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

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

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- 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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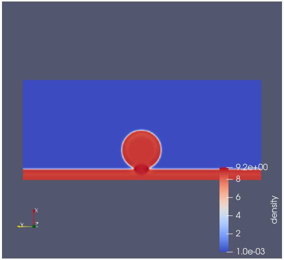
  - Surface wave
- DRY

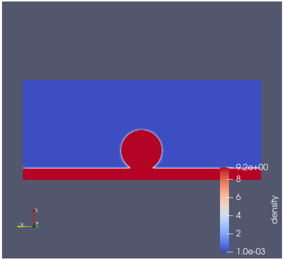
Cheng's paper

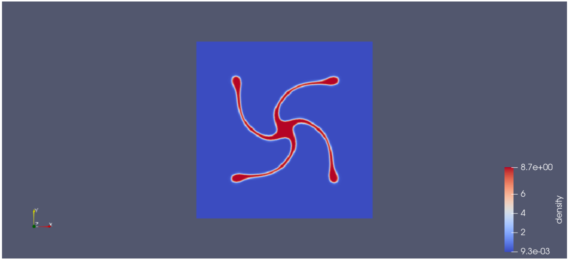
With these results we are able to:

- 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

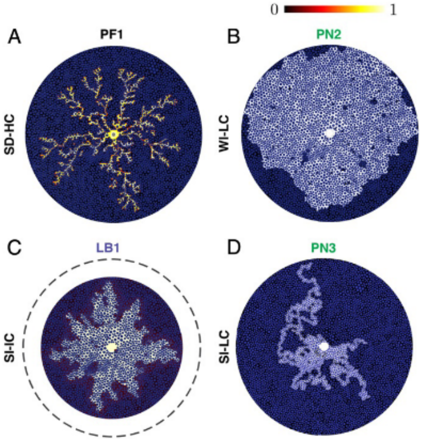


Fig. 3. Selection of simulated displacement patterns for the priority cases. (*A*) Strong drainage at high Ca (SD-HC) as simulated by a phase-field model. (*B*) Weak imbibition at low Ca (WI-LC) as simulated by a pore-network model. (*C*) Strong imbibition at intermediate Ca (SI-IC) as simulated by a 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 ~ 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.

Multiple phases in a single lattice

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?

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:

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

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

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

Macroscopic variables

Density and velocity are computed as follows:

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

Two important constitutive equations:

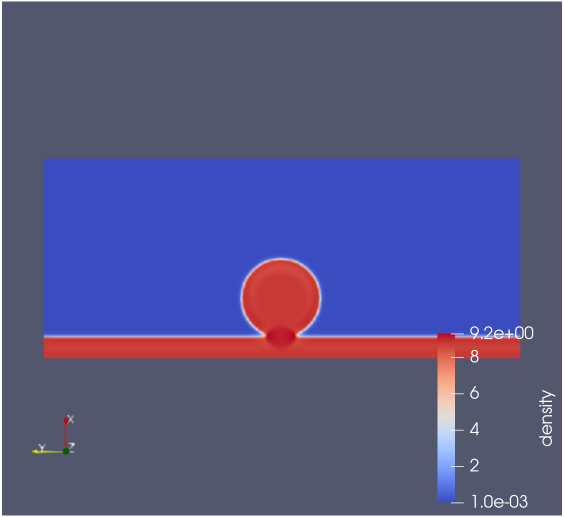
$$f_i^{\mathrm{eq}} = \rho\omega_i \left[1 + \frac{\vec{u}\cdot\vec{\mathbf{c}}_i}{c_s^2} + \frac{(\vec{u}\cdot\vec{\mathbf{c}}_i)^2}{2c_s^4} - \frac{\vec{u}\cdot\vec{u}}{2c_s^2}\right]$$

