Simulating a Droplet Within a Two-phase Viscous Flow

Matt Cho

CFD Methodology

Common Ground

We have a mental model. Is it closer to what we think is real or not?

CFD Methodology

Scientific Method

Analytical method where we go through an iterative process of:

Question $\rightarrow$ **Hypothesis** $\rightarrow$ **Experiment** $\rightarrow$ **Refinement**

(Engineering methodology is identical, but with cost constraints added.)

CFD Methodology

Scientific Method

CFD Methodology

Computational Math ("Post-Moore's Law")

We have a virtual model written in the form of an algorithm.
How do we make the most of it?

CFD Methodology

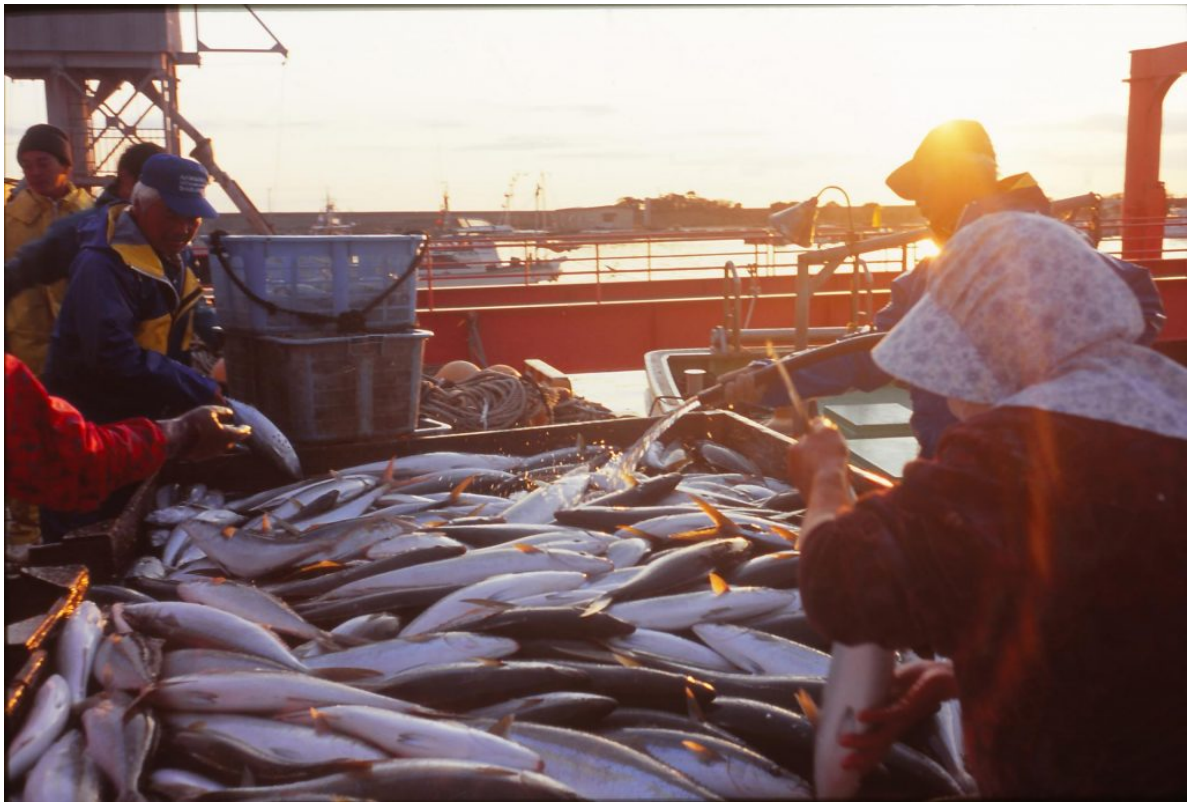
Computational Math ("Post-Moore's Law")

Process is fundamentally the same, but we now have 1000s of CPUs to do what we want:

Question $\rightarrow$ **Hypothesis** $\rightarrow$ **Experiment** $\rightarrow$ **Experiment** $\rightarrow$ **Experiment** $\rightarrow$ **Experiment** $\rightarrow$ **Experiment** $\rightarrow$ **...**

CFD Methodology

Computational Math ("Post-Moore's Law")



CFD Methodology

Computational Math ("Post-Moore's Law")

