

# PhD in Energy and Mineral Engineering at PSU

## Nicolás's Research - Reports

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**PennState**  
College of Earth  
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## 1 Spring 2022

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## Report Jan 24 - 2022

Main discussion points:

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

Bulk equation for the Shan-Chen force:

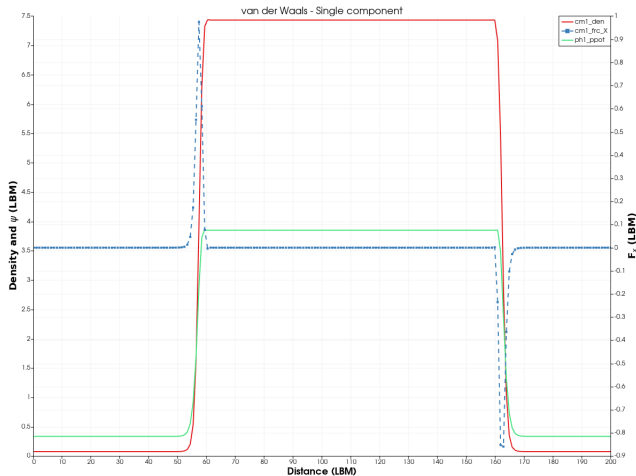
$$\mathbf{F} = -G\psi(x) \sum_i \omega_i \psi(x + \mathbf{c}_i \delta t) \mathbf{c}_i \quad \psi := \sqrt{\frac{2(P^{\text{EoS}} - c_s^2 \rho)}{G\delta t c_s^2}}$$

- MRT model
- Multi-component partially miscible

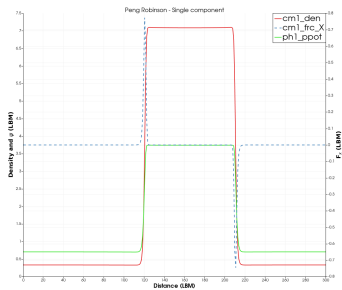
This I advanced before last state:

- 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

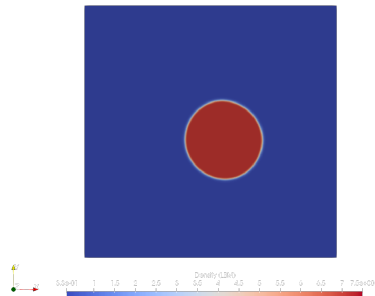
# van der Waals validation



# Peng Robinson validation



Figure





# Where I am going?

I was rediscovering the concept of  $\psi$  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  $\rho_i$ . Two components structure is ready to start building the 2-component case that Cheng uses for validation.

- 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

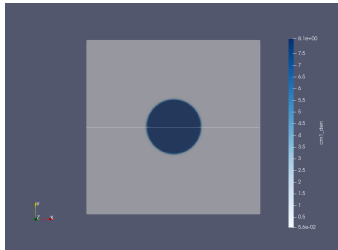
- Code and Cheng's paper
- SPH for EME 521
- Time demand
- Others
  - Dr. Mehmani meetings (I'll start slow).
  - Summer 2022
  - Almost null offer research-related. Italian courses.
  - STAP (Summer Tuition Assistance Program)
  - Penn State Vita (Taxes)
  - 2022 Fuel Science Graduate Awards
  - Own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

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

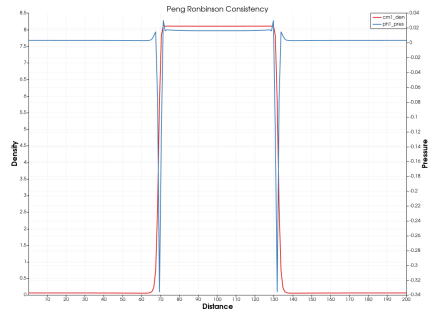
$$\mathbf{u}^{mod} = \mathbf{u} + \frac{\beta \mathbf{F}}{(\tau - 0.5)\psi^2} \quad (1)$$

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  $\psi^i$  and thus calculate a force per component.
- Each component relaxes with its own  $\tau^i$ , 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)

- 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  $\psi$  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  $\mathbf{A} \cdot \mathbf{x} = \mathbf{b}$ .

