PhD in Energy and Mineral Engineering at PSU

Nicolás's Research - Reports

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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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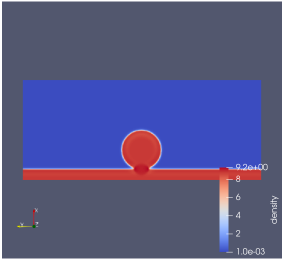
  - Droplet impacting surface (MCMP and IMM?)
  - Oscillating droplet
  - Rotating droplet
  - Surface wave
- DRY

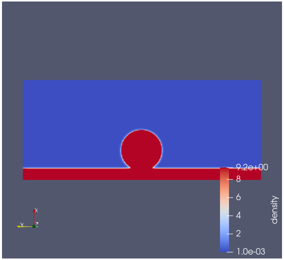
Cheng's paper

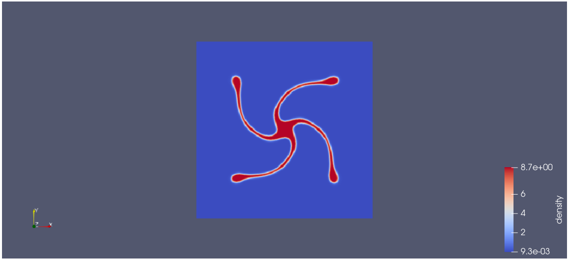
With these results we are able to:

- 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

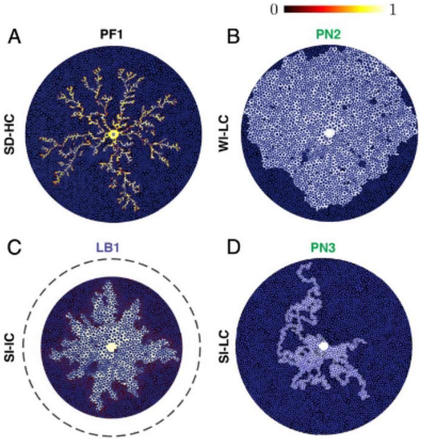


Fig. 3. Selection of simulated displacement patterns for the priority cases. (*A*) Strong drainage at high Ca (SD-HC) as simulated by a phase-field model. (*B*) Weak imbibition at low Ca (WI-LC) as simulated by a pore-network model. (*C*) Strong imbibition at intermediate Ca (SI-IC) as simulated by a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

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 book1

Report Oct 7 - 2021

Main discussion points:

- Generalities

EoS Results

```
nbuenoz@nbuenoz-asus:~/Documents/phd/privatePSU/immscible2D$ ./lbm
 Hello LBM World!
 ############  SCALING  ###########
 Length scale   8.5845885615224824E-010
 Time scale   1.4938819660023496E-012
 Pressure scale   2987.2706945477767
 Temp scale   1146.9129114303341
 R scale   8.3144600000000004
 MW scale   1.6043000000000002E-002
 Density scale   5.0256897140490541E-003
 Molar Density scale  0.31326371090500860
 ############  SCALING  ###########
 ############  VALIDATION  ###########

 EOS Validation
 a_lb, b_lb:   0.18367346938775514       0.10440000000000001
 a_lb, b_lb:    1.1054732634877027       0.28177392159094283
 Alpha function:   0.81953790010837613        1.2383568748075604
 Reduced temperature:    1.5437043078088137       0.69224941877171442
 m functions:    2.4142135623730949      -0.41421356237309515
 Initial pressue:   0.62706068232078038
 Factor Z and total molar density (lb units)   0.43867241207572677        3.0933126690097290
 Molar density cm 1, cm 2:    2.1142792092681497       0.97903345974157929
 Density 1:    2.1142792092681497
 Density 2:    3.5469900733911488


 EOS Validation
 a_lb, b_lb:   0.18367346938775514       0.10440000000000001
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 m functions:    2.4142135623730949      -0.41421356237309515
 Initial pressue:   0.62706068232078038
 Factor Z and total molar density (lb units)   0.59443319491561919        2.2827643903896107
 Molar density cm 1, cm 2:    1.9462849192461822       0.33647947114342858
 Density 1:    1.9462849192461822
 Density 2:    1.2190485750718592

 ############  VALIDATION  ###########
 data/output/lbmwrite0.vtk
 data/output/lbmwrite2.vtk
nbuenoz@nbuenoz-asus:~/Documents/phd/privatePSU/immscible2D$
```

```
**********************************************
Thermodynamic properties of carbonhydr components
**********************************************
P-R EOS, a, b, comp. 1 =  0.18367346938775511       0.10440000000000001
P-R EOS, a, b, comp. 2 =   1.1054370307926964       0.28176690995765424
R =   1.0000000000000000
Unit scales (P,T,R,M,rho) =   2987.2198023870678        1146.9219629738466        10.730000000000000        16.042999999999999
      0.24273566311481215        3.8942082433509313
Acentric coeffs (comp. 1&2) =   1.0400000000000000E-002  0.19950000000000001
Temp. corr. (comp. 1&2) =  0.81953790010837613        1.2383568748075604
Operation temp. =  0.46210641796915841
Critical temp. (comp. 1&2) =  0.29934904996481349       0.66754323721801334
Critical press. (comp. 1&2) =  0.22308368452414654       0.18431853429264117
Reduced temp. (comp. 1&2) =   1.5437043078088137       0.69224941877171442
P-R EOS, m1, m2 =   2.4142135623730949      -0.41421356237309515
pressinit =   1888.2000000000000
zz =   0.59081770517105570
init molar density =   1.9679054919622248       0.34727743975803982        2.3151829317202646
init mass density =   1.9679054919622248        1.2581690850250296        3.2260745769872541
zz liquid =  0.43867241858364858
amolemax =   3.0933897358710496
zz liquid =  0.59443319409087936
amolemin =   2.2828213002669662
denliquid =   2.1143318844678625        3.5470784452476125        5.6614103297154745
denvapor =   1.9463334406076154        1.2190789669625659        3.1654124075701811
coeff =    7.7518100258589587E-002
****************************************
```

Report XXX XX - 202X

Main discussion points:

- Topic 1
- Topic 2

Sample frame title

This is a text in second frame. For the sake of showing an example.

- Text visible on slide 1

Sample frame title

This is a text in second frame. For the sake of showing an example.

- Text visible on slide 1
- Text visible on slide 2

Sample frame title

This is a text in second frame. For the sake of showing an example.

- Text visible on slide 1
- Text visible on slide 2
- Text visible on slides 3

Sample frame title

This is a text in second frame. For the sake of showing an example.

- 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.