Software Framework

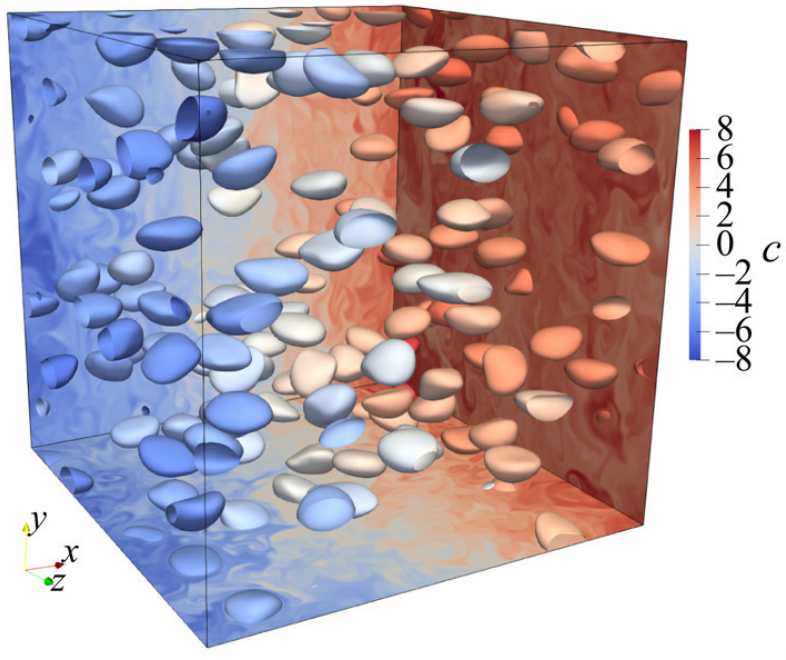
Introducing Basilisk

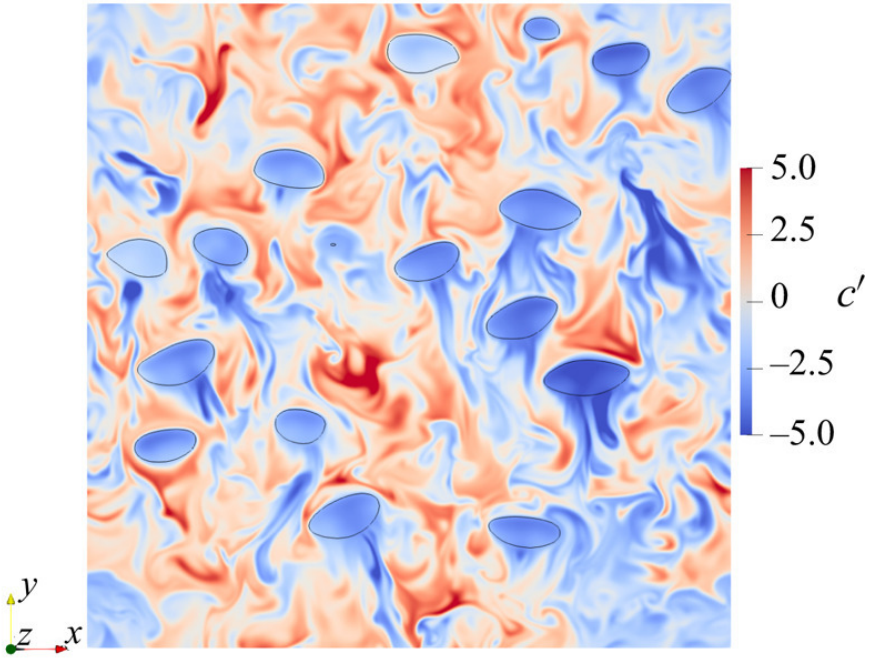
General Purpose PDE Solver specializing in solving over adaptive meshes.

Creator is Stéphane Popinet of Sorbonne Université (formerly Université Pierre-et-Marie-Curie) in Paris