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<sub>2</sub> plume generation.
- Interaction between fluids and rock (swelling, mineralization, adsorption)
- Rock deformation? Does imply FEM? Too complicated?
- Questions about  $\sigma$  in 3-P systems. I don't know? Nobody knows? Film drainage. Oil spills. Receding / advancing  $\theta$
- Can we derive a  $k_r$  label-blind with hysteresis, based on 3P simulations?



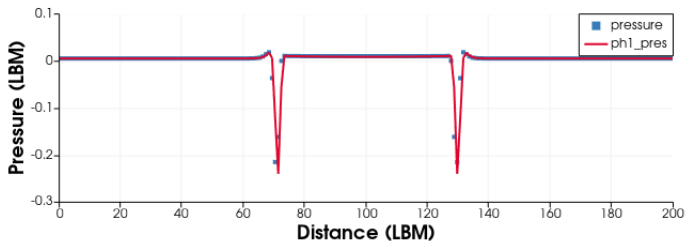
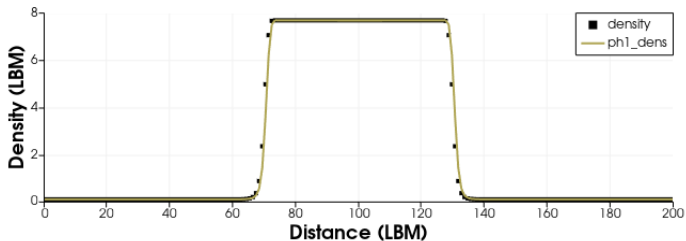
- Yes, start learning SPH.
- Look for internships in companies and research labs in the US. In Summer, if nothing appears, we will focus on research. Do not lose contacts and willingness to participate in new things.
- Apply to Fuel Award and Nico SPE Awards
- Go for MRT. Write equations. Pr. Orlando 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...

## Report Feb 7 - 2022

- Cheng's coding error in modified velocity.
- MRT implementation. Facts and difficulties:
  - Vectorized implementation. Still have problems with  $\mathbf{m}^{\text{eq}}$ . Works only in manual computing.
  - More validation cases. I only picked one.
  - Recent result: yesterday.
- Peng Robinson inconsistency: I have to revisit the PR results with BGK. I think it may be converging to densities slightly away from equilibrium.
- Dr. Mehmani suggestions.

# MRT Validation

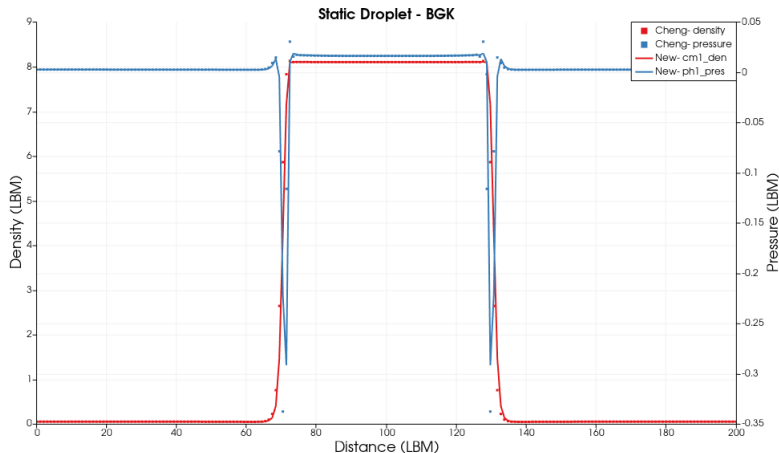


- Prepare meeting with Cheng: velocity modification, and MRT parameters. Source of validation.
- Trace a path for validation: Oscillating droplet, tube oscillation.
- Reading CO<sub>2</sub> with oil trapping and water different mechanisms and modeling.
- Share code.

