# PhD in Energy and Mineral Engineering at PSU

## Nicolás's Research - Reports

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## Report Sep 16 - 2021

Main discussion points:

- Generalities
- Cheng's paper
- Dr. Yashar and Miscible code
- Plausible models for thermodynamic coupling

# Generalities

Trip to New York next week (Friday)

Paper affiliation for paper recently accepted (yesterday)

Format of future presentations and meeting setup

# Cheng's paper

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  - Droplet impacting surface (MCMP and IMM?)
  - Oscillating droplet
  - Rotating droplet
  - Surface wave

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  - Droplet impacting surface (MCMP and IMM?)
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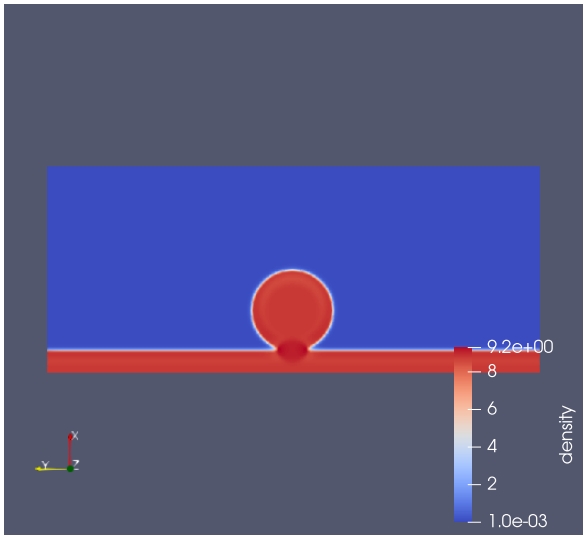
  - Rotating droplet
  - Surface wave
- DRY

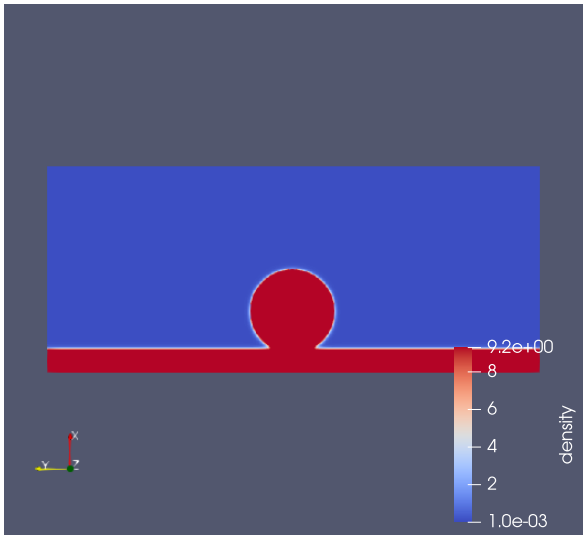
# Cheng's paper

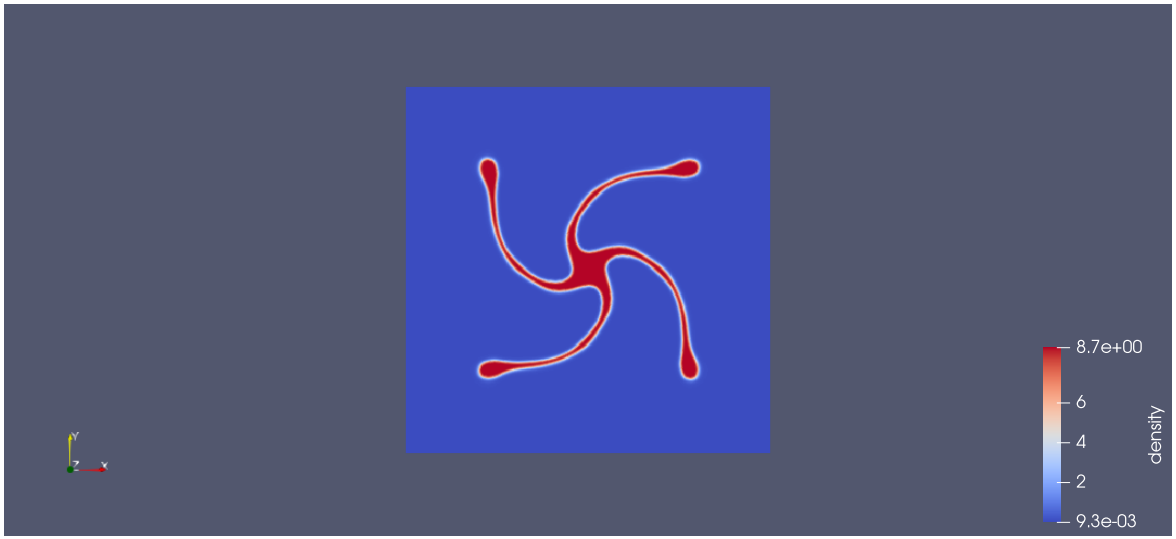
With these results we are able to:

