PhD in Energy and Mineral Engineering at PSU

Nicolás's Research - Reports

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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:

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

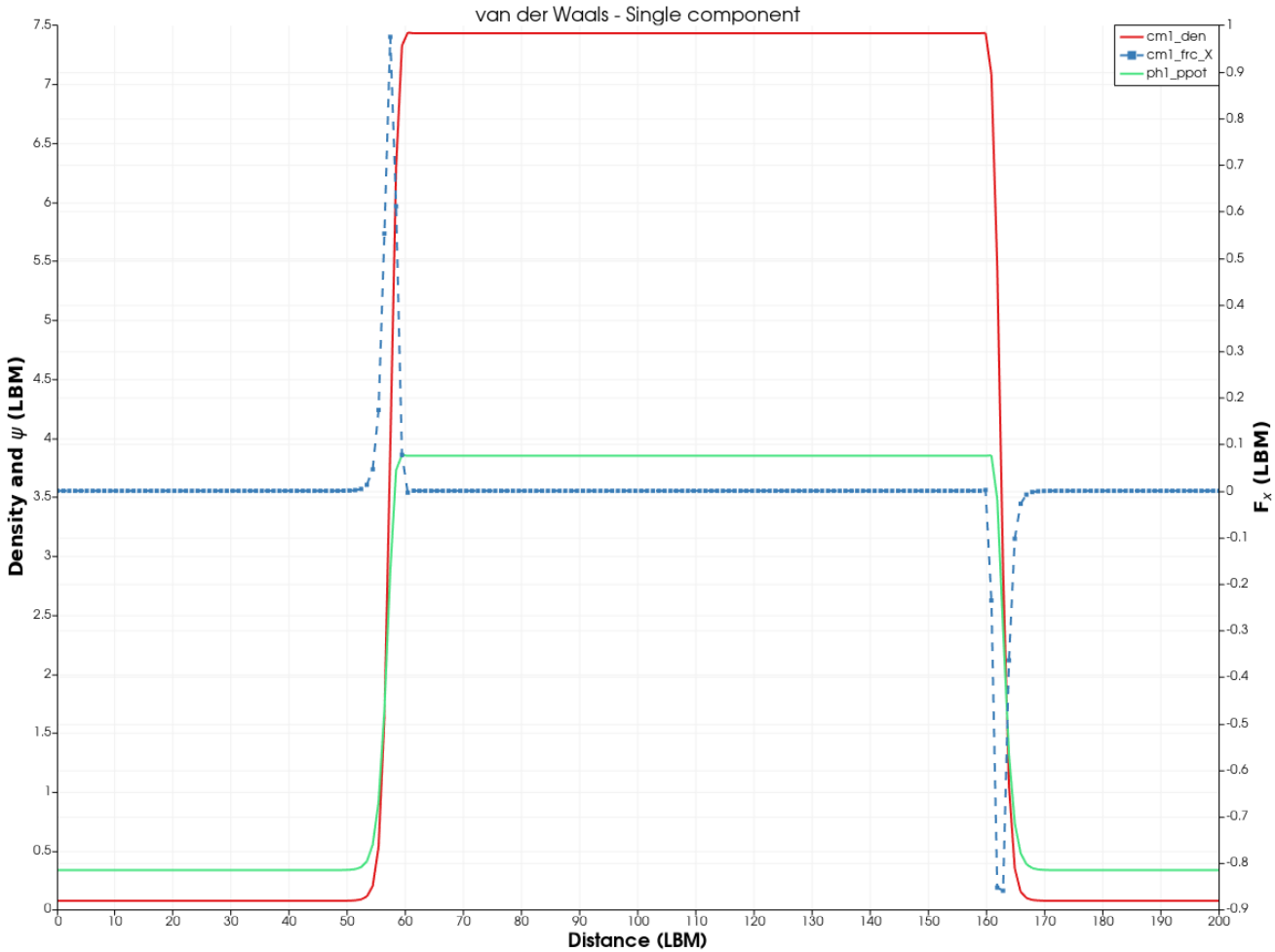
- MRT model
- Multi-component partially miscible

LBM state

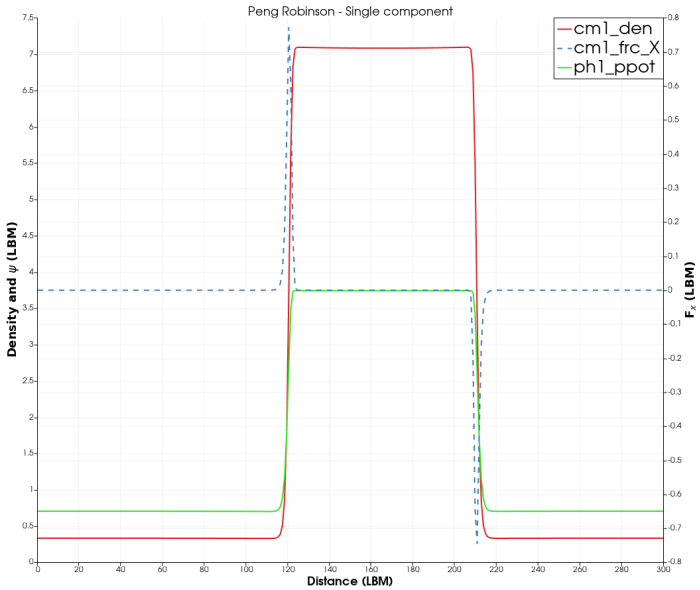
This I advanced before last state:

- 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

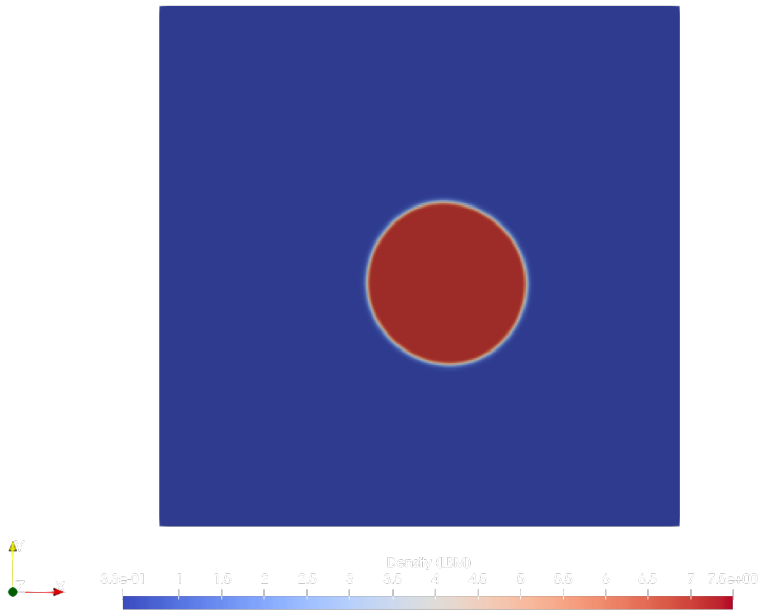
van der Waals validation



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.