Software Framework

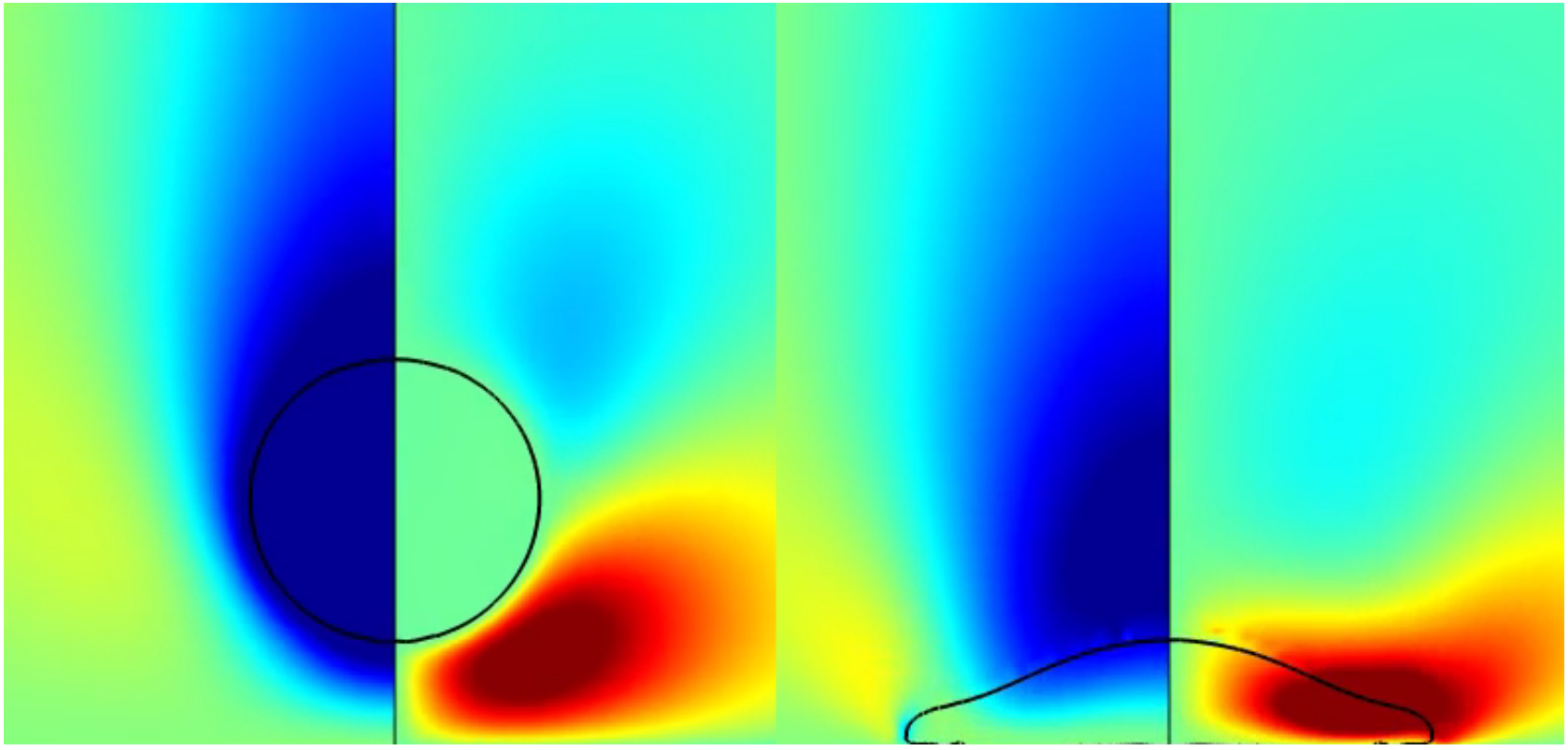
Introducing Basilisk





Software Framework

Introducing Basilisk



Software Framework

What is this really?

A solution to the Navier-Stokes equations, using the Volume-of-Fluid method (VOF).

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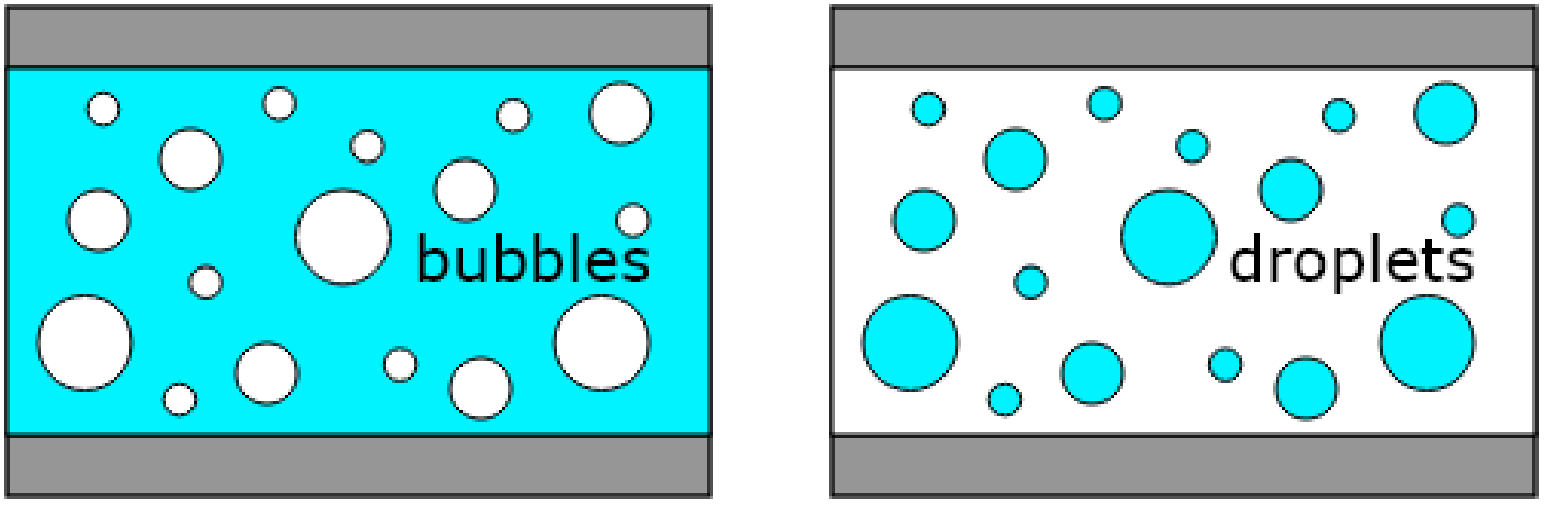
Problem of analysing real droplet behavior is a combination of problems. In isotropic conditions, this is essentially solving for a two-phase flow problem where the substrate is a solid boundary.

