Lattice Boltzmann Simulation of Gas Bubble Dynamics in Peat

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Outline

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  - Lattice Boltzmann Method (LBM) Basics
  - Multiphase LBM Types

- Bubbles with LBM
  - Laplace Law and surface tension
  - Bubble shape regimes
  - Single bubble simulations

- Bubbles in Porous Media/Peat
  - Contact angles
  - Early 2-D model vs. LBM model
  - Peat CT
  - 3-D bubble models

Ludwig Boltzmann
1844 - 1906
Motivation

- Peatlands may account for 5 to 10% of methane flux to the atmosphere
- Little known about role of peat structure on gas flux dynamics
  - Generation, accumulation, movement, release
- Peat methane
  - Episodic ebullition vs. diffusion (sampling)
  - Atmospheric pressure effects

LBM

- LBM is a mesoscopic method based on the scale between molecular dynamics and more familiar continuum approaches
- Particle stream–and–collide perspective with interparticle forces is adequate for most simulations
- LBMs are very versatile. Flow, solute/heat transport, and multiphase simulations can be carried out with the same model framework
- LBMs handle complex geometries well
LBM Basics

Discrete Velocities \( e_\alpha \)
Directional densities \( f_\alpha \)

Macroscopic density \( \rho = \sum_{\alpha=0}^{8} f_\alpha \)

Macroscopic velocity \( u = \frac{1}{\rho} \sum_{\alpha=0}^{8} f_\alpha e_\alpha \)
Streaming

\[ f_a(x + e_a \Delta t, t + \Delta t) = f_a(x, t) \]
Single Relaxation Time BGK (Bhatnagar-Gross-Krook) Approximation

\[
f_a(x + e_a \Delta t, t + \Delta t) = f_a(x, t) - \left[ f_a(x, t) - f_a^{eq}(x, t) \right] \frac{\tau}{2}
\]

Streaming

Collision (i.e., relaxation towards equilibrium)

\[
f_a^{eq}(x) = w_a \rho(x) \left[ 1 + 3 \frac{e_a \cdot u}{c^2} + \frac{9}{2} \frac{(e_a \cdot u)^2}{c^4} - \frac{3}{2} \frac{u^2}{c^2} \right]
\]

- \(w_a\) are 4/9 for the rest particles \((a = 0)\),
- 1/9 for \(a = 1, 2, 3, 4,\) and
- 1/36 for \(a = 5, 6, 7, 8.\)

- \(\tau\) relaxation time (viscosity)
- \(c\) speed on lattice (1 lu/time step)

Collision and streaming steps must be separated if solid boundaries present (bounce back boundary is a separate collision)
Multicomponent Multiphase LB Models

- Single Phase (No Interaction)
- Single Component Multiphase
- Miscible Fluids/Diffusion (No Interaction)
- Immiscible Fluids

Number of Components

Interaction Strength

Nature of Interaction

Attractive

Repulsive

Inherent Parallelism

High → Low
Phase Separation
Phase Separation
Interfacial Tension

- Laplace equation for circular bubbles and drops (2-D)

\[ \Delta P = P_{in} - P_{out} = \frac{\sigma}{r} \]
Single Bubble Observations

Re = 0.078
Eo = 8.67

Re = 0.232
Eo = 17.7

Re = 7.77
Eo = 243

Re = 94
Eo = 115

Re = 18.1
Eo = 339

Re = 30.3
Eo = 641

Re = 55.3
Eo = 32.2

Re = 259
Eo = 237

Bubble Shape Regime Map

Reynolds number

\[ R_e = \frac{V_b d_b \rho_L}{\mu_L} \]

Eötvös number

\[ E_o = \frac{g \Delta \rho d_b^2}{\sigma} \]

Morton number

\[ M = \frac{g \Delta \rho \mu_L^4}{\rho_L^2 \sigma^3} \]

Rising bubble dynamics: New effective buoyancy method

- Buoyant force per unit volume is

\[ F_B = g \Delta \rho \]  \hspace{1cm} (1)

- Apply equivalent effective buoyant force with upward body force only on bubble fluid component \( \kappa \) of density \( \rho_\kappa \):

\[ F_B = g_{applied} \rho_\kappa \]  \hspace{1cm} (2)