- Decide which dynamic metrics will be tracked to validate/analyze/compare
- Play around with some parameters to see how they impact the dynamic metrics

# Cheng's paper



# Dr. Yashar and Miscible Code

The new code already contains: scaling, two-phase equilibrium, initialization of parameters. Next step: DF initialization.

Before comparing programming languages, state its requirements:

- Parallelization. Garbage collector.
- 3D simulation (large memory usage)
- Maintainable and easy to couple with other tools

# Plausible models for thermodynamic coupling

**Comprehensive comparison of pore-scale models for multiphase flow in porous media**

Paper comparing bench-marking pore-scale methods against experimental data, varying $C_a$ and wettability.

- LBM higher resolution ($\sim$ 14 $\mu$m/lattice)
- Simulation metrics: fractal dimension ($D_f$), finger width ($W_f$)
- LBM captures thin films and corner flow (3D effect). Computationally costly.

**Phase Field (Quasi 3D method)**

Capture incomplete displacement (film flow) but not corner flow

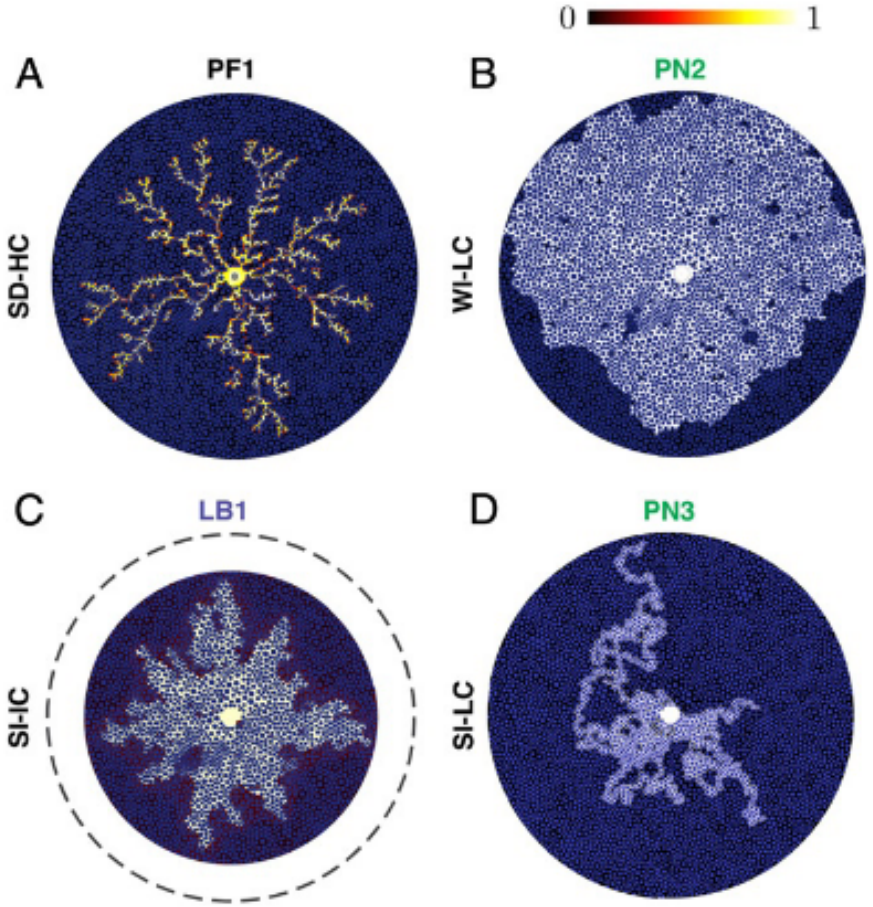



**Fig. 3.** Selection of simulated displacement patterns for the priority cases. (*A*) Strong drainage at high Ca (SD-HC) as simulated by a phase-field model. (*B*) Weak imbibition at low Ca (WI-LC) as simulated by a pore-network model. (*C*) Strong imbibition at intermediate Ca (SI-IC) as simulated by a lattice Boltzmann model at a reduced viscosity ratio ($\mathcal{M} = 40$). (*D*) Strong imbibition at low Ca (SI-LC) as simulated by a pore-network model.

Additional comments on phase field and LBM

- LBM requires $\sim$ 160 million cells. Limited by viscosity ratio $M$ and in the limit of thin films
- 3D simulation is recommended
- Phase field looks promising to capture 3D effects with reduced computational cost, at high $M$, depending on regime
- All of them capture viscous fingering in some degree
- Many-pore scale is the only way to capture flow dynamics

# Comments...

- Shared Google Drive
- Keep going fast with the new code
- Read last Cheng's paper and see how the simulations there can be connected with the needs in the second one
- Analytical solutions as a validation after comparing with Cheng's code
- Be ready for programming language discussion
- How different LBM models are formulated?
- Study in deep a phase field formulation to understand what it has inside
- PhD position

## Report Sep 30 - 2021

Main discussion points:

- Generalities
- Code state
- PhD position
- Communications with Cheng and Dr. Mehmani

# Generalities

- Courses:
  - Programming: Gained C++ proficiency: classes, pointers, functions (...). Weekly programming homework and quizzes.
  - Data mining: Exploring more classification algorithms, their cost functions, and implications. First project submitted on Sunday.
  - CHE 524: Entropy functional and probabilities. Final exam: Dec 13.
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- Paper about LBM for aneurysm (link)
- Worked for SIATA on Tuesday

# Code state

EoS partially validated.
Compressibility factor highly deviated from a particular pressure/compositi combination.
Changed functions to be vectorized

**Remark**

I didn't advance as expected (putting attention on other PhD tasks) but is ongoing. As I am comparing codes, the double screen will be a key point to me.

# Multiple phases in a single lattice

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If no, how to justify that a particular combination of composition and total density (or pressure) always honors thermodynamics in a stable phase.

If yes, shouldn't the model compute a split factor for each phase (as force is computed for phases) and then sum up the force for each component in each phase?

# PhD position

Hillmert Solano and Juliana Rueda

# Communications with Cheng and Dr. Mehmani

To Cheng's email:
Check Outlook

Dr. Mehmani email:

- 1-2 slides with governing equations.
- Simulation results
- Open discussion (methods, tools,...)

# Others

- Google Drive ready
- Screen received and waiting for the workstation
- Plan to incorporate Inkscape to these presentations

# Actions

- Advance in the code and prepare presentation with governing equations for Dr. Mehmani
- Send Fluid mechanics book
- Week ideas: validation cases can be found in the Paper 005.

## Meeting Nicolas - Dr. Mehmani - 2021

Main discussion points:

- Governing equations
- Results with current model
- State of new version

# Governing equations

The Lattice Boltzmann Method is based on kinetic theory, that states:

$$\underbrace{\frac{\partial f_i(x,t)}{\partial t} + \mathbf{c}_i \frac{\partial f_i(x,t)}{\partial x}}_{\text{Streaming - DF Advection}} = \underbrace{\mathbf{\Omega}}_{\text{Collision}} \tag{1}$$

What in its discretized form[1] becomes:

$$f_i(x + \mathbf{c}_i \Delta t, t + \Delta t) - f_i(x,t) = -\mathbf{M}^{-1}\mathbf{S}[\mathbf{m}(x,t) - \mathbf{m}^{\text{eq}}] + \hat{F}_i \tag{2}$$

where $\mathbf{m}$ are vectors of moments, $\mathbf{S}$ is a relaxation diagonal matrix, and $\mathbf{M}$ is a fixed matrix depending on DnQm. $\mathbf{m}^{\text{eq}} = f(f_i^{\text{eq}}, \mathbf{F})$.