(For now, we are interested in viscosity and advection more than heat transfer.)

Software Framework

What is this really?



c) Dispersed two-phase flow.

Software Framework

What is this really?

```
1  #include "navier-stokes/centered.h"
2  #include "two-phase.h"
3  #include "curvature.h"
4  #include "contact.h"
5  #include "vof.h"
6  #include "tension.h"
7  #include "log-conform.h"
8  #include "view.h"
```

Current Work: 2-D Simulation

Some Problems and Solutions:

- Even for symmetric problems, mirroring about an axis isn't sufficient.

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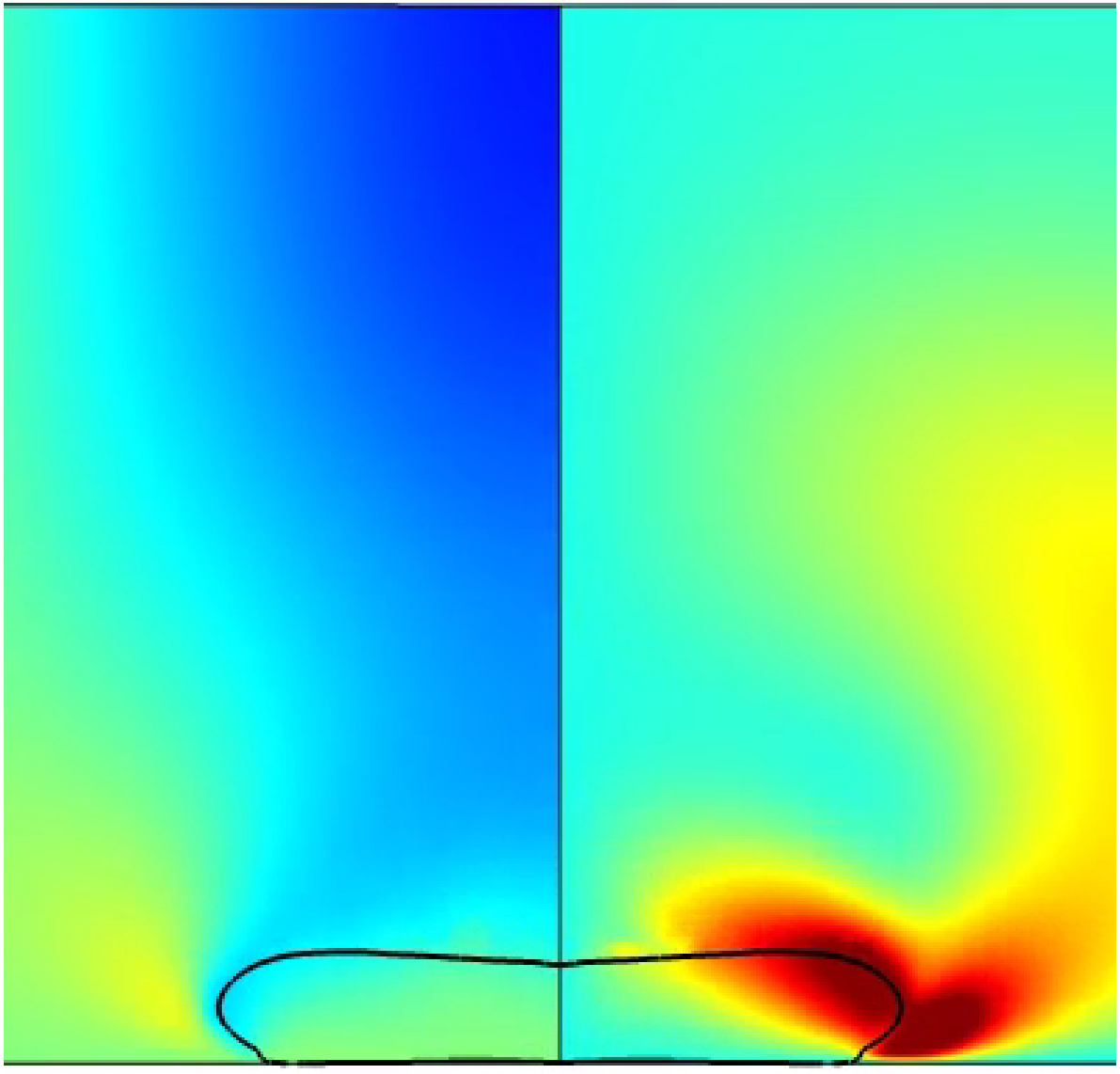