- Equate (1) and (2) to solve for appropriate acceleration:

\[ g_{applied} \rho_\kappa = g \Delta \rho \quad \Rightarrow \quad g_{applied} = g \frac{\Delta \rho}{\rho_\kappa} \]

- \( g_{applied} \rho_\kappa \) controls buoyancy and used in \( Eo \) and \( M \)
Air-Water Bubble During Rise

\[ PV = nRT = \text{Constant} \]

\[ P = \rho gh + \text{Patm} \]

\[ PV = \rho ghV + \text{Patm}V = \text{Constant} \]

\[ (\rho gh + \text{Patm}) \frac{4}{3} \pi r^3 = \text{Constant} \]

\[ r = \frac{3}{4} \sqrt[3]{\frac{3\pi}{4} (\rho gh + \text{Patm})} \]
Simulations

- $1 \leq Eo \leq 100$
- $3 \times 10^{-6} < M \leq 2.73 \times 10^{-3}$
- Viscosity ratio = $\nu_L / \nu_G = 1$
- Interfacial tension = $\sigma = 0.215 \text{ mu lu ts}^2$
- $d_0 = 80 \text{ lu}$
- Domain: fully closed

Fluid–Solid Interaction

- Simulation of fluid-solid interaction force [Martys and Chen, 1996]
  - $s$ function takes value 1 or 0
  - $G_{ads}$ is interaction strength between solid and each fluid component

$$F_{ads}^\kappa(r,t) = -G_{ads}^\kappa \rho^\kappa(r,t) \sum_a \omega_a s(r + e_a \delta t) e_a$$

- Interfacial tensions between different fluid components and solids

$$\cos \theta_1 = \frac{\sigma_{s2} - \sigma_{s1}}{\sigma_{12}}$$

- Sukop and Thorne [2006] substituted corresponding adhesion strengths for interfacial tensions

- Huang et al. [2007] proposed a simple equation to approximate contact angle in the SC LBM

$$\cos \theta_1 = \frac{G_{ads}^2 - G_{ads}^1}{G_{12} \rho_A - \rho_B}$$

$\rho_A$ main equilibrium density = 1
$\rho_B$ dissolved equilibrium density $\sim 10^{-3}$


Fluid/Solid Interaction (Wetting)

Initial condition

$15^\circ$

$45^\circ$

$90^\circ$

$135^\circ$

$0^\circ$

$30^\circ$

$60^\circ$

$120^\circ$

$150^\circ$
Peat bubbles: Reduced-complexity inverted sand pile model

LBM Model

180°  120°  15°
Bubble Frequency Distributions

![Graph showing bubble frequency distributions with various lines and equations]

- **LBM**: \( y = -11.991 \ln(x) + 23.281 \), \( R^2 = 0.8639 \)
- **Kellner et al. (2006)**: \( y = -11.003 \ln(x) + 19.957 \), \( R^2 = 0.9083 \)
- **Coulthard et al. (2009)**: \( y = -9.5348 \ln(x) + 16.146 \), \( R^2 = 0.8513 \)

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**Current study**

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Rule-based model

- Voxel-based pathway estimation
- Measure path length and tortuosity before trapping
- Average vector length from skeletonization

Computed Tomography of Peats

- Low density makes CT difficult
- Contrast agents: adsorbed Pb
- X-ray intensity $I$

$$I = I_0 e^{\mu x}$$

- $I_0$: Original beam intensity
- $x$: Path length through sample
- $\mu$: Linear attenuation coefficient

- Related to voxel gray scale distribution

Computed Tomography of Peats

- UK bogs
- 74 μm resolution (0.000074 m)
- Hierarchical tendril-like structure can make segmentation ambiguous
  - Give up and model fine scale as porous medium without distinct pore/solid structure?

Computed Tomography of Peats

- *S. magellanicum*

Application to Peat and other Porous Media

- Peat surface
- Living/minimally decomposed
Where the bugs are: source terms for gas

- Sensitive to Eh and other chemistry
- In micropores and/or on surfaces?
- First cuts:
  - Planar source
- Rates?
First 3D simulation
LBM Model (w/ porous medium)
Fluid-structure interactions

- Buoyancy can lead to peat structure deformation over range of scales
  - Cyclic and/or episodic ebullition events: Rupture
- Advanced modeling

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