PhD in Energy and Mineral Engineering at PSU

Nicolás's Research - Reports

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Table of Contents

Table of Contents

Report Jan 24 - 2022

Main discussion points:

- Cheng's paper
- LBM Code state
- Short-term Medium-term objectives

Cheng's paper

Bulk equation for the Shan-Chen force:

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

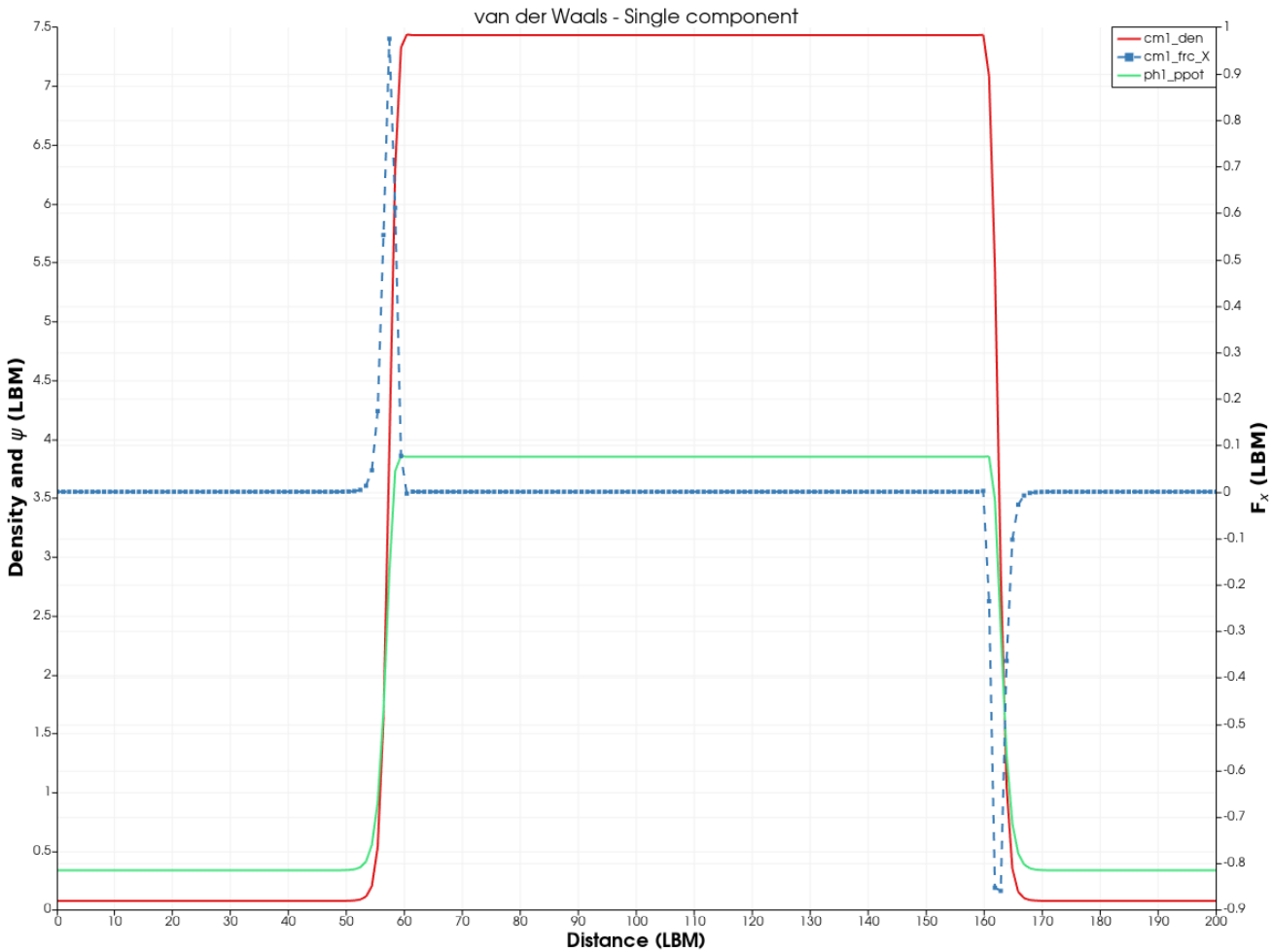
- MRT model
- Multi-component partially miscible

