Simulating a Droplet Within a Two-phase Viscous Flow

Matt Cho

CFD Methodology

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

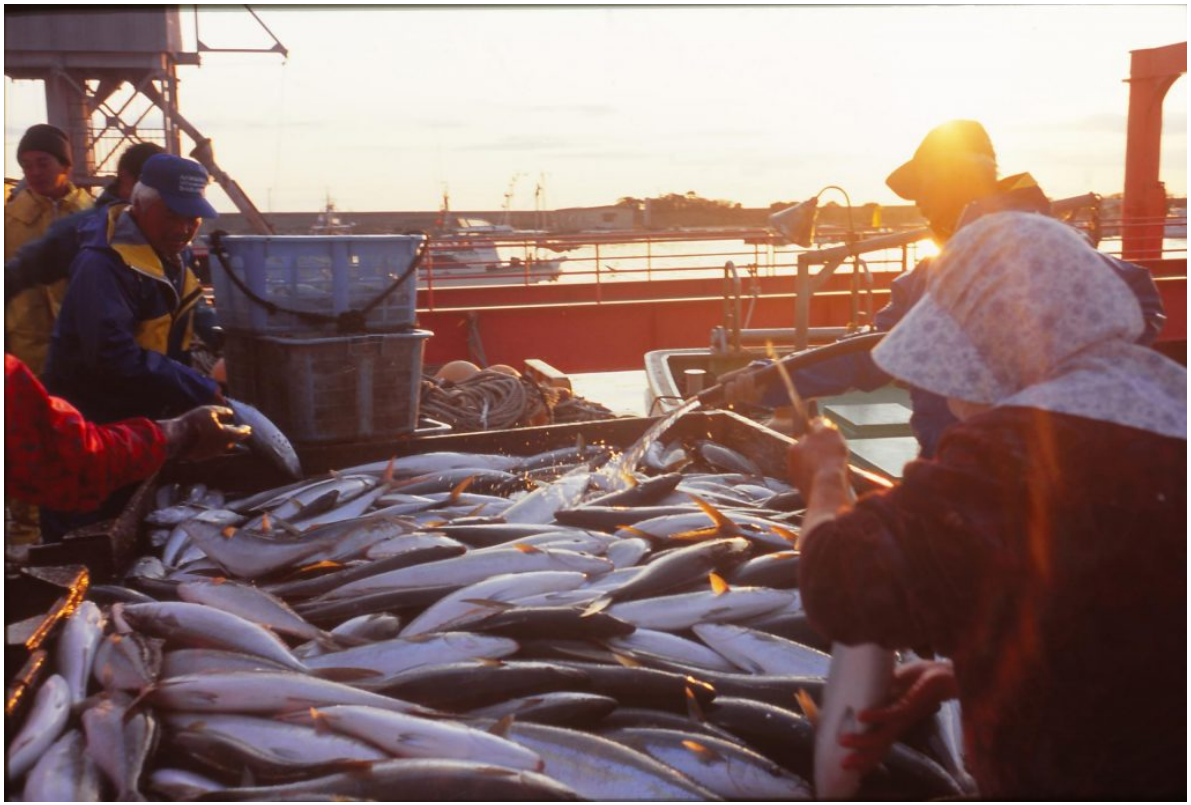
Computational Math ("Post-Moore's Law")

