Lattice Boltzmann Simulation of Gas Bubble Dynamics in Peat

FIU FLORIDA INTERNATIONAL UNIVERSITY

Earth and Environment

Applied Research Center

FAU FLORIDA ATLANTIC UNIVERSITY

Geosciences

UNIVERSITY OF BIRMINGHAM

Earth and Environmental Sciences

Mike Sukop, Seckin Gokaltun, Andy Pearson, Xavier Comas, and Nicholas Kettridge

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Outline

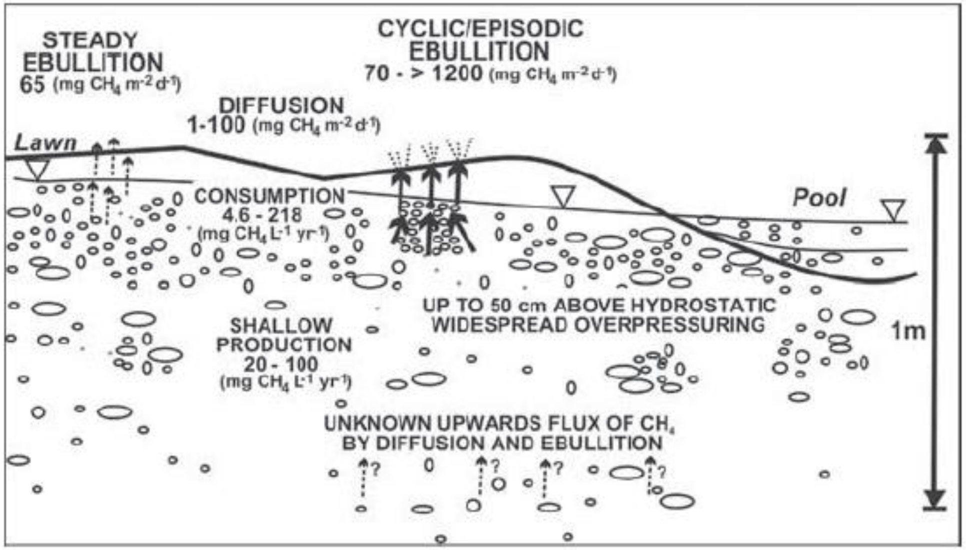
- Introduction
  - Motivation
  - Lattice Boltzmann Method (LBM) Basics
  - Multiphase LBM Types
- Bubbles with LBM
  - Laplace Law and surface tension
  - Bubble shape regimes
  - Single bubble simulations
- Bubbles in Porous Media/Peat
  - Contact angles
  - Early 2-D model vs. LBM model
  - Peat CT
  - 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



Coulthard, T., Baird, A. J., Ramirez, J. & Waddington, J. M. Methane dynamics in peat: the importance of shallow peats and a novel reduced-complexity approach for modeling ebullition. in Carbon Cycling in Northern Peatlands (eds. Baird, A. J., Belyea, L. R., Comas, X., Reeve, A. S. & Slater, L.) (AGU, 2009).