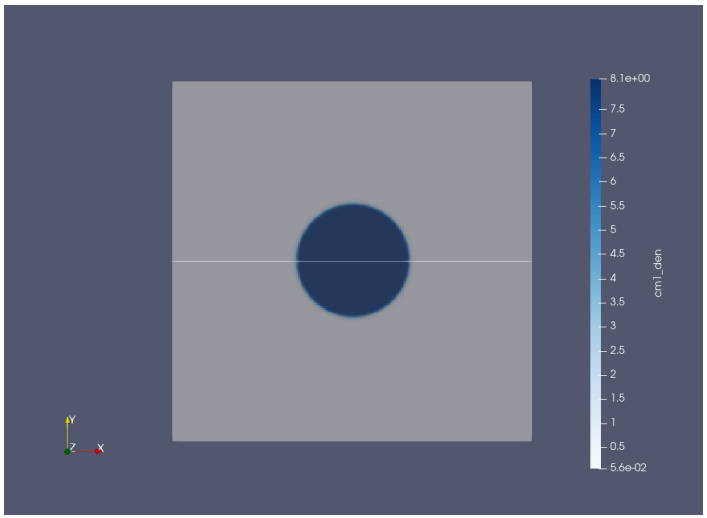
Code

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:

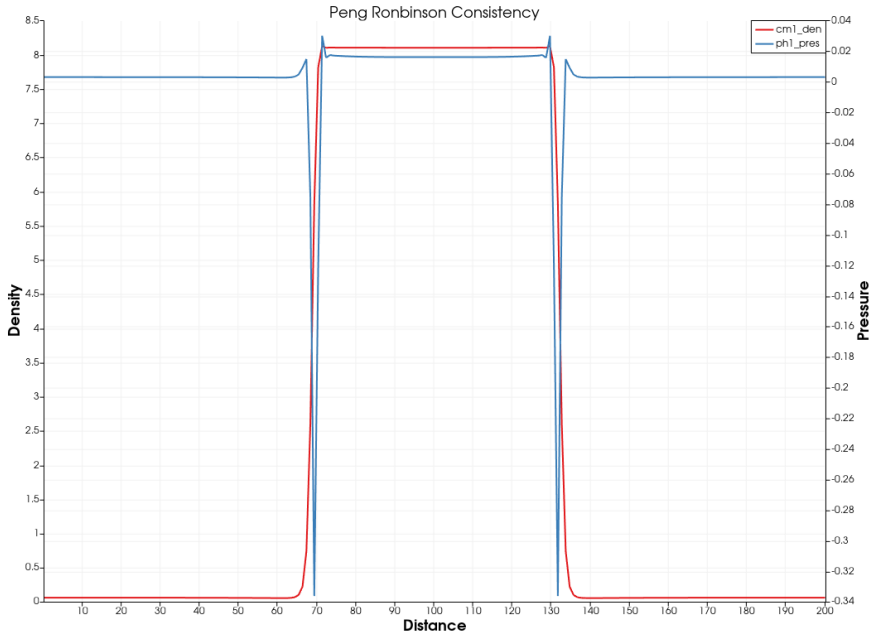
$$\mathbf{u}^{mod} = \mathbf{u} + \frac{\beta \mathbf{F}}{(\tau - 0.5)\psi^2} \tag{1}$$

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.

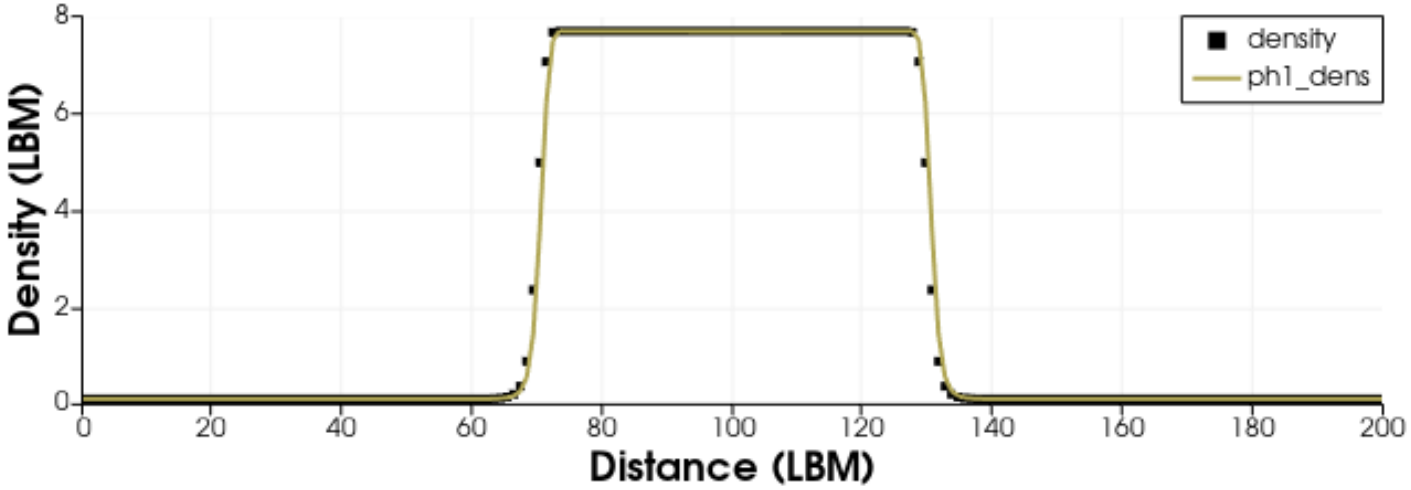
Discussion

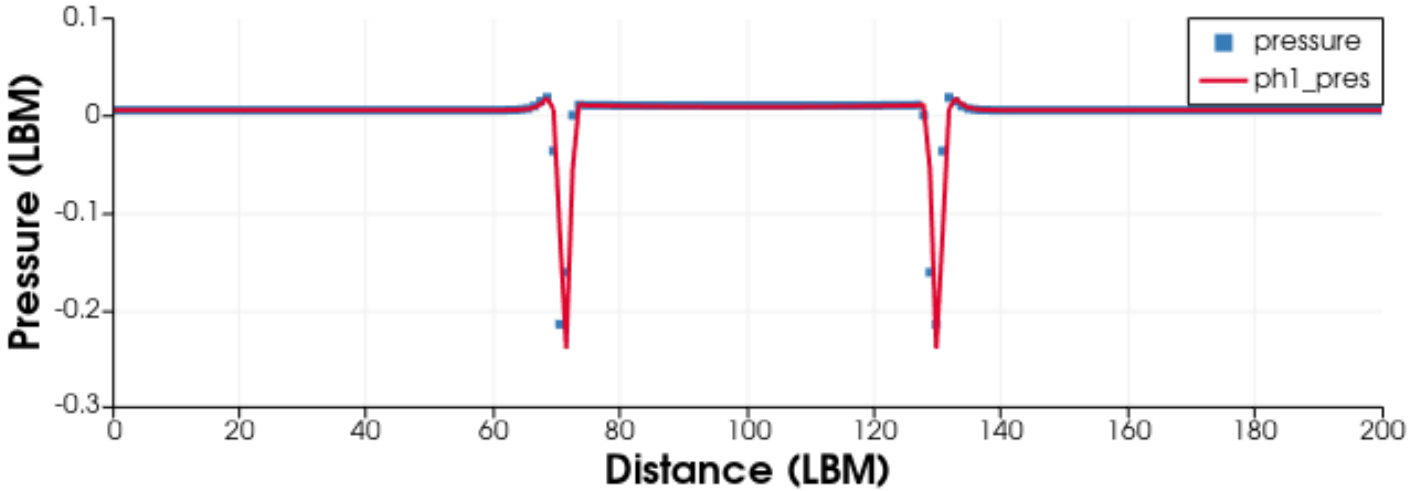
Discussion...

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 thing it may be converging to densities slightly away from equilibrium.
- Dr. Mehmani suggestions.