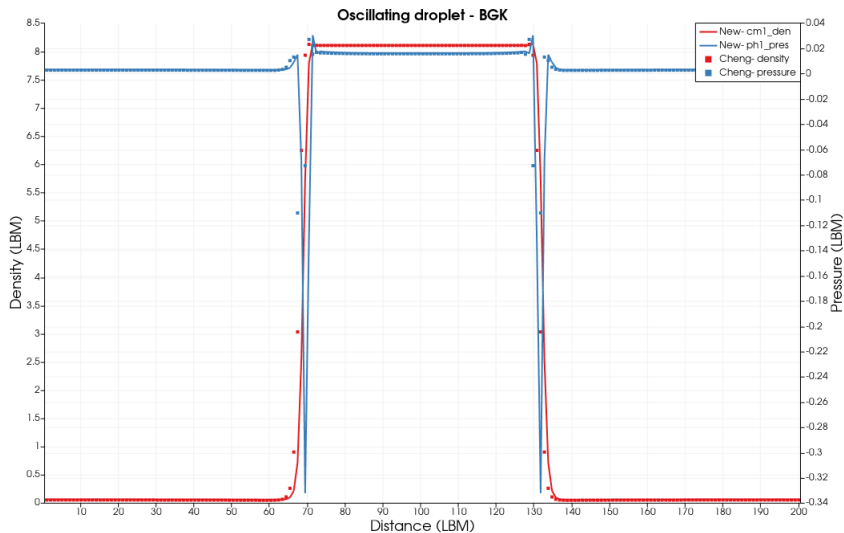
## Report Feb 7 - 2022

- BGK and MRT validations
  - Several cases tested: see the LBM private document
  - How to set fluid viscosity with MRT?
  - I had to change Cheng's diffuse width.
- Dr. Mehmani suggestions.
- Questions
  - Point-distributed parameter and point-centered (?) parameter
  - Fluid in tension LBM?
  - Motivation. Self-propulsion, drop collision, microemulsions: link to Youtube

