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

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Table of Contents

- **1** Spring 2022
 - Report Jan 24 2022
 - Report Jan 31 2022
 - \bullet Meeting with LBM questions
 - template

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 - \bullet Report Jan 24 2022
 - Report Jan 31 2022
 - \bullet Meeting with LBM questions
 - template

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:

$$\mathbf{F} = -G\psi(x)\sum_{i}\omega_{i}\psi(x+\mathbf{c}_{i}\delta t)\mathbf{c}_{i} \quad \psi := \sqrt{\frac{2(P^{\text{EoS}} - c_{s}^{2}\rho)}{G\delta tc_{s}^{2}}}$$

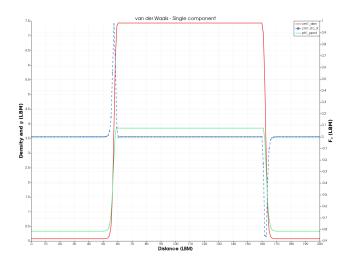
- MRT model
- Multi-component partially miscible

LBM state

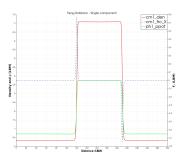
This I advanced before last state:

- 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

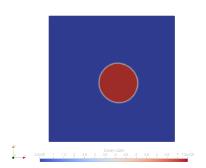
van der Waals validation



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.

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.

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

Code - 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
- CO₂ 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

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

Present

Present...

template

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- A

Report XXX XX - 202X

Main discussion points:

- Topic 1
- Topic 2

21 / 27

23 / 27

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- Text visible on slides 3

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- Text visible on slide 4

In this slide

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

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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