LBM state

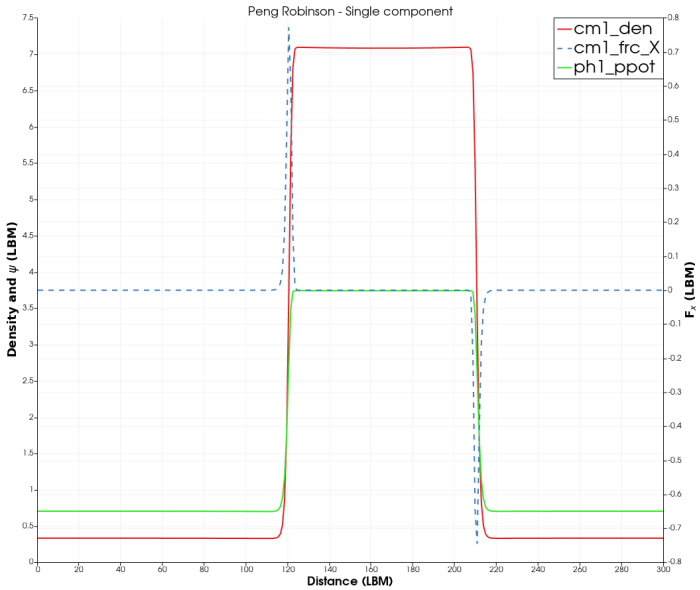
This I advanced before last state:

- Tried the binary printing (unsuccessful)
- Run the single component multi-phase model (successful)
- Equation to count the number of molecules in a lattice.
- Short-term mid-term objectives

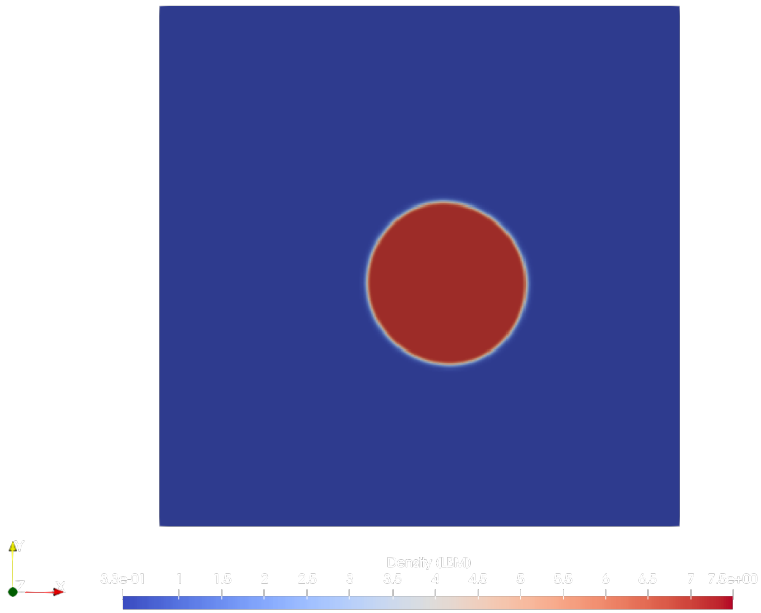
van der Waals validation



Peng Robinson validation



Figure



Where I am going?

I was rediscovering the concept of ψ that now belongs to the bulk (phase) entity. In Kruger's book is assigned to each component, so each components computes its own SC force. Other forces split according to ρ_i.
Two components structure is ready to start building the 2-component case that Cheng uses for validation.

Actions

- Dry-run of research proposal for qualifying exam.Deep dive into literature looking for problems in current problems and interesting applications (reactions-solute transport-energy-multiphase).
- LBM tutorials is the next short-term project
- Finish my own code to run the Cheng's cases in our simulator.
- Long-term: evaluate the Kruger's perspective of calculating SC per component.

Report Jan 31 - 2022

- Code and Cheng's paper
- SPH for EME 521
- Time demand
- Others
  - Dr. Mehmani meetings (I'll start slow).
  - Summer 2022
  - Almost null offer research-related. Italian courses.
  - STAP (Summer Tuition Assistance Program)
  - Penn State Vita (Taxes)
  - 2022 Fuel Science Graduate Awards
  - Own website
- Lost.

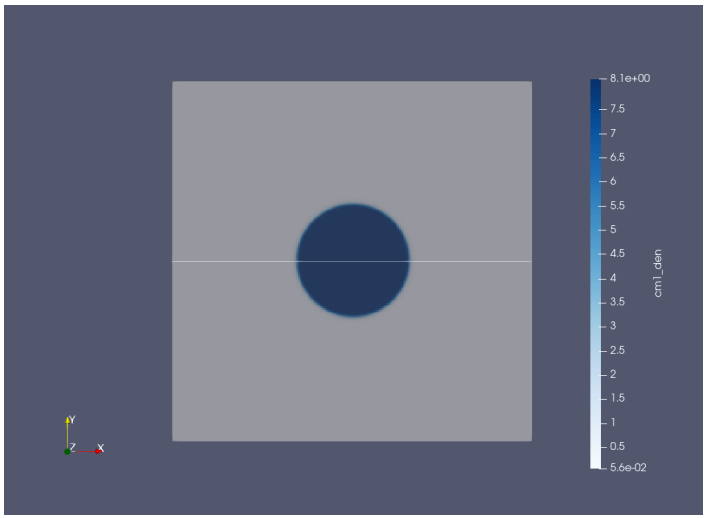
Code

Multiphase validations: van der Waals (flat interface, droplet), Peng-Robinson (making use of velocity redefinition and β parameter).
Cheng redefined the velocity for the Guo's scheme as:

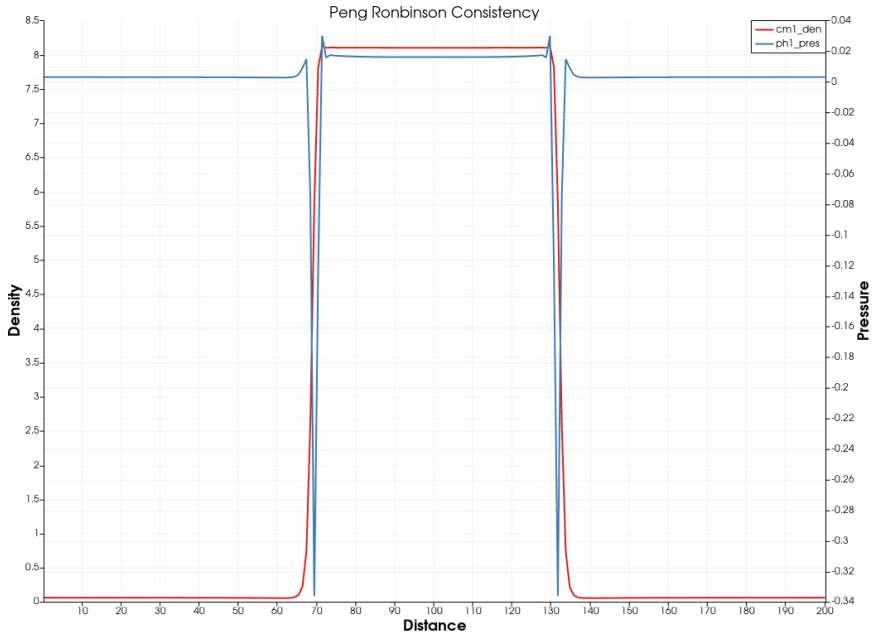
$$\mathbf{u}^{mod} = \mathbf{u} + \frac{\beta \mathbf{F}}{(\tau - 0.5)\psi^2} \tag{1}$$

The other velocity definitions remain. Without this term, the PR case diverges. Also G affects stability.

Code - Peng Robinson validation



Figure



Code - New features

- Now we can have N_F forces of different nature. All are grouped and discretized in the velocity space together.
- We have now a new force to compute ψ^i and thus calculate a force per component.
- Each component relaxes with its own τ^i, allowing different viscosities.
- Reading density/pressure fields for every component, and a common velocity field.

Current problems:

- Force only working for periodic BC.
- Still not implemented the force fluid/solid
- Instability (due to BGK)

Code

- Can the pressure of the gas be higher than the liquid? What if we initialize a bubble instead of a droplet?
- Validate Young-Laplace?
- I am now setting a 2C 2P problem to validate the code. I can try both, immiscible and miscible, as both implementations are there and the only change is the ψ definition.
- Injecting A into a system full of B. How does it look like?
- What 1C complex systems can we simulate? Water hammer effect?

Ready for meeting with Pr. Orlando for program. language discussions, questions about implementations, and possible feedback (I need the time to compile the material).

PBM: RR procedure. I'll program the minimization algorithm, but try to implement Eigen, a library to solve $\mathbf{A} \cdot \mathbf{x} = \mathbf{b}$.

Research

I definitely want to use my research for applying the LBM to a particular field. In contrast, my Master's Thesis was only computational, with validations, but did not include any experimental/real data of any type. Questions I have:

- Bubbles, coalescence, and their viscosity effect
- CO_2 plume generation.
- Interaction between fluids and rock (swelling, mineralization, adsorption)
- Rock deformation? Does imply FEM? Too complicated?
- Questions about σ in 3-P systems. I don't know? Nobody knows? Film drainage. Oil spills. Receding / advancing θ
- Can we derive a k_r label-blind with hysteresis, based on 3P simulations?

Actions

- Yes, start learning SPH.
- Look for internships in companies and research labs in the US. In Summer, if nothing appears, we will focus on research. Do not lose contacts and willingness to participate in new things.
- Apply to Fuel Award and Nico SPE Awards
- Go for MRT. Write equations. Pr. Orlando presentation. Think in 2C cases that validates our understanding. 2 non interacting components (miscible). Then partially miscible.
- Bubbles as an interesting topic to work with in LBM. There may be other options.

Discussion

Discussion...

Meeting with LBM questions

Questions:

- LBM Formulation
  - Are the equations molar/mass based? Which one should it be for efficiency?
- Boundary conditions
  - Composition for pressure BC at outlet or inlet

Discussion

Discussion...

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Report XXX XX - 202X

Main discussion points:

- Topic 1
- Topic 2

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Sample frame title

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Remark

Sample text

Important theorem

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Examples

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Two-column slide

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$$E = mc^2$$

- First item
- Second item

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