – Ice Formation Calculations

- A python script was written to work with the boundary condition `timeVaryingMappedFixedValue` to define the scalar field `pointMotionUx`

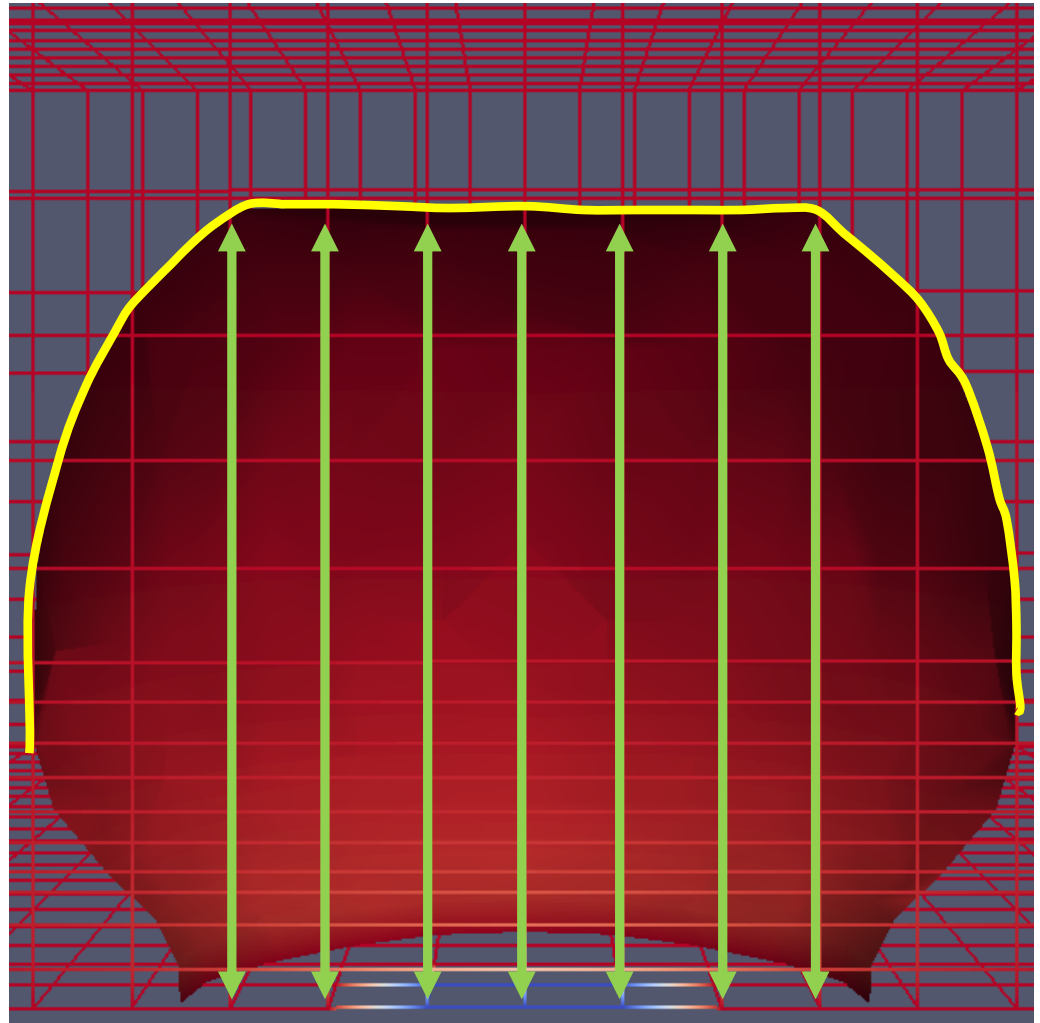
# Model – Ice Formation Calculations

- The fixed normal distance to the top surface of the water at each mesh point in the boundary was calculated