MRT Validation





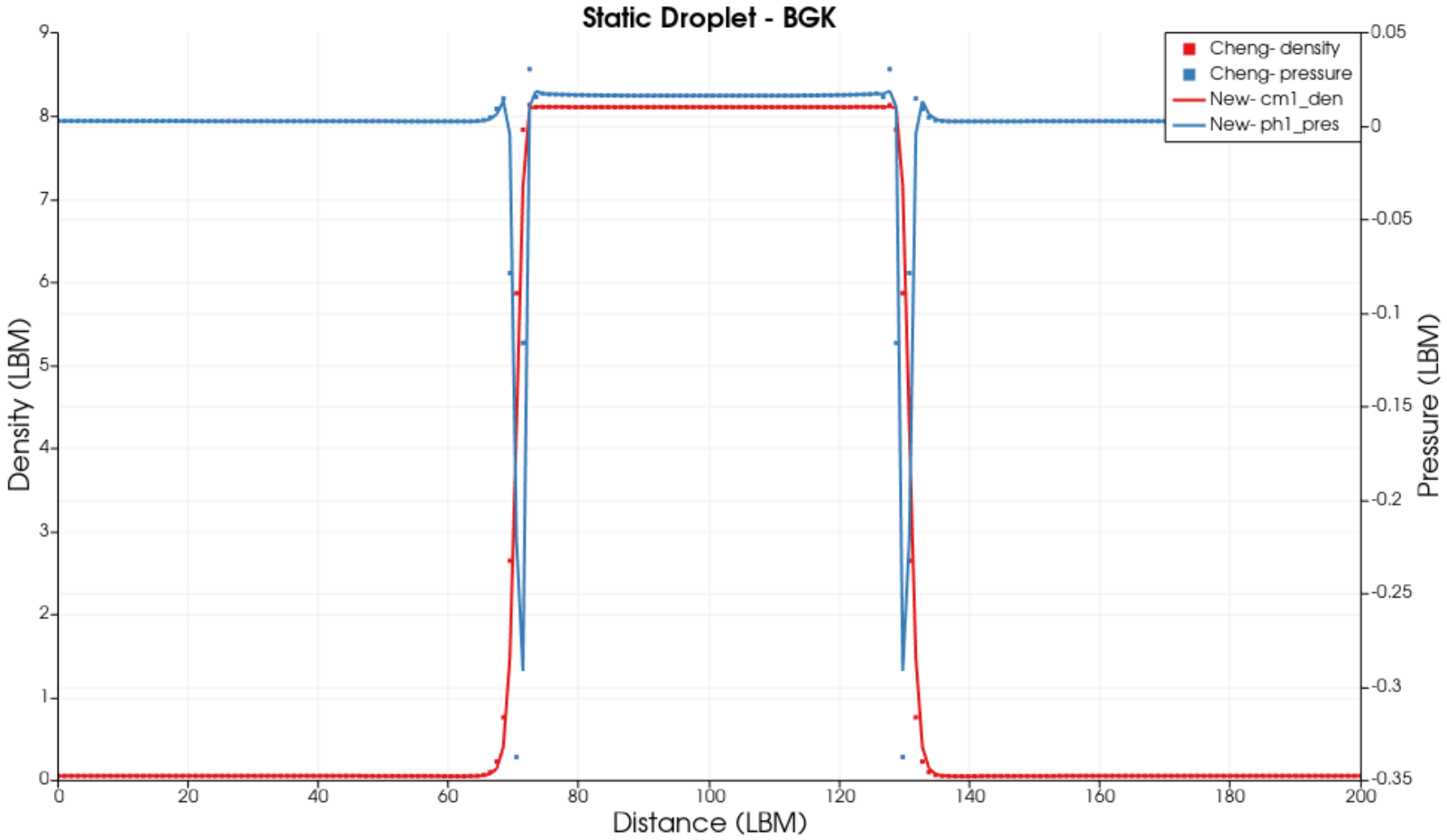
Actions

- Prepare meeting with Cheng: velocity modification, and MRT parameters. Source of validation.
- Trace a path for validation: Oscillating droplet, tube oscillation.
- Reading CO_2 with oil trapping and water different mechanisms and modeling.
- Share code.