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

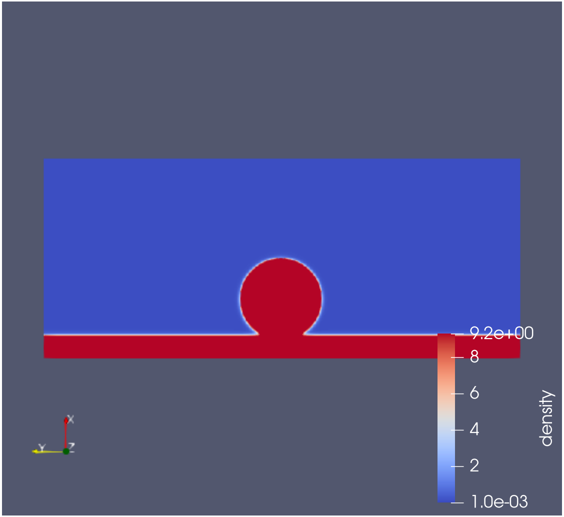
where $\mathbf{F}$ is defined in the multiphase problem, as the Shan Cheng force:

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

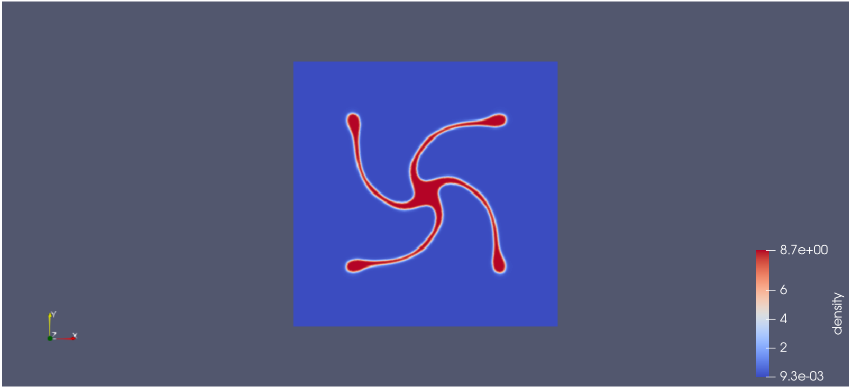
Droplet impacting on a surface - Immiscible



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?

CVs: Hillmert and Felipe. Upgrading paper.

Report Oct 14 - 2021

Main discussion points:

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

Courses

Code state

- 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.

Code state

- 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

Code state

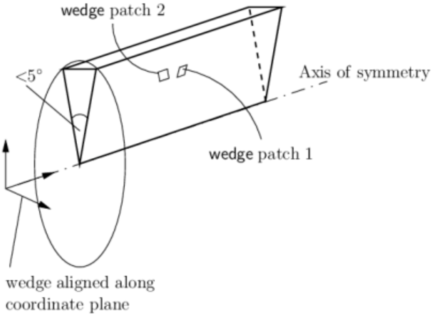


Figure 4.3: Axi-symmetric geometry using the *wedge* patch type.

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

- Validate first the channel case

Report Oct 28 - 2021

Main discussion points:

- Courses
- Spring courses / CS Minor
- Code state
- Generalities

Courses

- Adv. Programming: Exam next week.
- Data mining: Final project in two weeks.
- Stat. Thermo: Towards molecular dynamics.
- Found. Fluids M.: I started to go again this week.

Spring Courses

- PNG 501 - Flow in Porous Media - Yashar Mehmani
- PNG 520 - Thermodynamics of Hydrocarbon Fluids - Luis Ayala
- PNG 518 - Design of Miscible Recovery Projects.
- EME 521 - Mathematical Modeling of Energy and Mineral Systems - Derek Elsworth

CS Minor

CS Minor Website

Requirements:

- Research Doctorate, the doctoral minor requires a total of 15 credits with at least 6 credits at the 500-level. These 15 credits must be in addition to the credits applied towards the major Ph.D. program, i.e. they cannot be double-counted.
- While courses offered by the student's graduate major program cannot be used to satisfy the minor requirements, up to 6 (M.S.) /9 (Ph.D.) credits may be courses cross listed with the student's graduate major program, provided the student registers for the cross-listed section of the course (not the graduate major section of the course).
- Ph.D. students pursuing the Minor also need to have a CSCI faculty member on their Ph.D. committee.