[1] Going from 1 to 2, what about spatial derivative?

# Macroscopic variables

Density and velocity are computed as follows:

$$\rho = \sum_i f_i \qquad \mathbf{u} = \sum_i \mathbf{c}_i f_i \tag{3}$$

Two important constitutive equations:

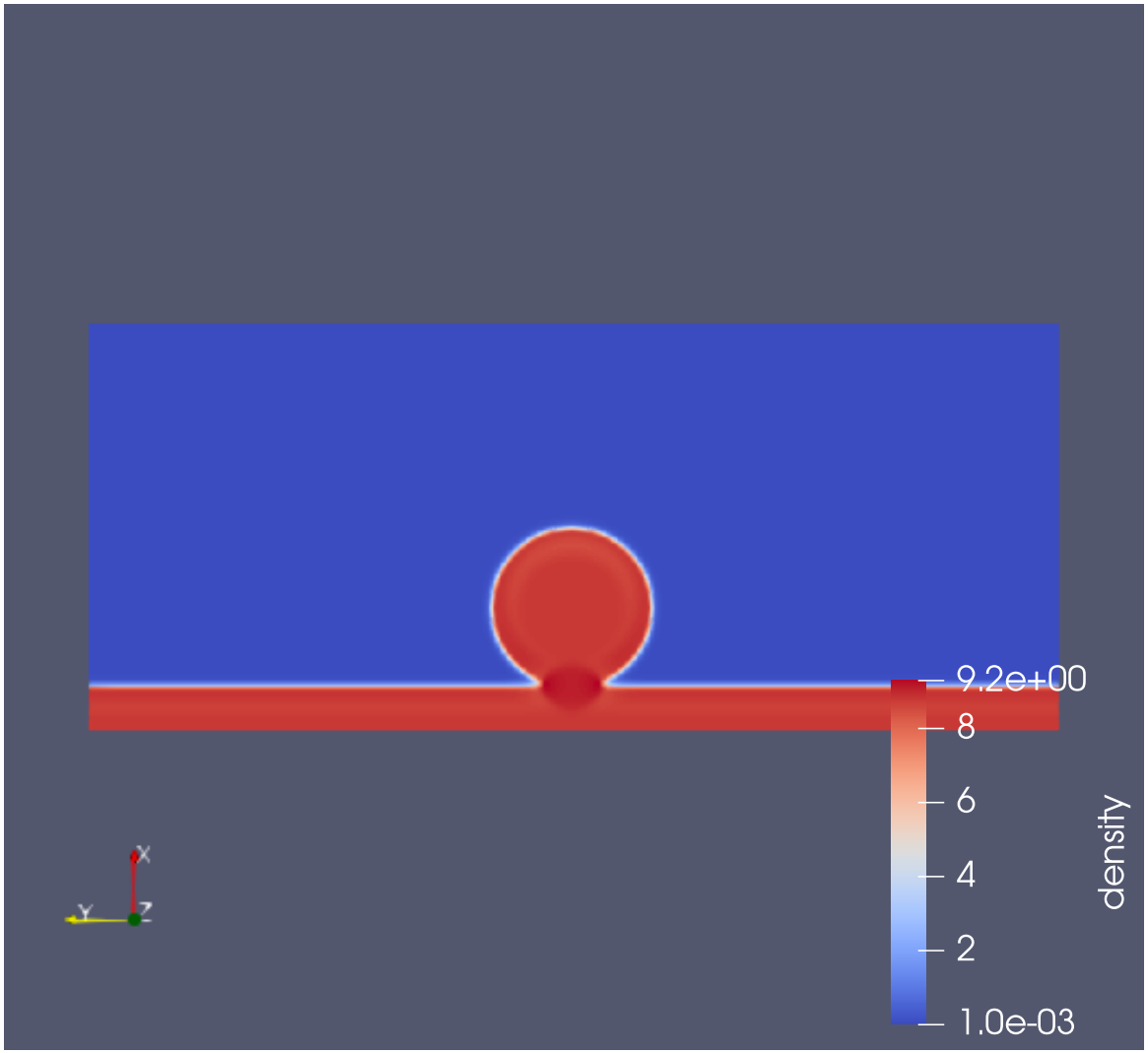
$$f_i^{\text{eq}} = \rho\omega_i \left[1 + \frac{\vec{u}\cdot\vec{\mathbf{c}_i}}{c_s^2} + \frac{(\vec{u}\cdot\vec{\mathbf{c}_i})^2}{2c_s^4} - \frac{\vec{u}\cdot\vec{u}}{2c_s^2}\right]$$

$$\hat{F}_i = \frac{\mathbf{F}}{\rho}\frac{\vec{u}-\vec{\mathbf{c}_i}}{c_s^2} f_i^{\text{eq}}$$