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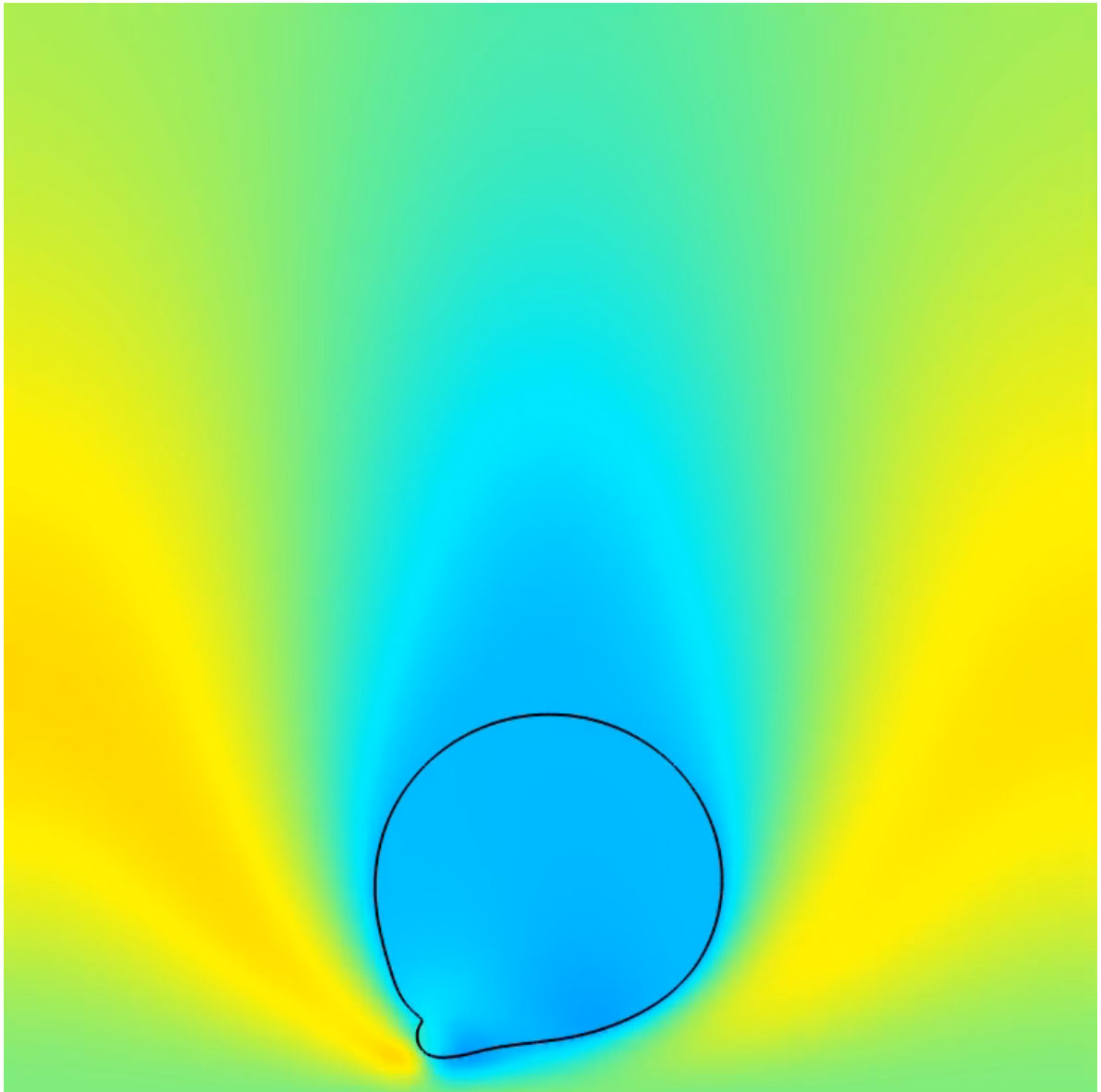

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$\rightarrow$ Use an adaptive grid and tune it.