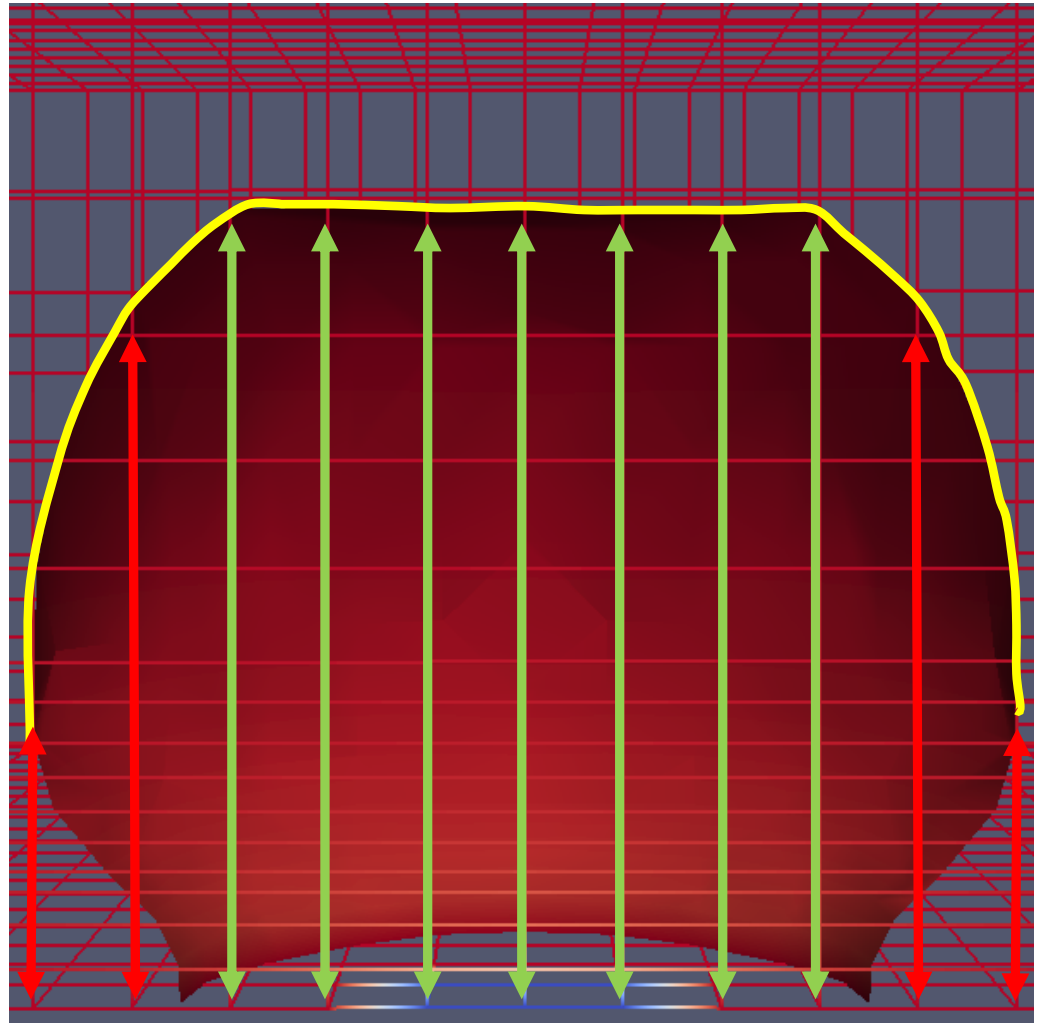
# Model – Ice Formation Calculations

- The fixed normal distance to the top surface of the water at each mesh point in the boundary was calculated



# Model – Ice Formation Calculations

- The fixed normal distance to the top surface of the water at each mesh point in the boundary was calculated
- Dry points were excluded

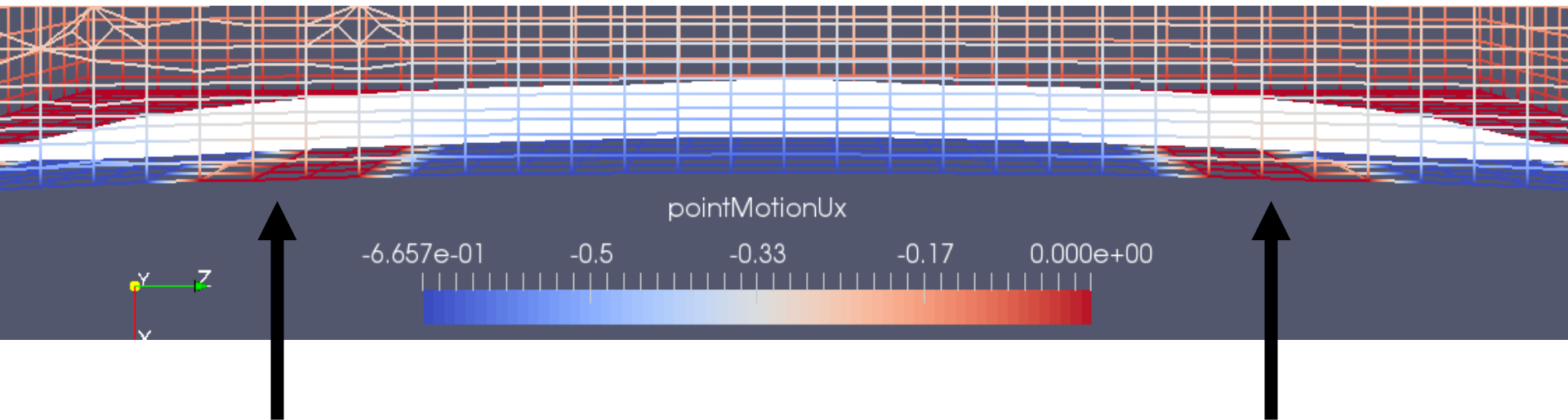


# Model – Ice Formation Calculations

- For most mobile points,  $x'$  was set to  $v\_transf$
- If the distance was smaller than  $v\_transf * del\_t$ ,  $x'$  was set to the  $distance / del\_t$
- If the distance was 0 or less,  $x'$  was set to 0