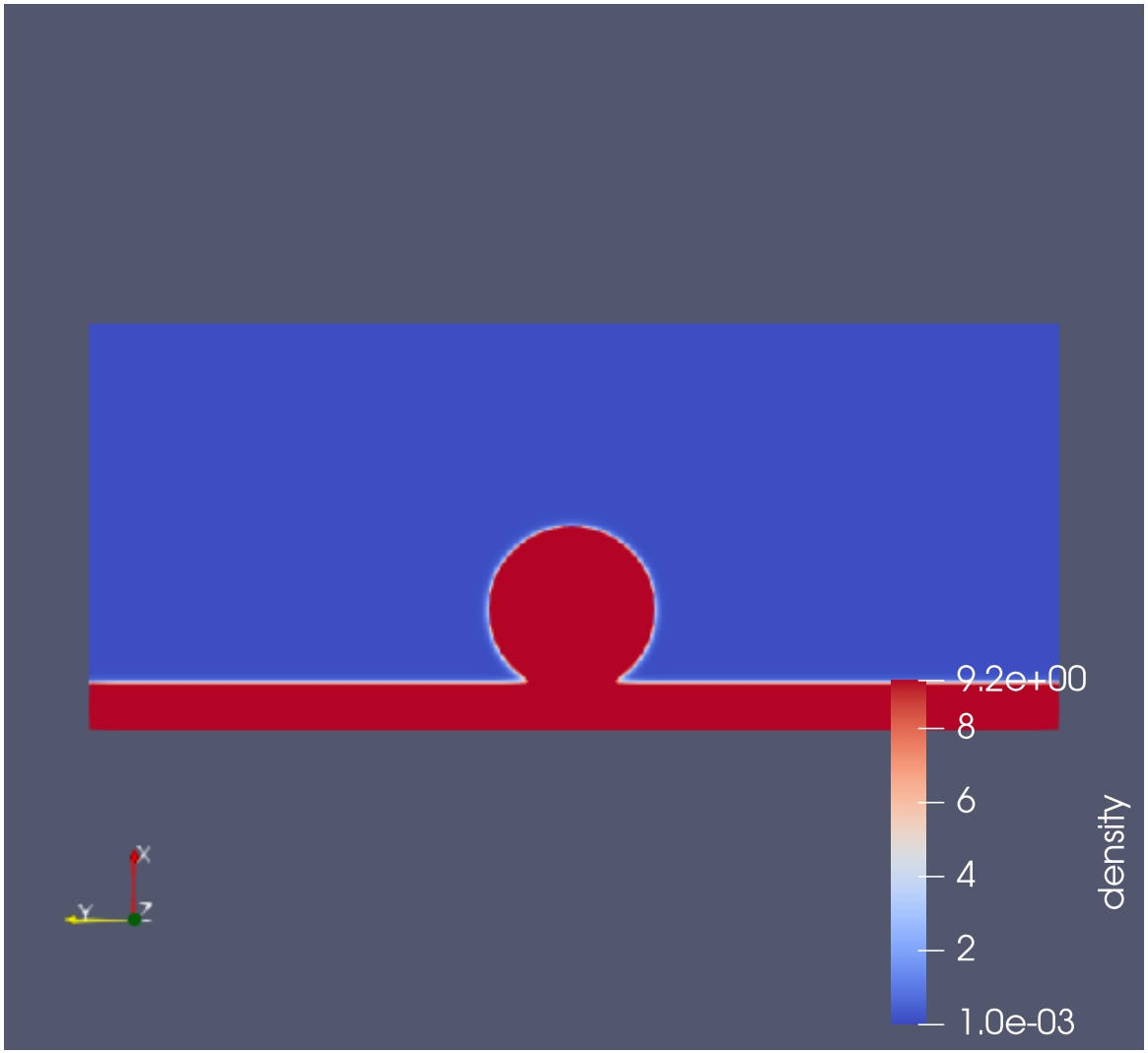
where $\mathbf{F}$ is defined in the multiphase problem, as the Shan Cheng force:

$$\mathbf{F} = -G\psi(x)\sum_i \omega_i \psi(x + \mathbf{c}_i\delta t)\mathbf{c}_i \quad \psi := \sqrt{\frac{2(P^{\text{EoS}} - c_s^2\rho)}{G\delta t c_s^2}} \tag{4}$$

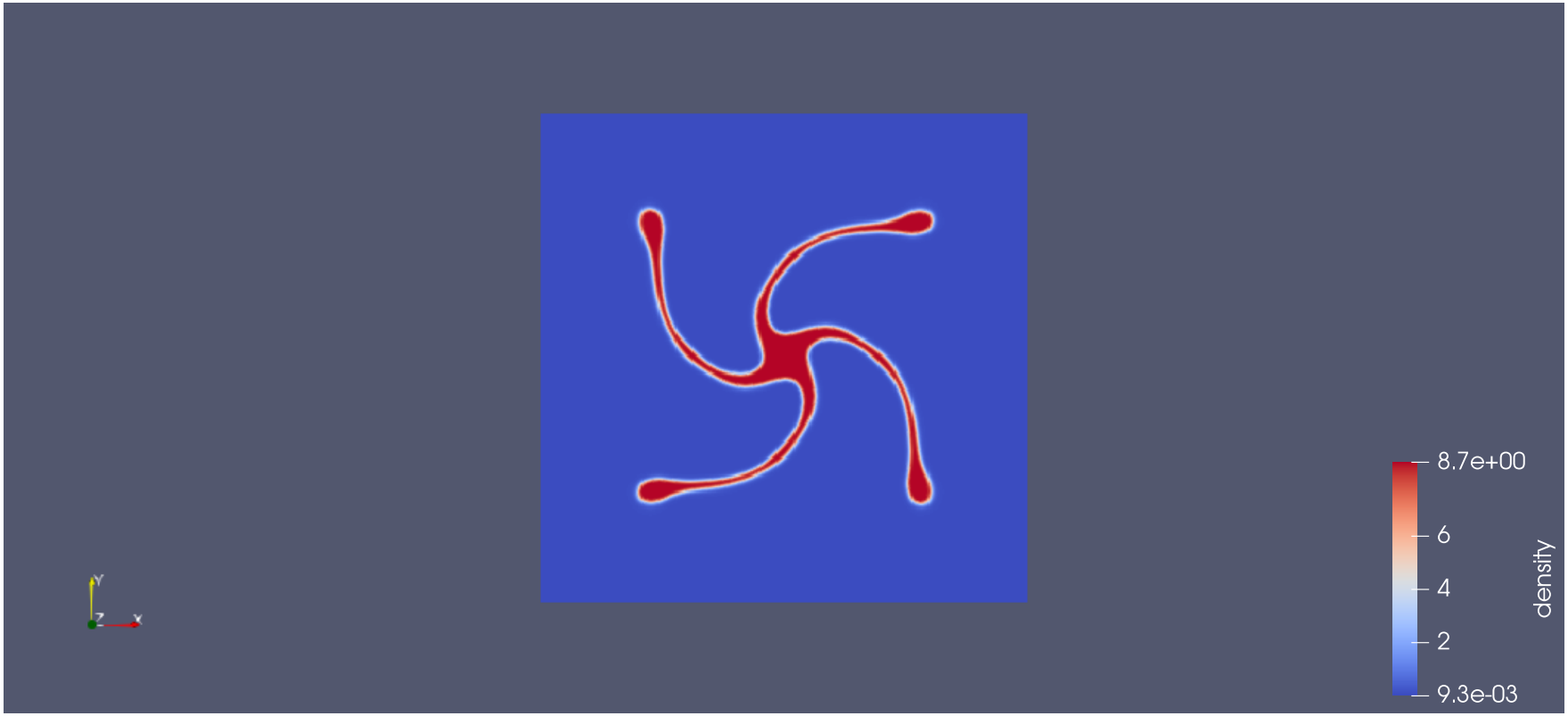
# Droplet impacting on a surface - Immiscible