$\rightarrow$ There is no avoiding going smaller without approximation, which is not a suitable solution.

Current Work: 2-D Simulation

Some Problems and Solutions:

- Even for symmetric problems, mirroring about an axis isn't sufficient.

- At small length scales, numerical errors dominate the physics unless if they are mitigated.

- Experiment Design: Trying to match real conditions is incredibly computationally intensive, have to settle for simpler/coarser model with respective changes in non-dimensional numbers.

Results and Future Work

Currently have a fairly reasonable simulation of a "nanodroplet" (micro and nanometer length scale) that agrees with constants reported in literature:

(Wang et. al. "Phase diagram for nanodroplet impact on solid surfaces" 2021).

Results and Future Work

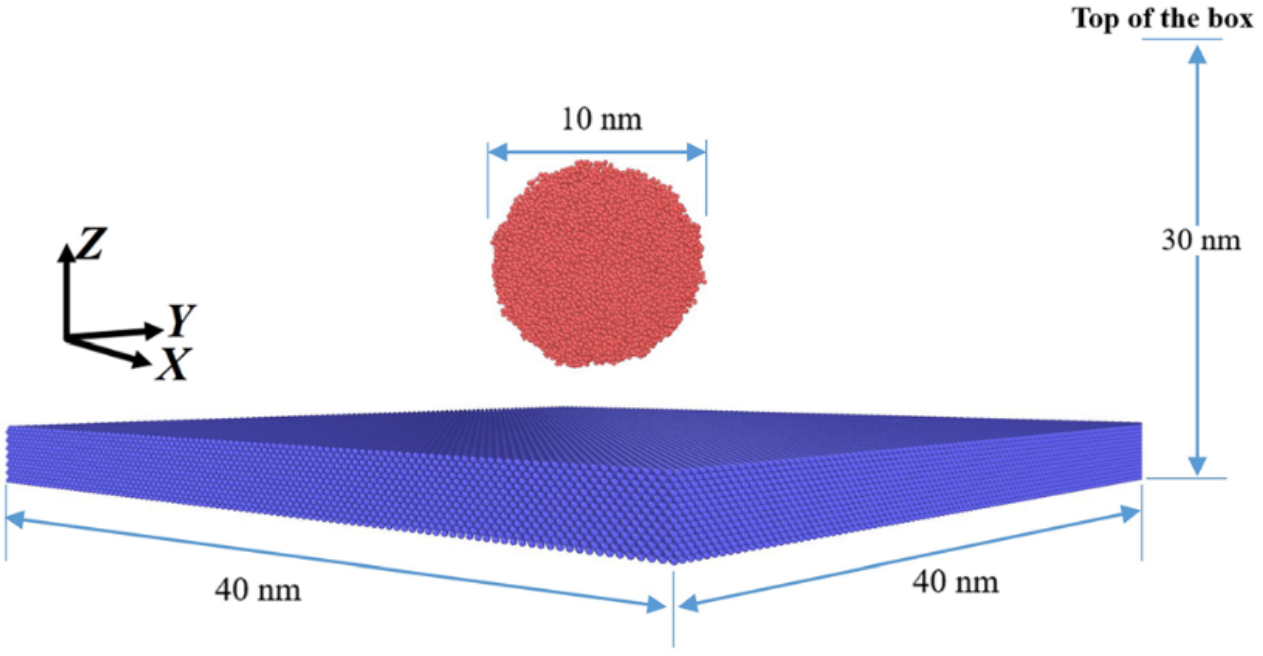
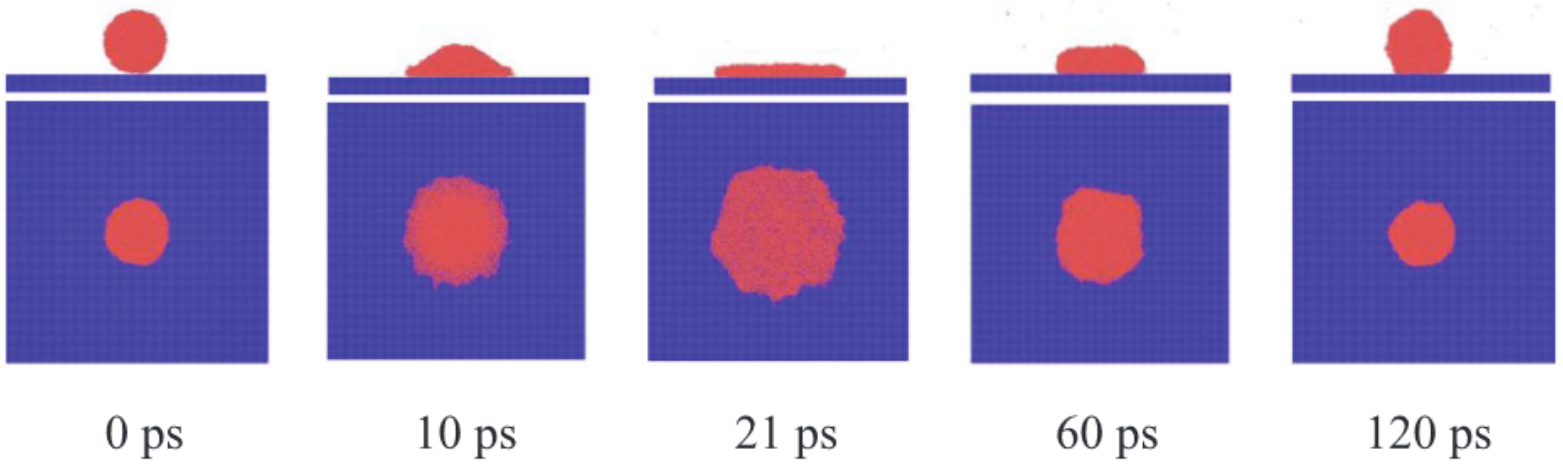


