

Simulating a Droplet Within a Two-phase Viscous Flow

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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 → **Hypothesis** → **Experiment** → **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 → Hypothesis → Experiment → Experiment
→ Experiment → Experiment → Experiment → ...**

CFD Methodology

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



CFD Methodology

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



Software Framework

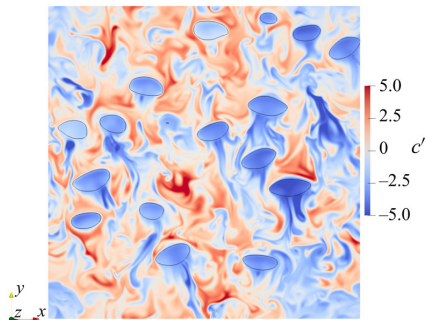
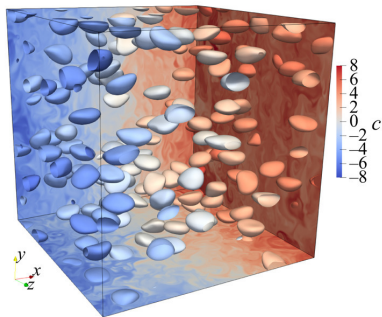
Introducing Basilisk

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

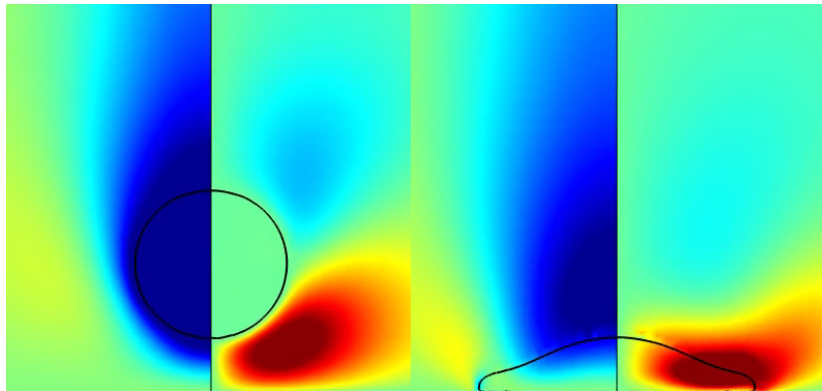
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What is this really?

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

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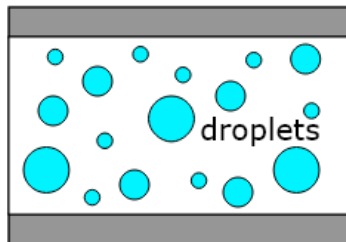
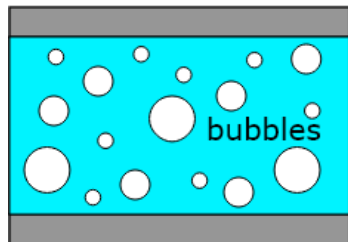
A solution to the Navier-Stokes equations, using the Volume-of-Fluid method (VOF).

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.)

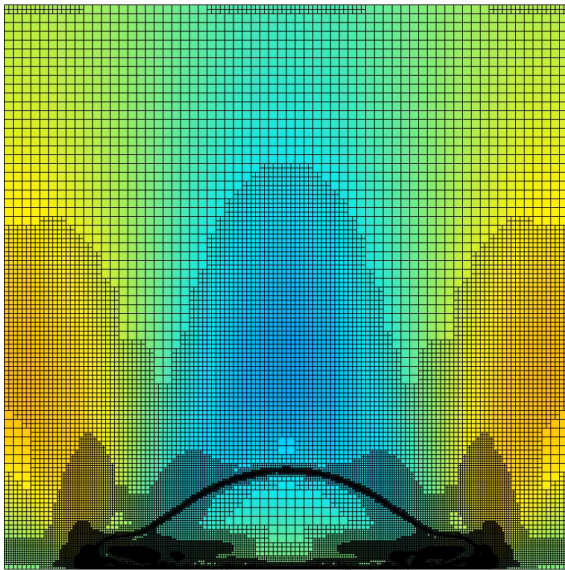
Software Framework

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c) Dispersed two-phase flow.

Current Work: 2-D Simulation



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Some Problems and Solutions:

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Some Problems and Solutions:

- Even for symmetric problems, mirroring a simpler domain 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 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

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JOBID PARTITION NAME USER ST TIME NODES Nodelist(REASON)
29903 gpu basillisk mc462 PD 0:00 1 (AssocGrpBillingMinutes)
29902 gpu basillisk mc462 PD 0:00 1 (AssocGrpBillingMinutes)
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29898 gpu basillisk mc462 R 1:00 1 n0089
29899 gpu basillisk mc462 R 1:00 1 n0024
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29884 gpu basillisk mc462 R 2:50 1 n0002
29883 gpu basillisk mc462 R 2:53 1 n0090
29882 gpu basillisk mc462 R 2:57 1 n0089
29881 gpu basillisk mc462 R 3:00 1 n0088
29880 gpu basillisk mc462 R 5:18 1 n0069
mc462@login02 basillisk-tx]$
```

Results and Future Work

```
mattcho@mc462:~$ ./wulver.sh  
mc462@wulver.njit.edu's password:  
Connection closed by 128.235.212.9 port 22
```

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