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

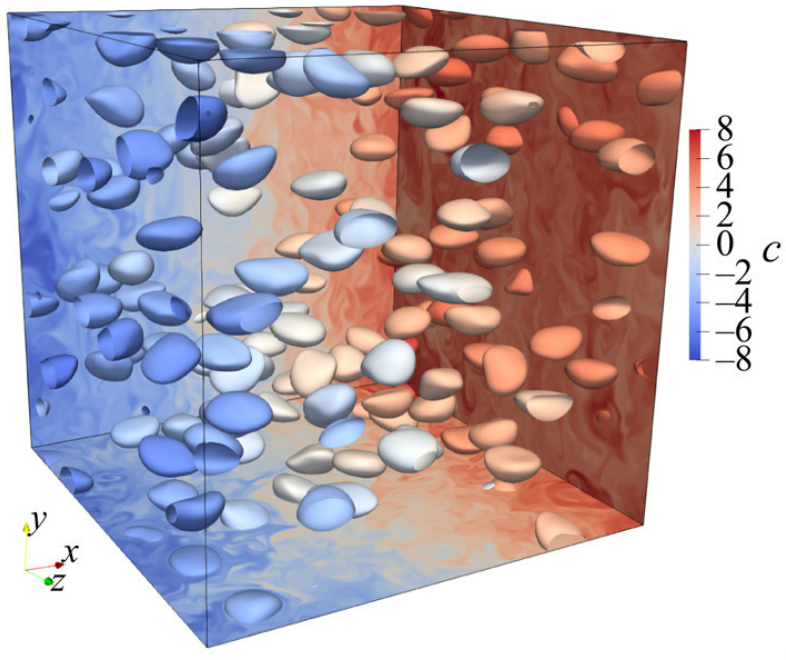
Introducing Basilisk

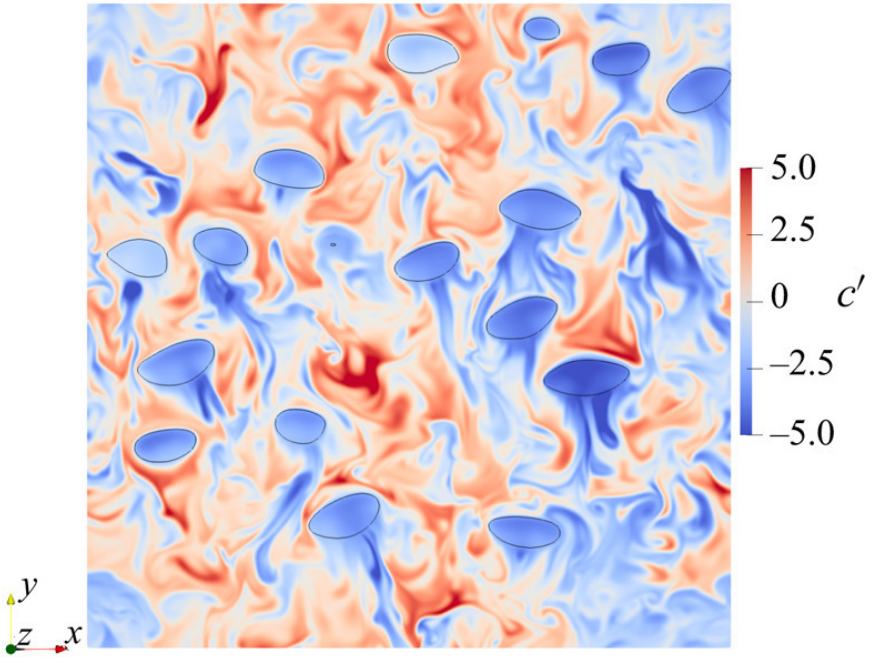
General Purpose PDE Solver specializing in solving over adaptive meshes.