FIG. 1. Initial configuration of the simulated system, where Pt atoms are in blue and water molecules are in red.

Results and Future Work



(a)

Results and Future Work

Literature Example:

under the following conditions:
$We = 0.02$ to 220, $Re = 0.33$ to 40,

Results and Future Work

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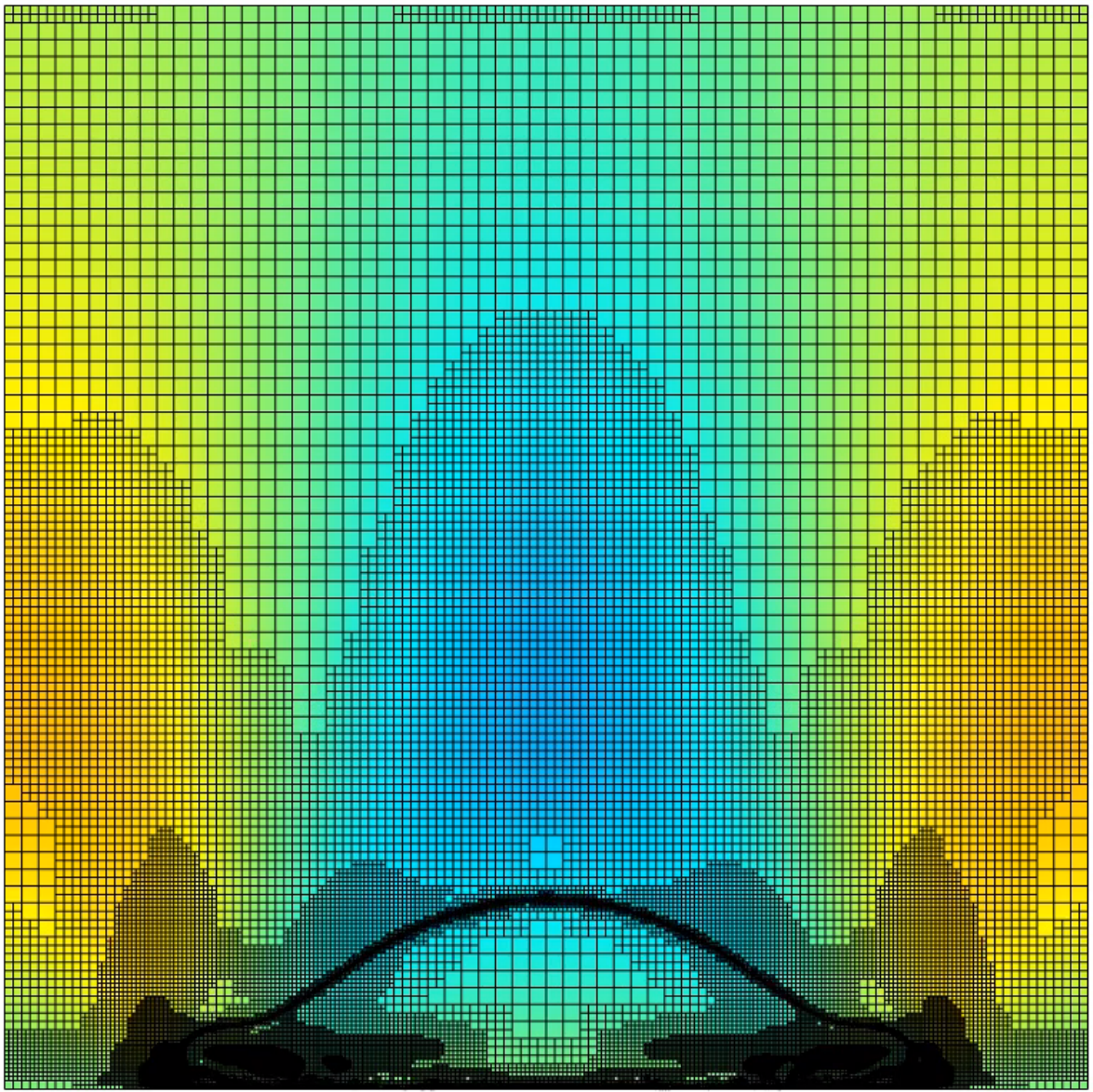
Our Constants:

Reynolds $= 5.0$

$$\text{Weber} = \frac{\rho v^2 l}{\sigma} = \frac{(0.001)(2.0)(0.5)}{0.05} = 0.02 \text{ (nice!)}$$

Results and Future Work



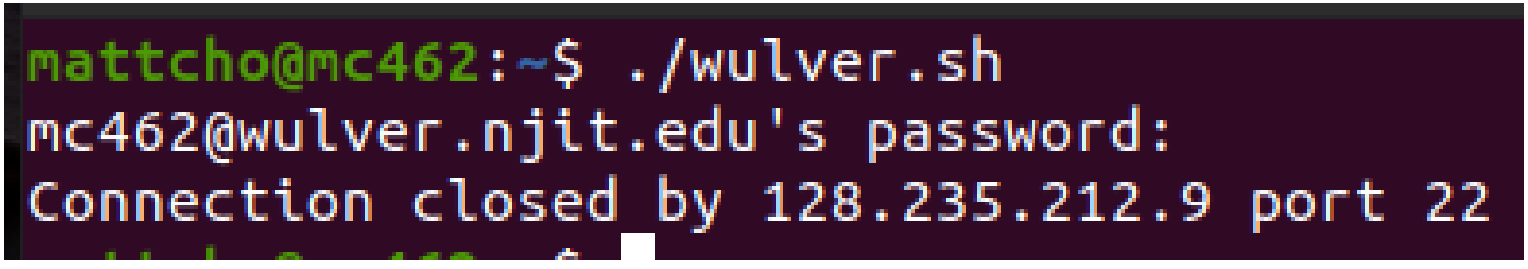
Results and Future Work

Okay, that's cool, but where are your numbers?

Results and Future Work

```
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
             29903       gpu basilisk    mc462 PD       0:00      1 (AssocGrpBillingMinutes)
             29902       gpu basilisk    mc462 PD       0:00      1 (AssocGrpBillingMinutes)
             29901       gpu basilisk    mc462 PD       0:00      1 (AssocGrpBillingMinutes)
             29900       gpu basilisk    mc462 PD       0:00      1 (AssocGrpBillingMinutes)
             29896       gpu basilisk    mc462  R       1:00      1 n0027
             29897       gpu basilisk    mc462  R       1:00      1 n0091
             29898       gpu basilisk    mc462  R       1:00      1 n0089
             29899       gpu basilisk    mc462  R       1:00      1 n0024
             29895       gpu basilisk    mc462  R       1:34      1 n0068
             29892       gpu basilisk    mc462  R       1:37      1 n0047
             29893       gpu basilisk    mc462  R       1:37      1 n0047
             29894       gpu basilisk    mc462  R       1:37      1 n0068
             29890       gpu basilisk    mc462  R       1:56      1 n0046
             29889       gpu basilisk    mc462  R       2:31      1 n0069
             29888       gpu basilisk    mc462  R       2:34      1 n0027
             29887       gpu basilisk    mc462  R       2:37      1 n0005
             29886       gpu basilisk    mc462  R       2:40      1 n0004
             29885       gpu basilisk    mc462  R       2:46      1 n0002
             29884       gpu basilisk    mc462  R       2:50      1 n0002
             29883       gpu basilisk    mc462  R       2:53      1 n0090
             29882       gpu basilisk    mc462  R       2:57      1 n0089
             29881       gpu basilisk    mc462  R       3:00      1 n0088
             29880       gpu basilisk    mc462  R       5:18      1 n0069
[mc462@login02 basilisk-tx]$
```

Results and Future Work



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Natural thing to do would be to incrementally approach larger scale (mm-scale drops).

The way forward is simply applying known computer programming/engineering techniques to make computational problem tractable.