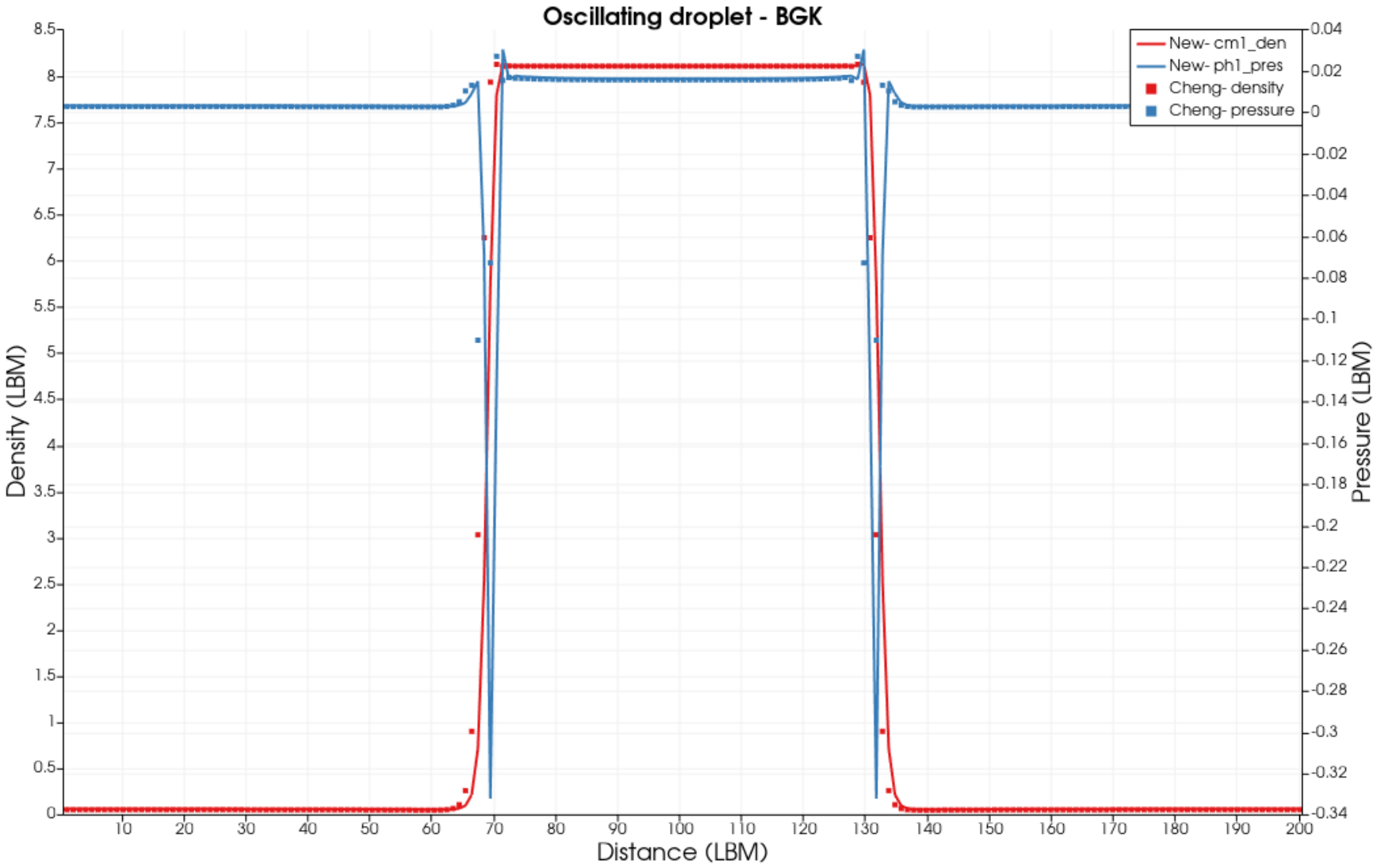
Report Feb 14 - 2022

- 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

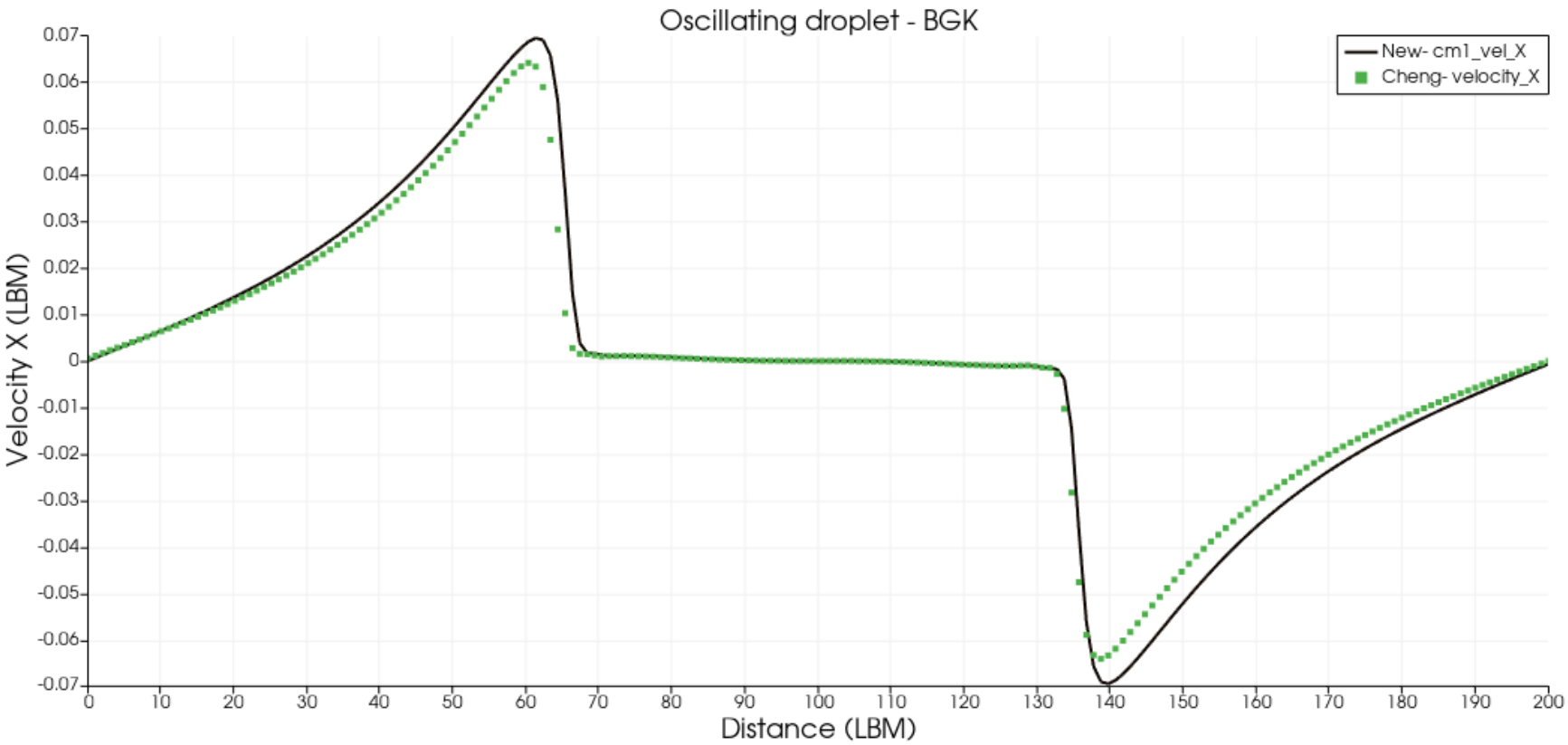
BGK Validation - Cheng's code



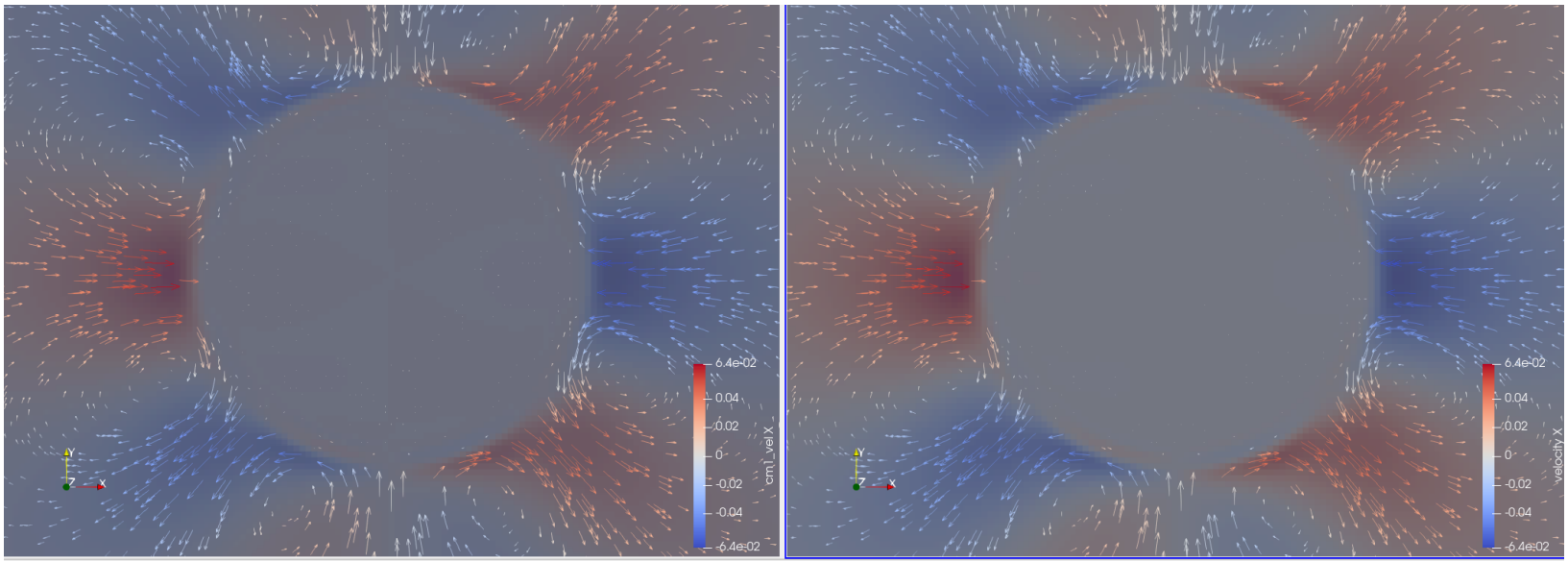
BGK Validation - Cheng's code



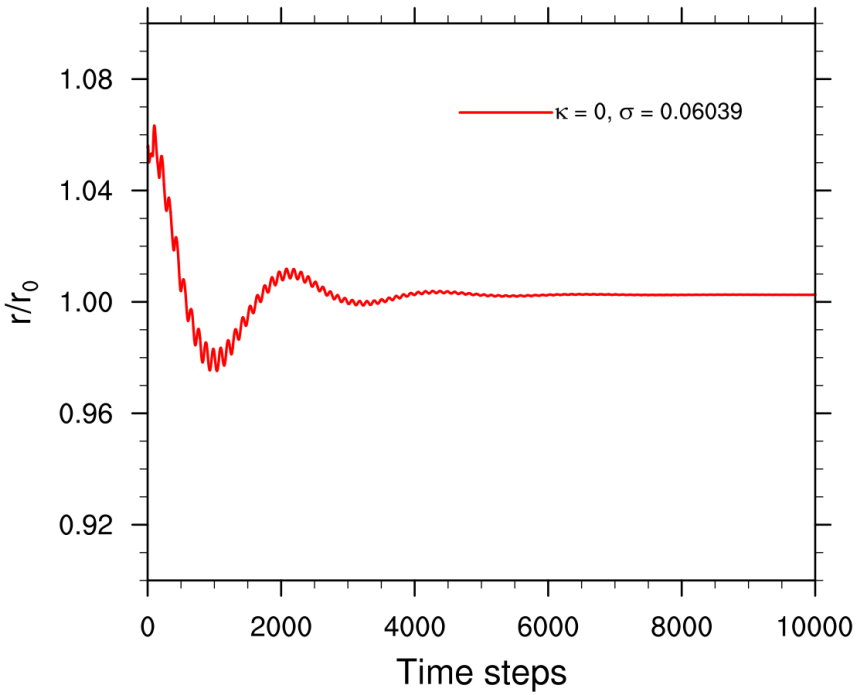
BGK Validation - Cheng's code

