PhD in Energy and Mineral Engineering at PSU
Nicolás's Research - Reports

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and Mineral Sciences

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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

I was running some codes (those with more than 1 time step). They are now stored in my OneDrive and my laptop. What I found:

- Different versions of the same code

Cheng's paper

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- Different versions of the same code
- They compile and run correctly (the tested ones). Visualization adapted from the code I developed for William's cases. Run cases:
  - 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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  - Surface wave
- DRY

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

Dr. Yashar and Miscible Code
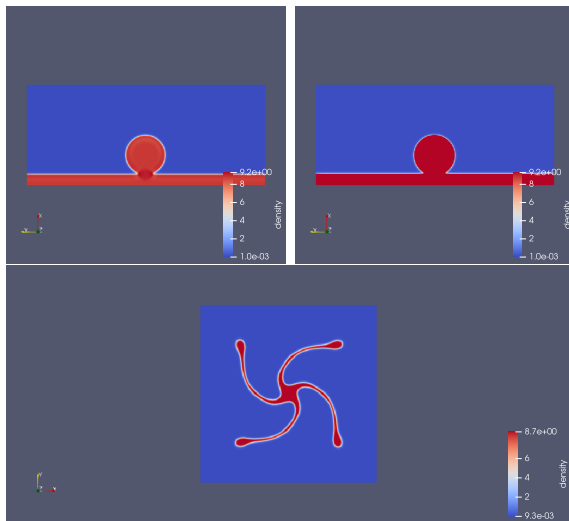
The new code already contains: scaling, two-phase equilibrium, initialization of parameters. Next step: DF initialization.

Before comparing programming languages, state its requirements:

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

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)

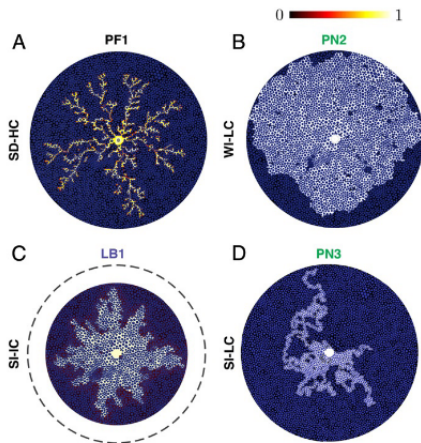Capture incomplete displacement (film flow) but not corner flow

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 ~ 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.
    - AERSP 508: Solving analytically flow for inviscid-incompressible flow.

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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.

Do you agree that in a single lattice, multiple phases may coexist in a particular time step?

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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.

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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?

Hillmert Solano and Juliana Rueda

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. $\mathbf{m}^{\text{eq}} = f(f_i^{\text{eq}}, \mathbf{F})$.

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

Macroscopic variables

Density and velocity are computed as follows:

$$\rho = \sum_i f_i \quad \mathbf{u} = \sum_i \mathbf{c}_i f_i \quad (3)$$
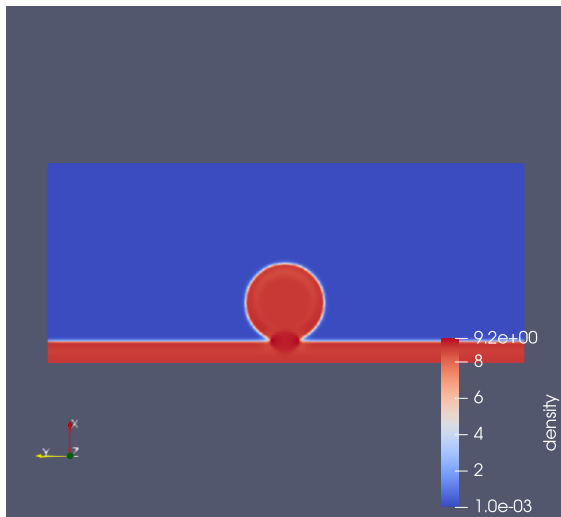
Two important constitutive equations:

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

$$\hat{F}_i = \frac{\mathbf{F}}{\rho} \frac{\vec{u} - \vec{\mathbf{c}_i}}{c_s^2} f_i^{\text{eq}}$$
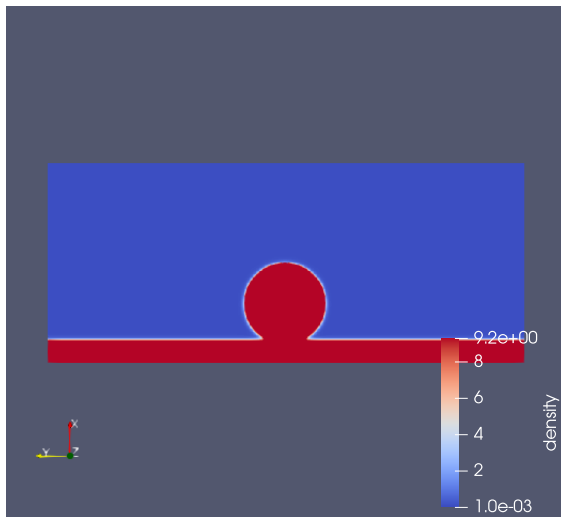
where $\mathbf{F}$ is defined in the multiphase problem, as the Shan Cheng force:

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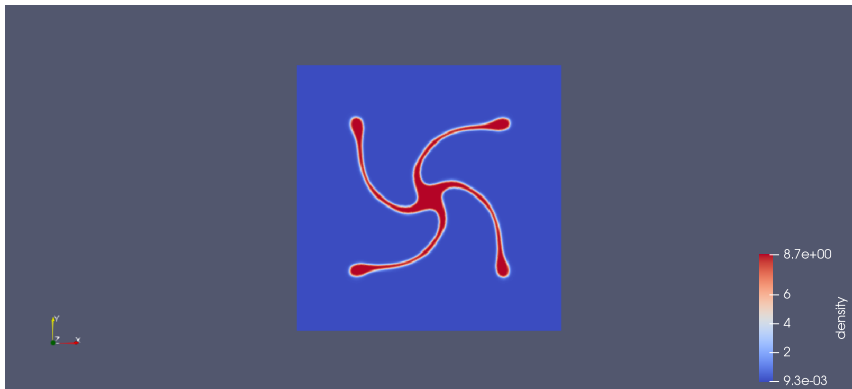
Droplet impacting on a surface - Immiscible

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

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[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?

- 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?

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

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

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?

CVs: Hillmert and Felipe. Upgrading paper.

Report Oct 14 - 2021

Main discussion points:

- Courses
- Review the last week missing points
- Code state

Courses

- I ran the fractured porous media simulation from William. I plan to compare against this case first.
- New implementations: pseudo potential calculation, Shan-Cheng force, and collision (50%).

Actions

- Validate first single component multiphase and multicomponent multiphase immiscible cases.
- Review the mathematical form of those equations more than implementation.
- Keep doing best effort with the courses

Report Oct 21 - 2021

Main discussion points:

- Generality: trip to Colombia: Dec 14th. Bus tickets Dec 13th.
- Generality: correcting Fuel paper. SIATA on weekends and night.
- Courses
- Code state

Courses

- Adv. Programming: Covering topics about software development and software architecture.
- Data mining: Incredible connection to statistical thermodynamics, about a method to classify entities with unknown labels, by maximizing an entropy functional (posterior probability).
- CHE 524: Midterm yesterday. Interesting connection with statistics and LBM concepts. Still not sure where it will arrive.
- AERSP 508: I wasn't able to review the topics. Keep going next week.

- I have been checking the tutorials and books, to review the LBM math.
- New implementations: run time report, collision BGK, MRT, decoupling more some functions. Right now, in Streaming step.
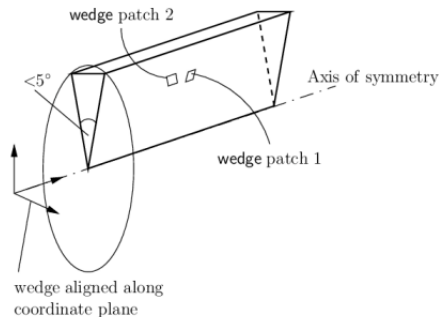- Still not sure how to treat boundaries

Figure 4.3: Axi-symmetric geometry using the *wedge* patch type.

Definition of patches in OpenFOAM

Code state

- Lost time in setting up CMake. Tool to facilitate (?) compilation of large projects, allowing for compiling external libraries with own software. Designed for C++.

- I decided to go for an small prize first: turbulent flow around cylinder (I have a solution which to compare with). Then single component multiphase. Then multicomponent immiscible.

Actions

-
-

Present

Present...

Report XXX XX - 202X

Main discussion points:

- Topic 1
- Topic 2

Sample frame title

This is a text in second frame. For the sake of showing an example.

- Text visible on slide 1

Sample frame title

This is a text in second frame. For the sake of showing an example.

- Text visible on slide 1
- Text visible on slide 2

Sample frame title

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- Text visible on slide 1
- Text visible on slide 2
- Text visible on slides 3

Sample frame title

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- Text visible on slide 1
- Text visible on slide 2

- Text visible on slide 4

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.