CS Minor

I already took 6 credits. Next semester options:

- AERSP 524 - Turbulence and Applications to CFD: DNS and LES - Xiang Yang
- STAT 515 - Stochastic Processes and Monte Carlo Methods - Bharath Kumar Sriperumbudur

Code state

The code is now in a beta version, where different runs can be performed varying: domain, BCs, basic LBM, some thermodynamic coupling with LBM (to be tested). Results to be validated soon: channel flow. Already running. I haven't validated.
Main difficulty now: how to impose BCs to corner nodes.

Not related to PSU:

The rebuttal to Fuel was sent.
Received email from Juan Manuel. Invited me to do a presentation on any Saturday to his students.

Actions

- Look for EME 521 Lectures
- Late registration email
- Plan: Minor (15) + PhD (12 course+12 res) = 39 credits
  - FA 21: 9 cd. in courses (minor) + 3 cd. in research (late)
  - SP 22: 12 cd. in courses from EME (ready for QUAL)
  - FA 22: 6 cd. in clases (minor) + 3 cd. in research
  - SP 23: 6 cd. in research (Ready for COMP)
- Check Cheng's corner implementation and validate against tutorial

Report Nov 4 - 2021

Main discussion points:

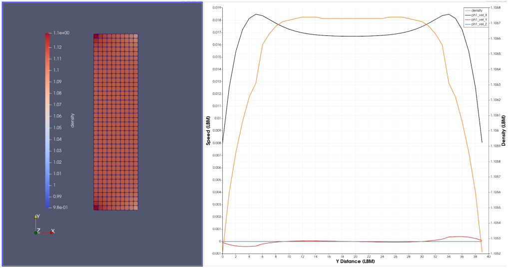
- Courses
- Code state
- Research collaboration

Courses

- Adv. Programming: Midterm done.
- Data mining: Final project in one weeks.
- Stat. Thermo: Midterm done. Kinetic theory called my attention to understand the connection with LBM or limitations (such as that Boltzmann proposed a collision operator more complex than BGK. How it relates to MRT?). Kruger's book mention that LBM can handle incompressible NS, but I haven't read it in detail.
- Found. Fluids M: Reference for analytical solutions.

I realized that Cheng handles the boundary conditions at corners depending on the application. See diagrams I draw.

The corners were corrected, but something is missing that makes the density to diverge. I had to implement forcing schemes, as the channel works with imposed force.



Missing: periodic boundary conditions, which Cheng uses in channel. Scaling for the basic LBM.

Code state

What I still have to understand better before implementation:

- Should we use the concept of phase inside the code? Two components with different f_i, should they move at the same bulk velocity? I think so, but which density should enter to calculate f^{eq}? Never two components move at different $\vec{u}$? If they move together, force correction must use total force.
- Viscosity-time relationship, constant for all components (phases?)
- I recall that some simulations have different weighting factors for the force. What should we implement?
- Mastering Chapman-Enskog will be the key to understand consequences of each approach.

Research collaboration

Physics

- Single component with customized EoS (Xenon)
- Solid attraction (no fixed density, depends on local values and thermodynamics. Solid can not ask for more than is available)

Computational implications:

- 3D model. Currently, the code has a 70% 3D implementation
- What are the geometries of the experiment and its boundary conditions?
- Include simple validation cases in 3D (No surface tension)

We receive data for validation, but, what are we validating/representing? How can we give back? What I propose to do next:

- Rethink the scaling for generalized $\Delta x, \Delta t$
- Establish the main dimensionless numbers for experiments and suggest a scaling procedure

Actions

Present

Present...

Report XXX XX - 202X

Main discussion points:

- Topic 1
- Topic 2

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Sample frame title

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- Text visible on slide 2

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- 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.