# Mesh movement effects

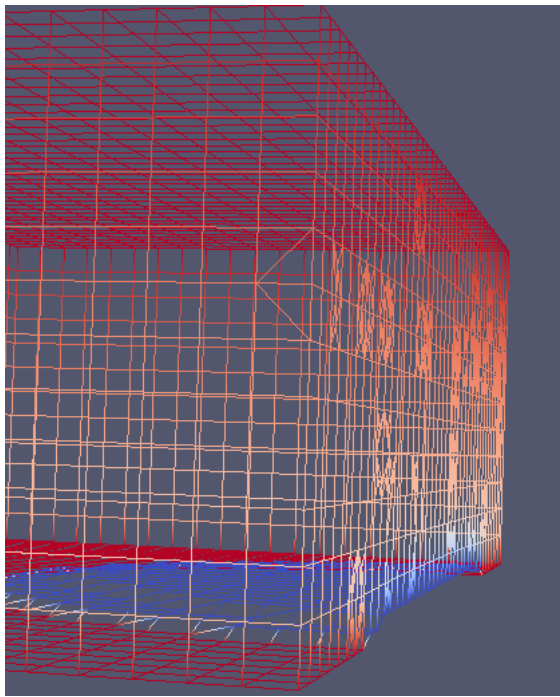
- The droplet surface is displaced along with the mesh
- Extracting water surface using the latest mesh causes a runaway ice growth
- To prevent this, the current water region was imposed on the original mesh to calculate the water surface



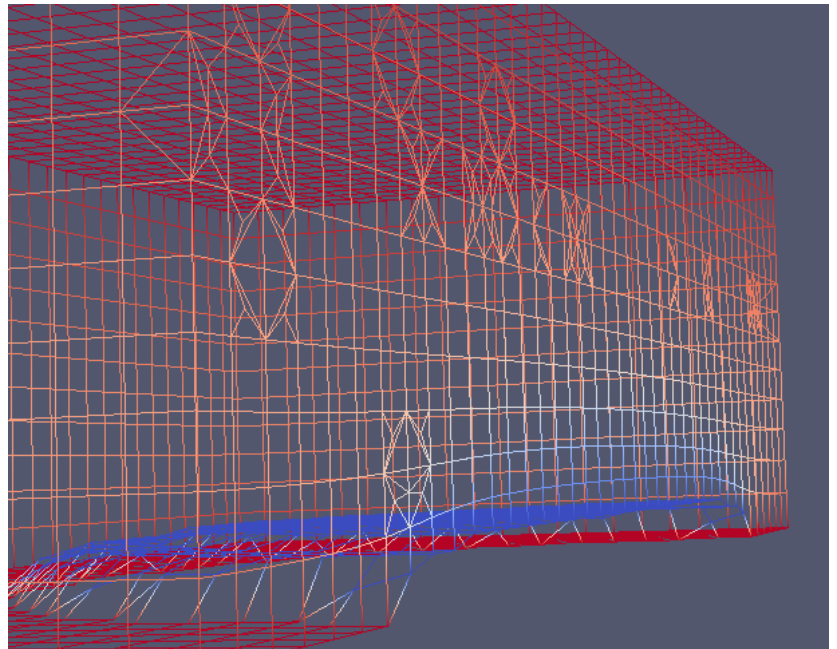
These regions of 0 motion are found, despite the water surface (shown in white) shown to be more than a cell away from the boundary

# 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

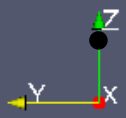


↑ Straighter horizontal lines

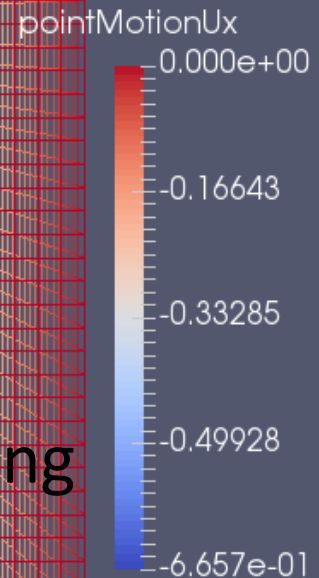


# Mesh Density Limitations

- 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  $\mu\text{m}$ , impacting a surface at 40 m/s