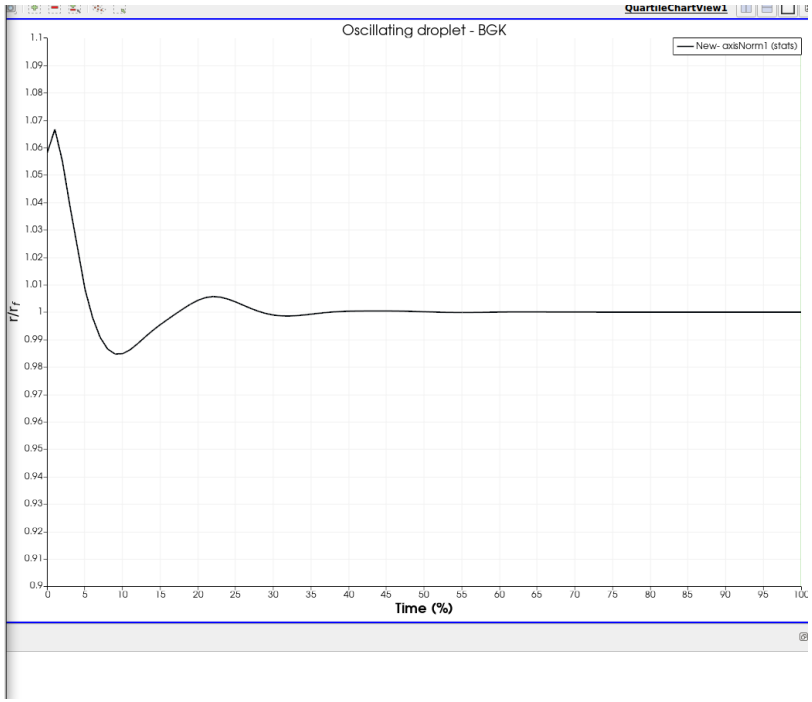


BGK Validation - Cheng's code

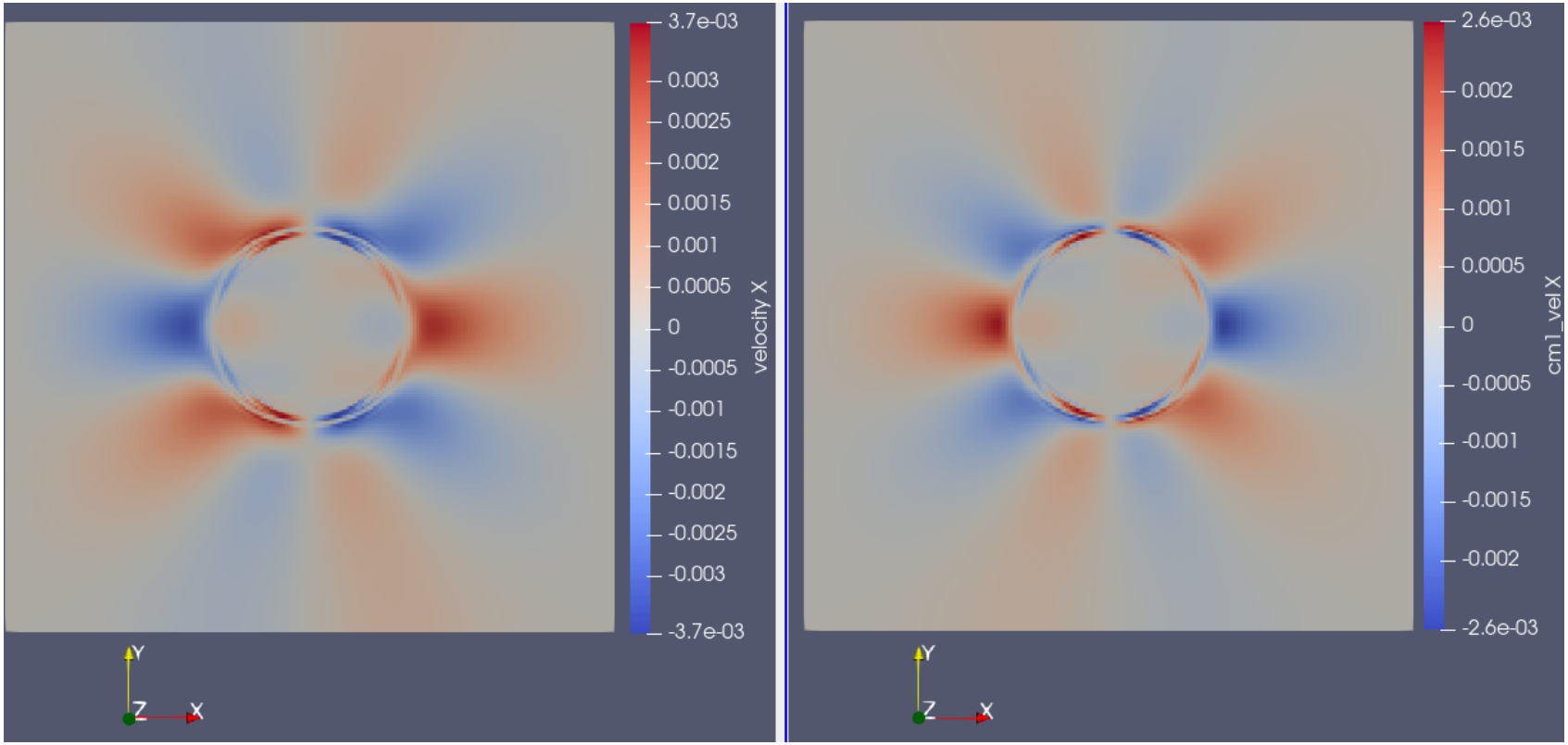


BGK Validation - Cheng's code



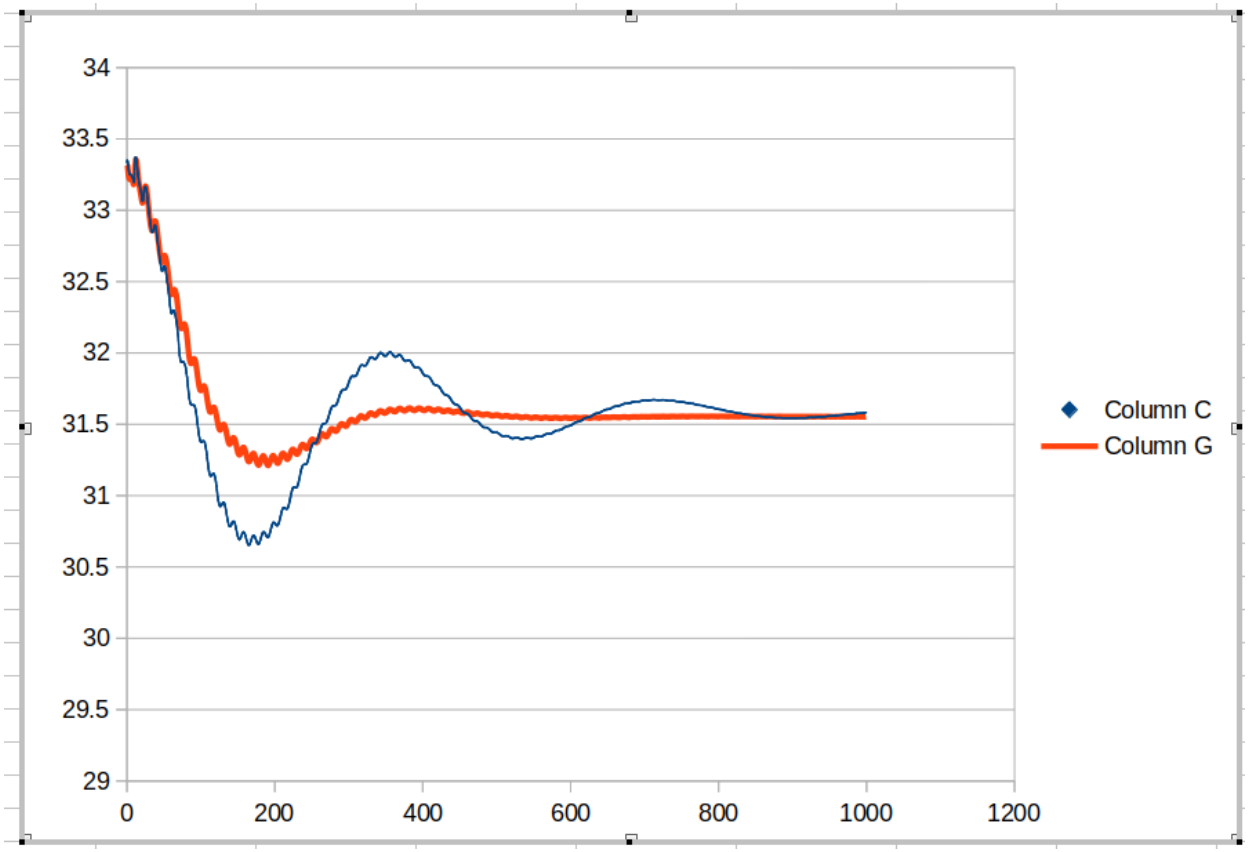


MRT Validation - Cheng's code



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 σ field)
  - Bubble break-up due to variable $\sigma field$