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

Software Framework

Introducing Basilisk





Software Framework

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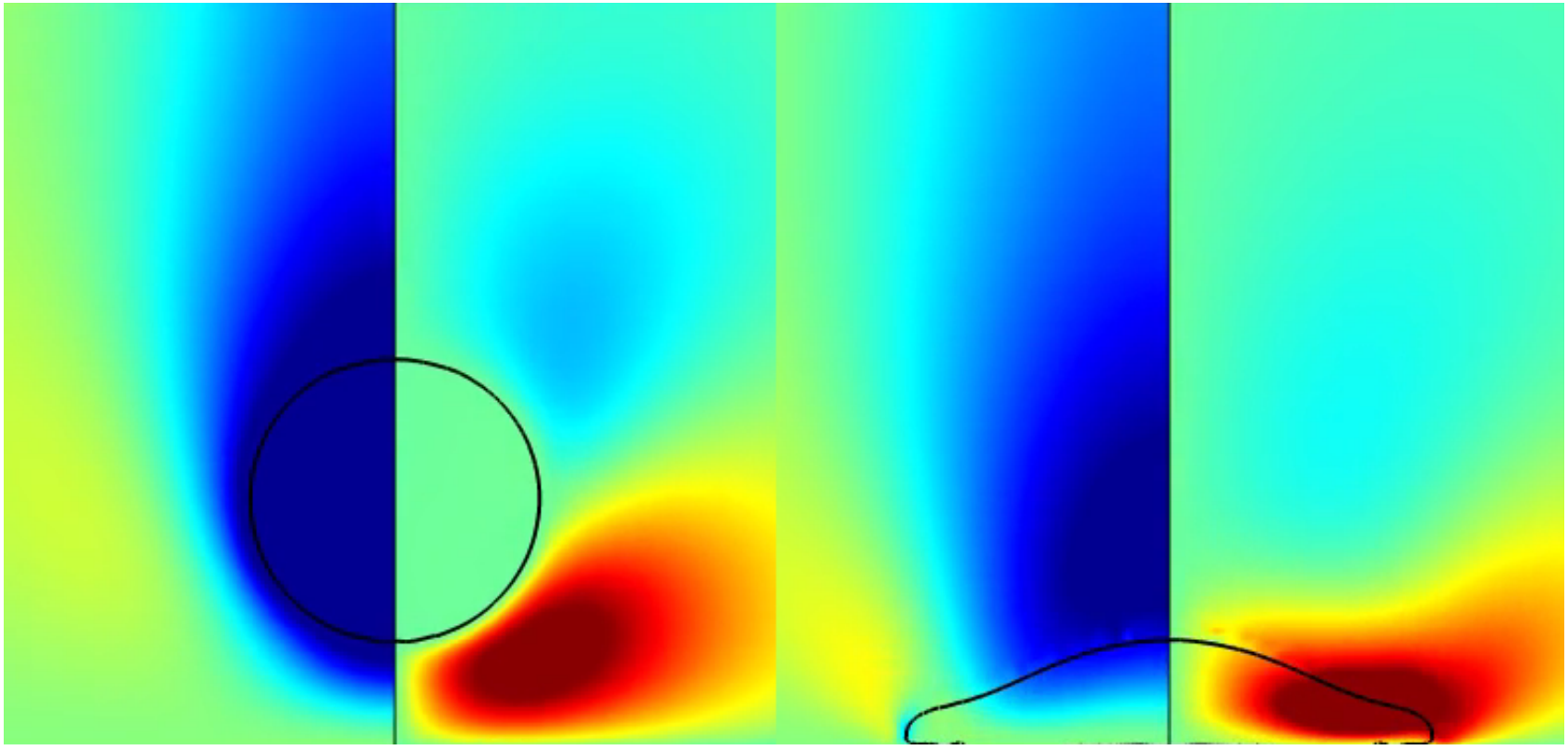

Software Framework

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.

(We are interested in viscosity and advection more than heat transfer.)