# BGK Validation - Cheng's code

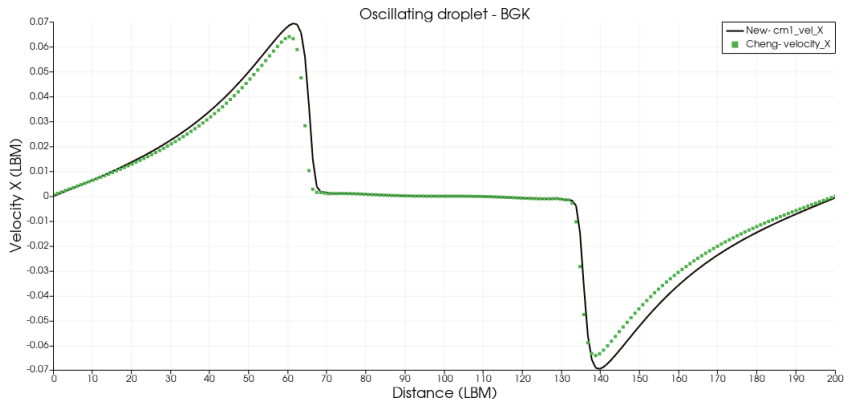


# BGK Validation - Cheng's code

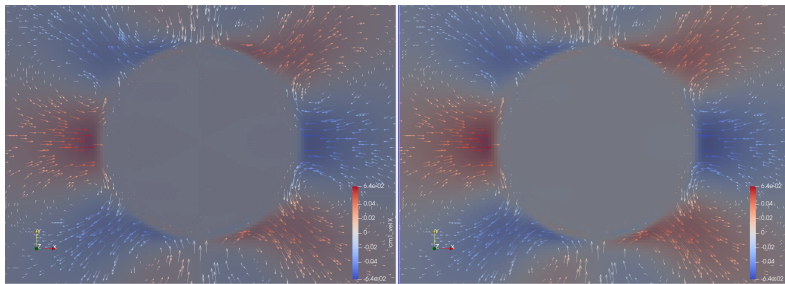




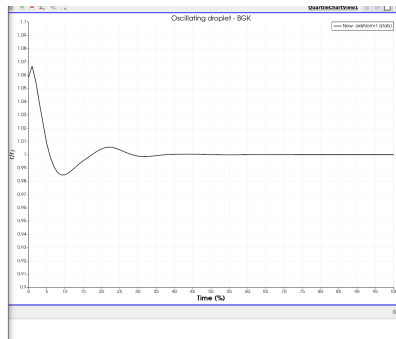
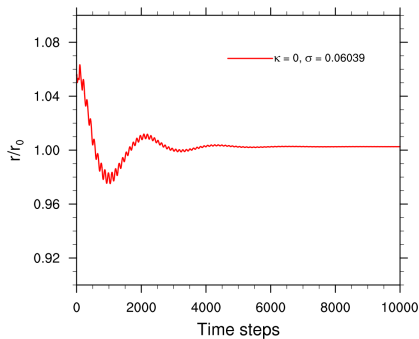
# BGK Validation - Cheng's code



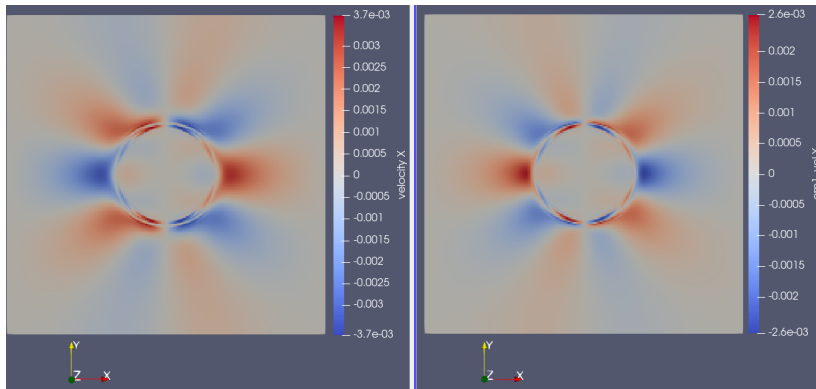
# BGK Validation - Cheng's code



# BGK Validation - Cheng's code

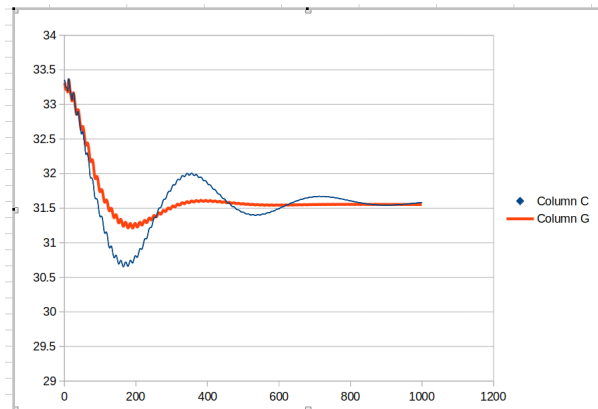


# MRT Validation - Cheng's code



# MRT Validation - Cheng's code

Attached video.



# For analytical solutions

- How to convert a single component droplet surrounded by its vapor, to a droplet surrounded by empty space? Is the frequency of the oscillation the same in both cases.
- Analytical solutions and reported cases:
  - Oscillating droplet
  - Rising bubble (very interesting!)
  - Square drop as IC
  - Rayleigh-Taylor instability (heavy fluid supported against gravity)
  - Induced translation by Marangoni-effect (variable  $\sigma$  field)
  - Bubble break-up due to variable  $\sigma$  field

# Actions



# Meeting with LBM questions

## Main topics

- Short questions:
  - Molar/mass formulation. Which one should be used for efficiency?
- Boundary conditions
  - Mass increasing when imposing velocity/outflow.
  - Over-constraining for fixed  $P$  and  $\mathbf{u}$  at the same boundary.
  - Outflow boundary conditions. Assumptions and implications.
  - General treatment for corners
  - Composition for pressure BC at outlet or inlet
  - Pseudopotential per component



Discussion...

**a**

• A

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Discussion...

## Report XXX XX - 202X

Main discussion points:

- Topic 1
- Topic 2









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In this slide  
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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

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## Examples

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$$E = mc^2$$

- First item
- Second item

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