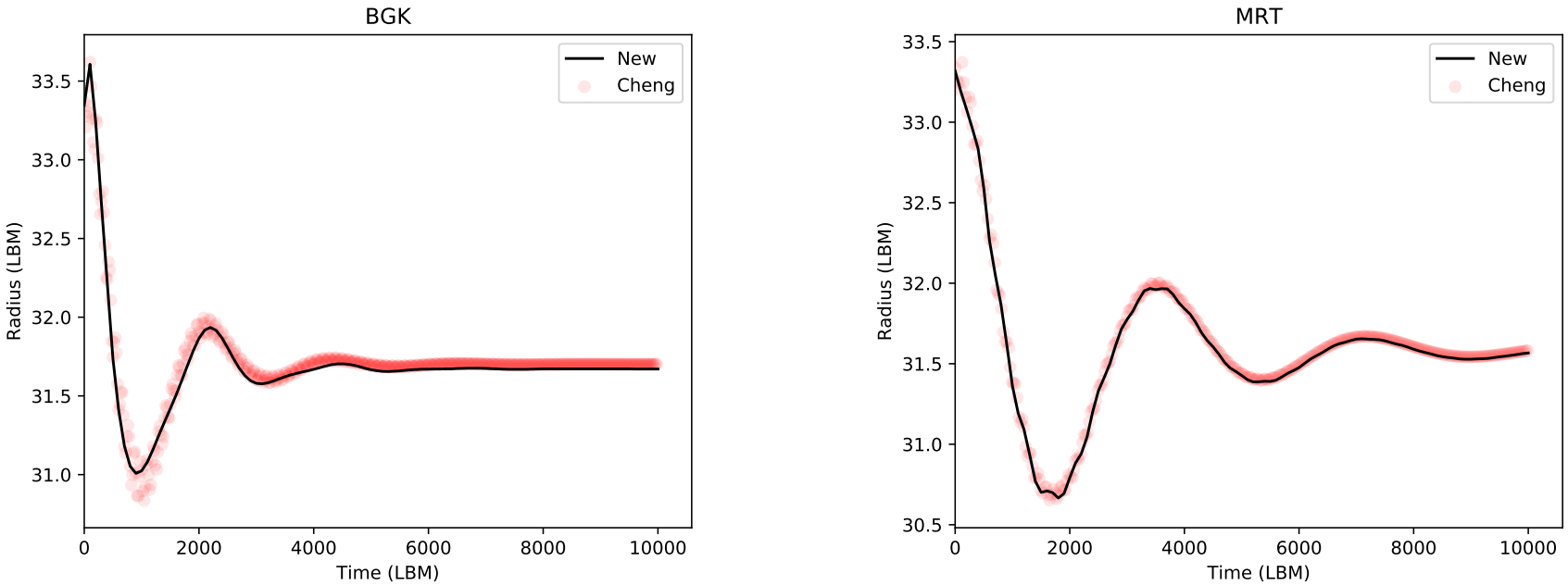
Actions

- Keep preparing Cheng's meeting
- Go back to BGK and compare oscillations
- Find differences with MRT for oscillating droplet
- Start reading LAMP reference and Cheng's reports to compare against analytical solution
- Go for the 2 components case

Report Feb 21 - 2022

- BGK and MRT validations
- Viscosity per phase-per component
- Rising droplet (video)
- Marangoni flow (papers based on Phase-Field and Free energy)
- Questions
  - Point-distributed parameter and point-centered (?) parameter
  - Fluid in tension LBM?
  - Motivation. Self-propulsion, drop collision, microemulsions: link to Youtube
- What to present in next meeting?

Oscillating droplet



(a) BGK

(b) MRT

Figure: Oscillation droplet case. Viscosities are different in each case.

Thursday meeting

- Motivation of new code
- Current validations
- Current status
- Questions about: boundary conditions, global density increase, dynamic validations:
  - Oscillating droplet (ready). For which conditions, an analytical solution exists? Droplet in void space?
  - Rayleigh-Taylor instability (oscillating capillary tube)
  - Rotating droplet (any analytical solution)

Actions

Weekly meeting - LBM

Feb 24 - 2022

- LBM Code - New version (motivation, state, and validation)
- Questions about the LBM formulation
- Paper (Dynamic validations)

LBM Code

Motivation:

- 3D version for arbitrary porous media and boundary conditions
- Parallelization
- Possible coupling with other transport equations

General description:Fortran 90 Object Oriented LBM code for multi-component (N_c) mixtures. Output in VTK format. Main classes:

- Components - Phase - Mixture - Equation of state
- LBM Functions (Parameters - Coll. Operators - Steps)
- Domain - Global Properties
- Forces - Boundaries

Desired simulation setup is given through input files (parameters, domain, initial conditions).

Validations

The main validation sources have been: analytical solutions, Cheng's codes, and a priori physics understanding (qualitatively).

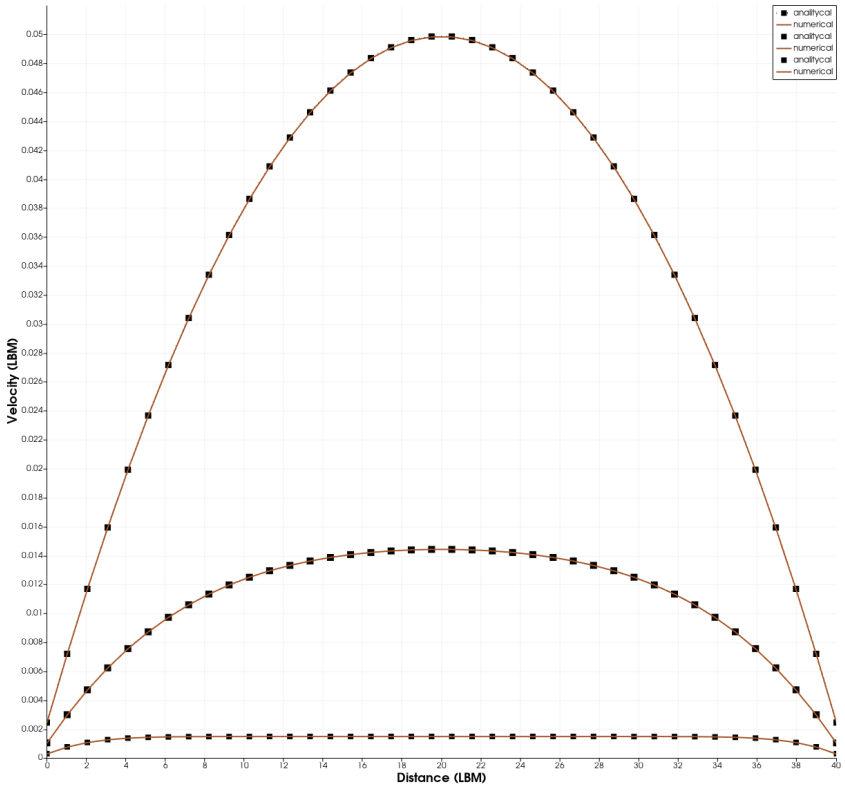
Single phase:

- Channel flow ($\mathbf{F}$ & ∇p-driven)
- Couette flow (plates)
- Cylinder (turbulent)
- Cavity flow
- Porous medium

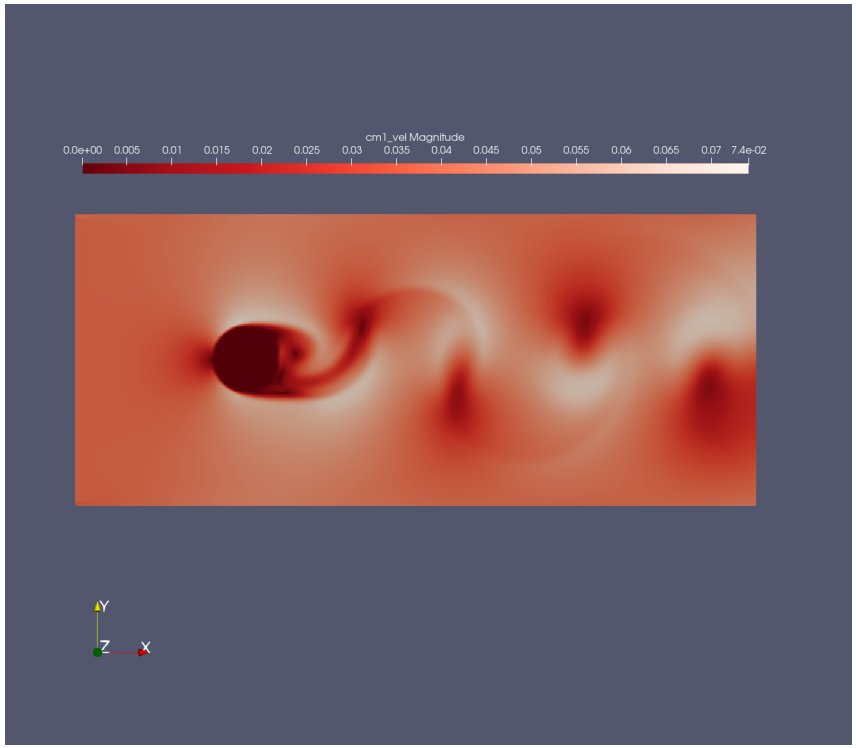
Multiphase:

- Static droplet
- Oscillation droplet
- Falling droplet

Single phase validations (quantitative)



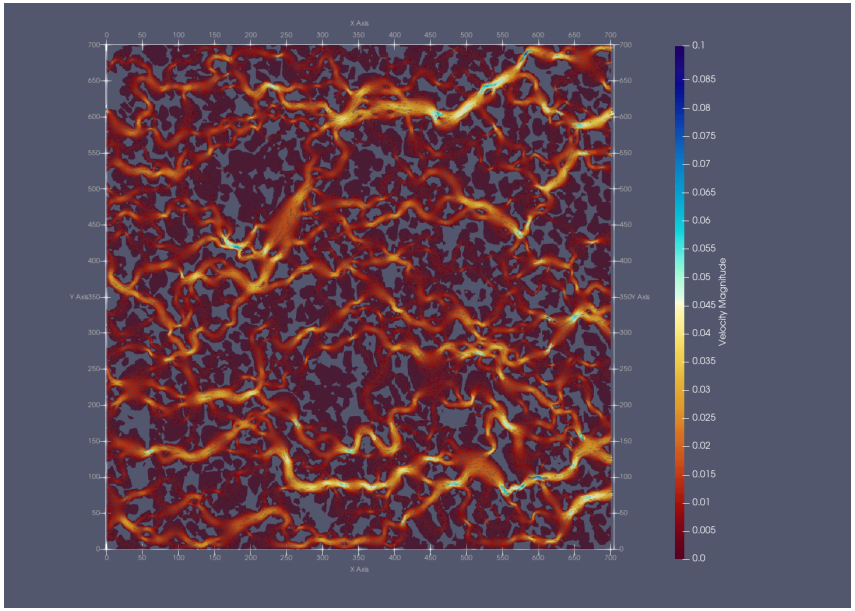
(a) **F**-driven channel flow



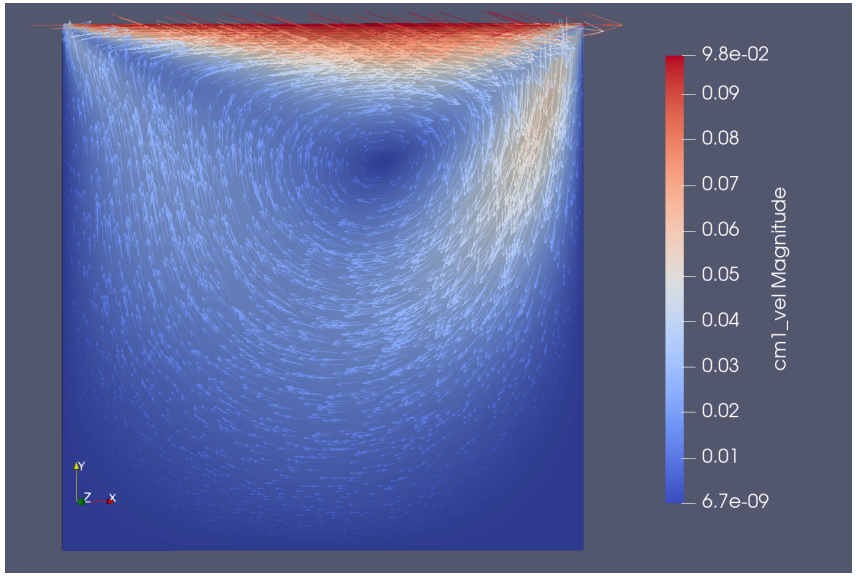
(b) Turbulent flow around cylinder

Figure: Results with direct source for quantitative comparisons.

Single phase validations (qualitative)



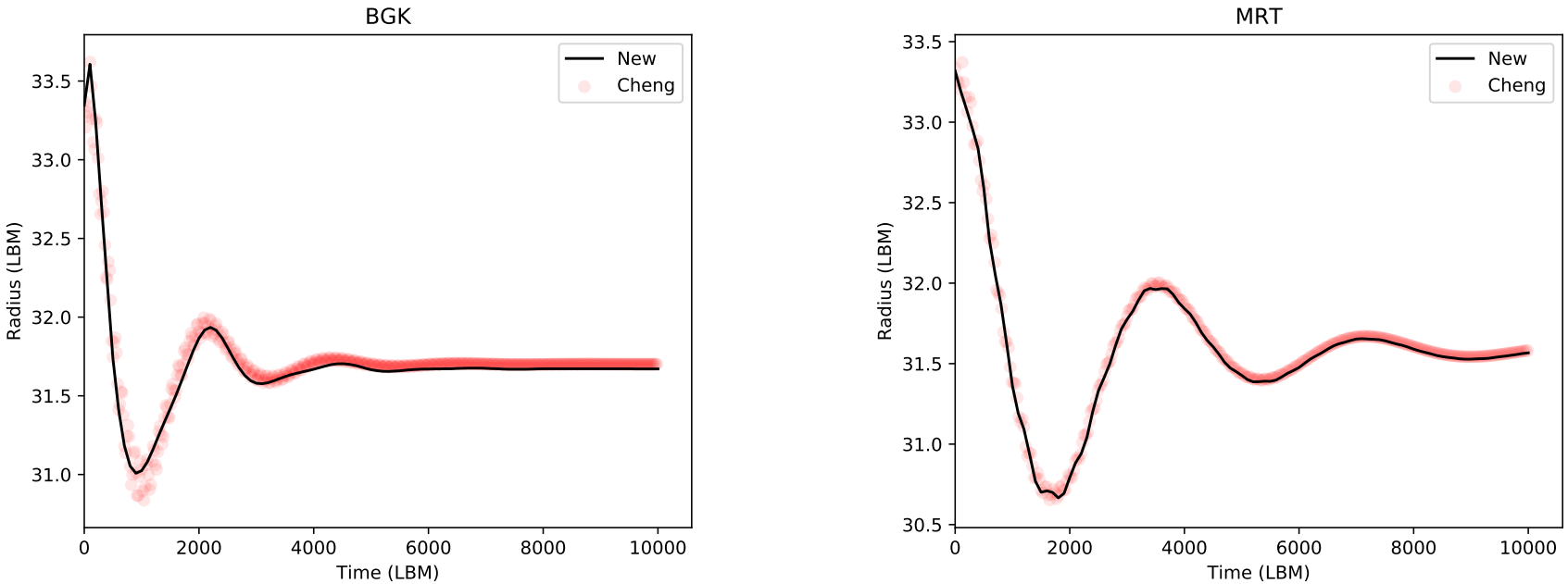
(a) Arbitrary porous medium (from real imaging).



(b) Cavity flow, imposing a velocity on the upper wall.

Figure: Single phase cases qualitatively demonstrating the ability of modeling arbitrary porous media and arbitrary boundary conditions.

Multiphase single component - Oscillating droplet



(a) BGK

(b) MRT

Figure: Oscillation droplet case. Viscosities are different in each case.

Ongoing work

- Two-component validation case
- Generalizing the Shan-Chen force at boundary blocks
- Viscosity per phase, to reproduce falling and raising droplet/bubble within LBM velocity ranges (see falling droplet video).