Software Framework

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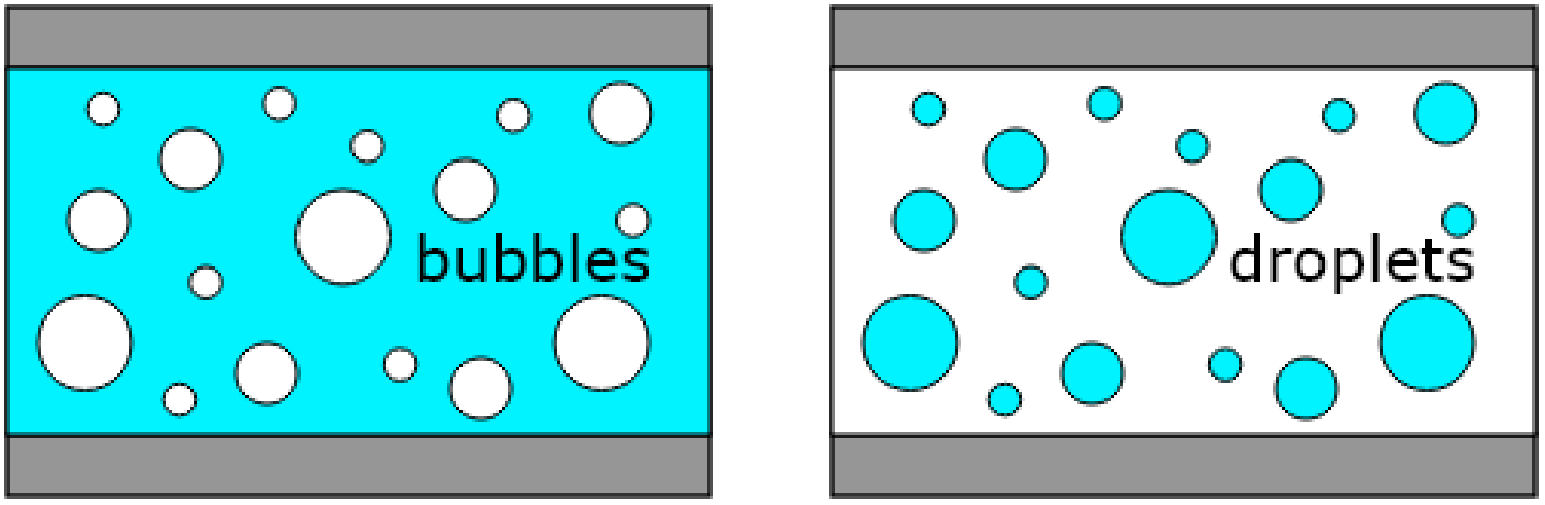