# Droplet impacting on a surface - Miscible



# Rotating droplet



# State of new version

- Object oriented Fortran code
- VTK-format printing to visualize with Paraview
- EoS completely detached from LBM: using inheritance for classes[2]
- Tools being used:
  - Visual Studio Code as interface. Compiler: gfortran
  - Visualization: ParaView. Not using VTK libraries yet
  - Makefiles. Not CMake yet

**Philosophy**

Decouple physical concepts from numerical concepts
Flexible code for future implementations

[2] Developed in international system of units

# Questions

Clarification. I am attempting to finish the code for 3 reasons: unify versions and capabilities, having fun, and: materialize on my code the possible PhD projects. Should I attempt to take advantage of this stage to program in parallel other methods?
My concerns: should I start now in C++? Should I start with OF as well? What about other modern/promising methods? Will this be my entry point to the academia?

# Questions

- If you were to start your PhD again, which topic/method/language/project would you start?
- Pore-scale phenomenology, most relevant set of equations and ideal solutions for pore-scale modeling, origin of Young Laplace equation, assumptions, etc...

End...

# Actions

- Is F representing other possible forces? van der Waals, Coulomb, walls.
- Write down here the derivation on the board.
- Yashar has a code for level-set and volume-of-fluid which to contrast with if I want to develop those methods by myself.
- Get used to those methods, derivations, force definitions and the core of the solution: coloring function
- C++ with an automatic differentiation library? Can I connect it to Python library? This may reduce my coding time by a factor of 4!
- Memorize advection equation, stress tensor definition, forces...
- Concise but better detailed LBM explanation. How surface tension force arises in LBM? Also, do not show results if there is not a good reason to show them (happened with ready simulations).

## Report Oct 7 - 2021

Main discussion points:

- Generalities
- Code state

# Generalities

- New machine status:
  - Working as expected (really well!)
  - Need to contact John: installation in limited/storage disk (remote)
  - Need permissions to set up my Google Drive account
  - Compilers working well! gfortran and g++

# Generalities

- New machine status:
  - Working as expected (really well!)
  - Need to contact John: installation in limited/storage disk (remote)
  - Need permissions to set up my Google Drive account
  - Compilers working well! gfortran and g++
- Question: without having to solve two distribution functions per component, can we solve an isochoric version of the EoS for every node?

# Code state

Show code status and results connected to ParaView.

# Comparison of EoS Results

| Variable | Old | New | Decimal Pos. Diff |
|---|---|---|---|
| $P$ scale | 2987.2198 | 2987.2707 | 2 |
| $T$ scale | 1146.9220 | 1146.9129 | 2 |
| $a_1$ scale | 0.18367 | 0.18367 | 14 |
| $b_2$ scale | 0.28177 | 0.28177 | 6 |
| $Z$ liquid | 0.438672 | 0.438672 | 9 |
| $Z$ gas | 0.59443 | 0.59443 | 10 |

Table: The results related to a thermodynamic conditions, were evaluated at 1888.2 psi

# Validation of the code

- Cheng's version and William's version
- Closed tube to see linearity of capillary pressure and contact angle
- Evaporation from a channel (analytical solution)

# How to keep the momentum?

Should I...

- Start visualizing a particular method as potential for us? How to approach to it?
- Accelerate any process in which I am being slow?

## Report XXX XX - 202X

Main discussion points:

- Topic 1
- Topic 2

# Sample frame title

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- Text visible on slide 1

# Sample frame title

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- Text visible on slide 2

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- Text visible on slides 3

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In this slide

In this slide
the text will be partially visible

In this slide
the text will be partially visible
And finally everything will be there

# Sample frame title

In this slide, some important text will be highlighted because it's important. Please, don't abuse it.

**Remark**

Sample text

**Important theorem**

Sample text in red box

**Examples**

Sample text in green box. The title of the block is "Examples".

# Two-column slide

This is a text in first column.

$$E = mc^2$$

- First item
- Second item

This text will be in the second column and on a second tought this is a nice looking layout in some cases.