Questions

- Mass increasing when imposing velocity/outflow.

$$f_{i,\text{in}}^{\text{bndry}} = f_{i,\text{in}}^{\text{neighbor}} \quad \text{vs.}$$

$$f_{i,\text{in}}^{\text{bndry}} = f_{\bar{i},\text{in}}^{\text{bndry}} - g(\mathbf{u}_n^{\text{neighbor}})$$

- Over-constraining P and $\mathbf{u}$ with outflow, may solve the increasing density?

Questions

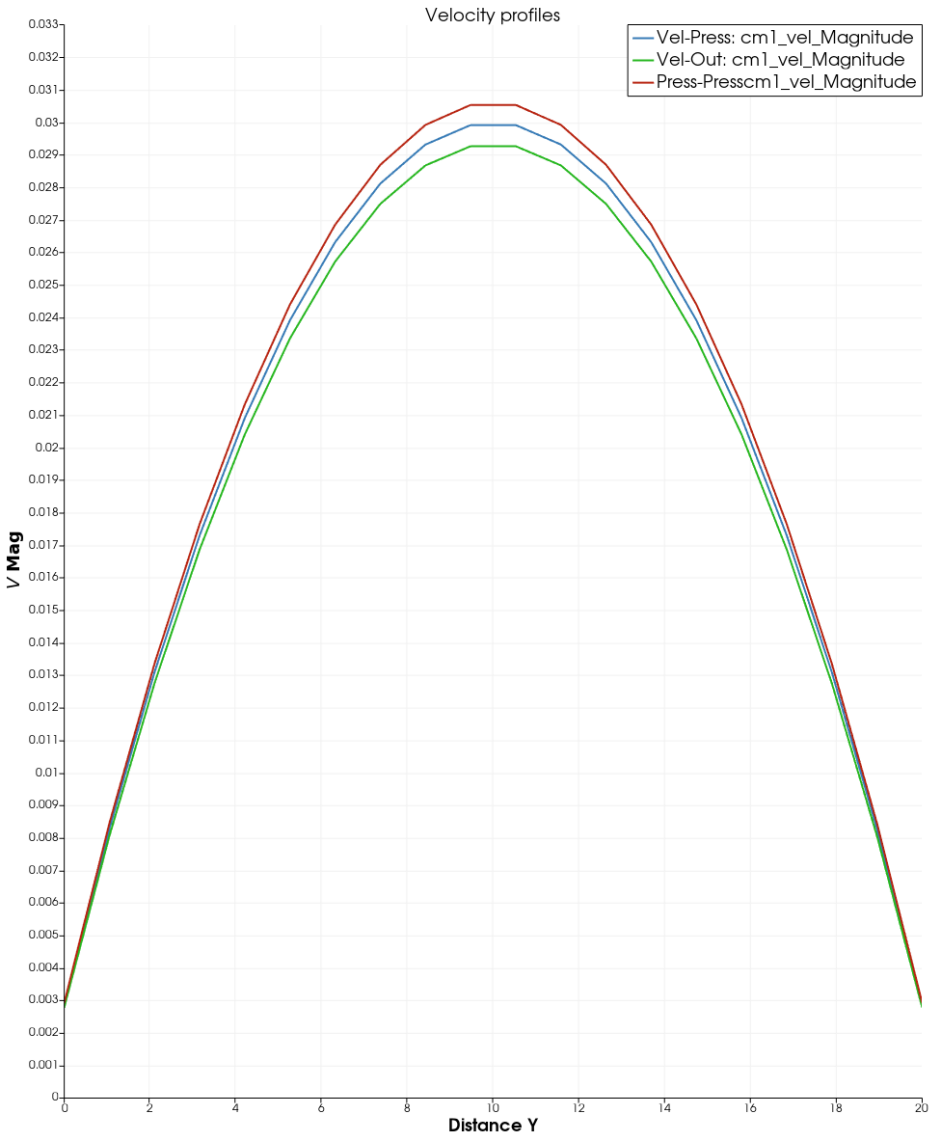
- Outflow boundary conditions. Assumptions and implications. How many layers for averaging?
- Density variations in velocity/pressure are common in LBM?

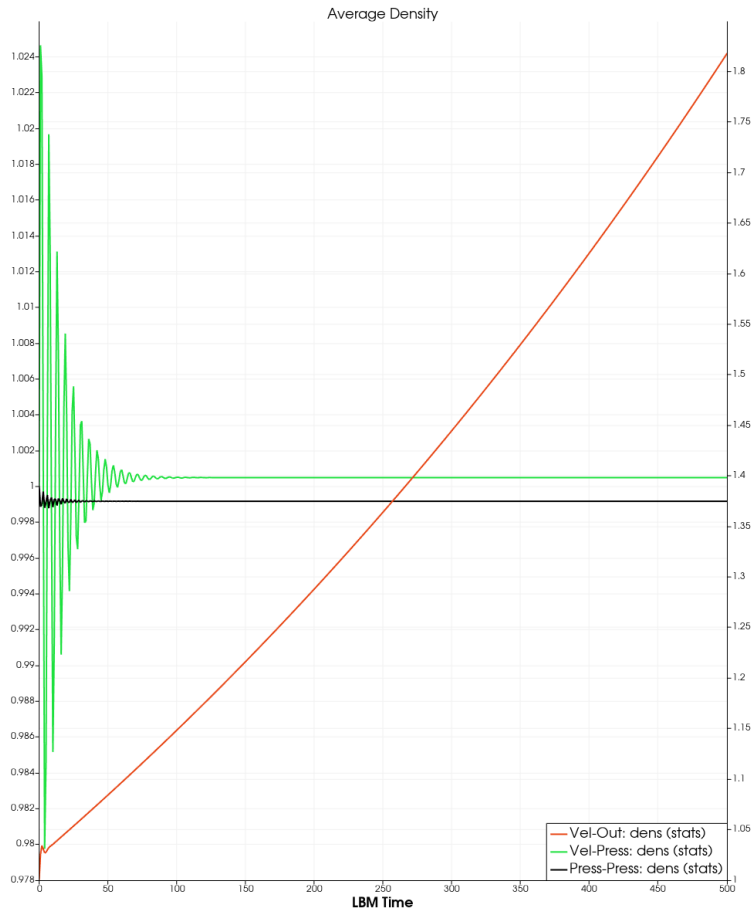
Questions

- Is there a general treatment for corners, no matter what the BCs are?
- Pseudopotential per component. Was this tried and what were the difficulties?
- Reason for applying:

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

Density variations





Paper

Which are the cases initially thought to serve as validation?

Current ideas/tasks for dynamic validations:

- Young-Laplace equation
- Identify analytical expression for oscillation frequency
- Rayler-Taylor instability (surface waves)
- Rising bubble/falling droplet (easy analytical solution!)
- Impacting droplet

Starting with the Young-Laplace case is straightforward, if this case will go in the paper.

Discussion

Discussion...

Input

```
###################### LBM INPUT ######################
############## Mixture Description ############
Ncm, 1
Nph, 1
############## Discrete Domain and Initial Conditions ##############
InitialP, 0.333
InitialT, 1.000
InitialComp, 1.0, 1.0
TimeSteps, 10000
nBound, 4
MeshReading, 'UNIFORM'
############## Boundaries ##############
cornerPatch, 3, 4, 3, 4
###### Conditions ######
1, 'PRESS', 0.335, 0.0, 0.0
2, 'VEL', 0.05, 0.0, 0.0
3, 'WALL', 0.0, 0.0, 0.0
4, 'WALL', 0.0, 0.0, 0.0
############## Forcing ##############
nForces, 1
###### Forces ######
1, 'UNIF', 0.0e-5, 0.0, 0.0
############## Numerical parameters ##############
printFreq, 500
diagnostic, 1
simuName, 'PV'
############## LBM parameters ##############
taoNorm, 0.6
###### Scaling ######
printReport, .true.
type, 'VDL'
deltaX, 9.0e-6
############## EoS ##############
type, 'IDEAL'
realDen, 1000.0
###### phases ######
1
kinVisc, 1.0e-6
###### Components ######
'Omega Tc Pc Mw'
1
1.0, 1.0, 1.0, 1.0
EOF
###################### LBM INPUT ######################
```

Discussion

Discussion...

template

a

- A
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Discussion

Discussion...

Report XXX XX - 202X

Main discussion points:

- Topic 1
- Topic 2

Sample frame title

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- Text visible on slide 1

Sample frame title

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- 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.