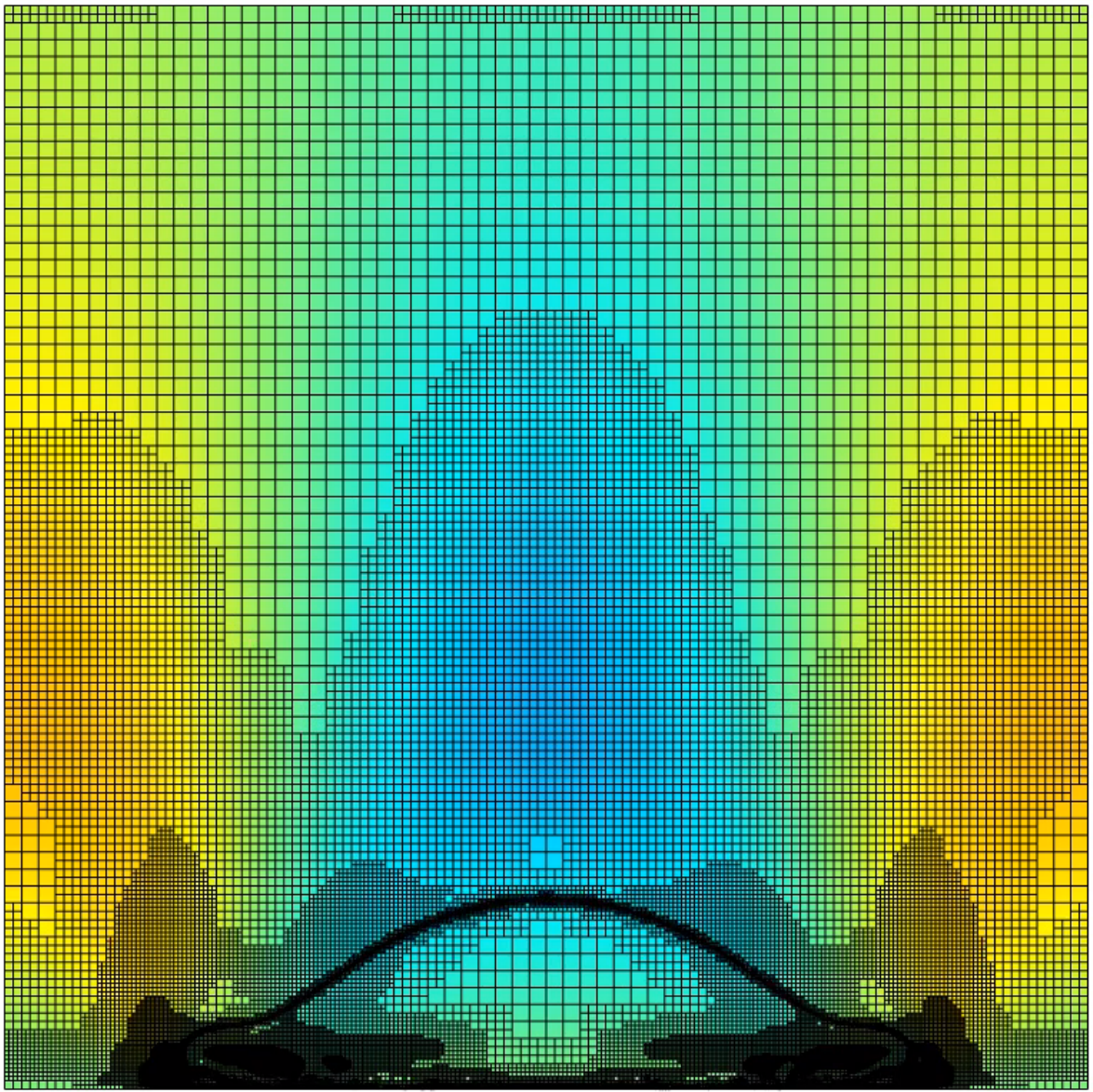
c) Dispersed two-phase flow.

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



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- 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 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.

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)
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             29897       gpu basilisk    mc462  R       1:00      1 n0091
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             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
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             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
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[mc462@login02 basilisk-tx]$
```
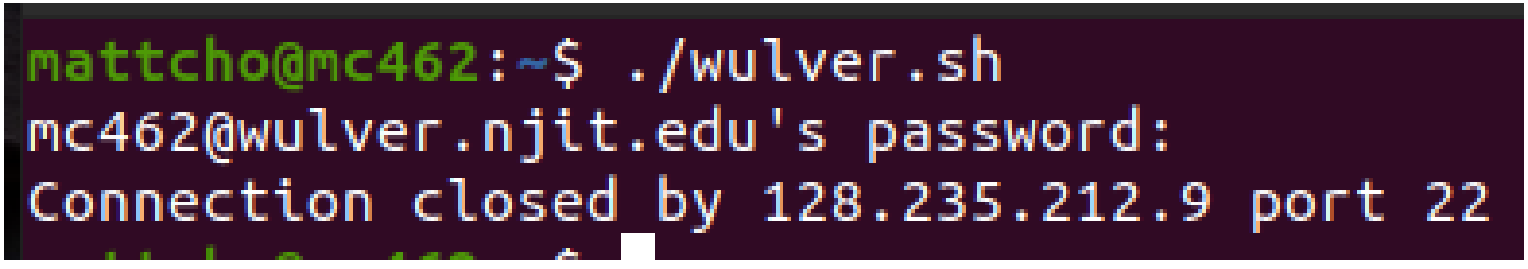

Results and Future Work



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The way forward is then to apply tried and true computer programming/engineering techniques to make computational problem tractable.