LBM

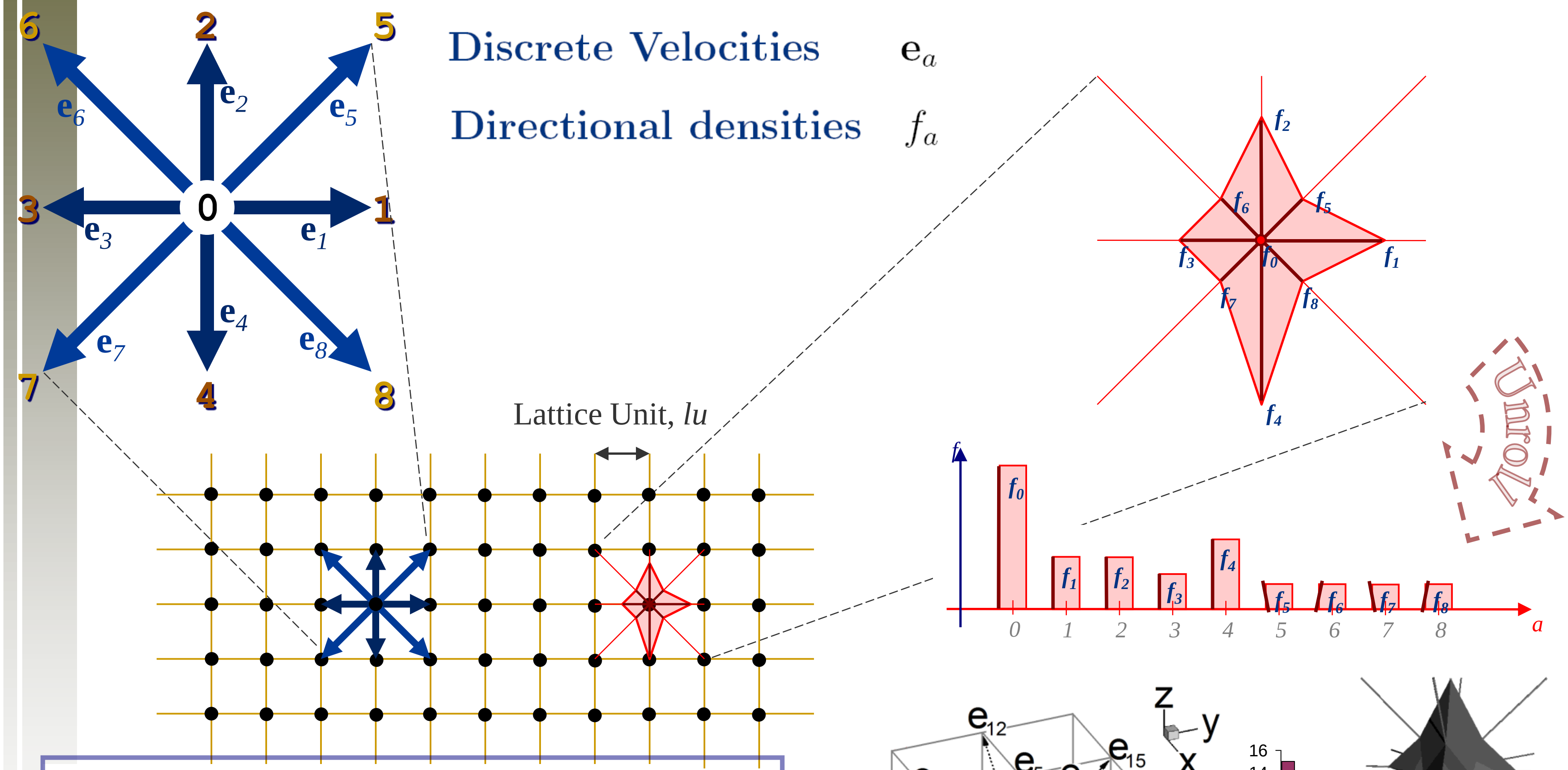
- LBM is a mesoscopic method based on the scale between molecular dynamics and more familiar continuum approaches
- Particle stream-and-collide perspective with interparticle forces is adequate for most simulations
- LBMs are very versatile. Flow, solute/heat transport, and multiphase simulations can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

LBM Basics

D2Q9

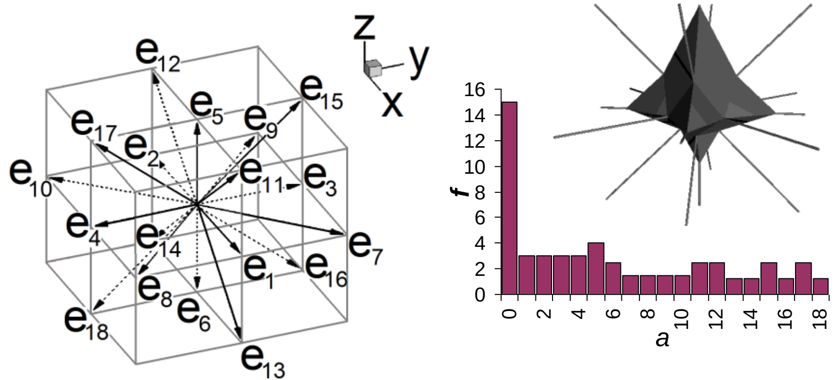
Discrete Velocities $\mathbf{e}_a$

Directional densities f_a



Macroscopic density
$$\rho = \sum_{a=0}^{8} f_a$$

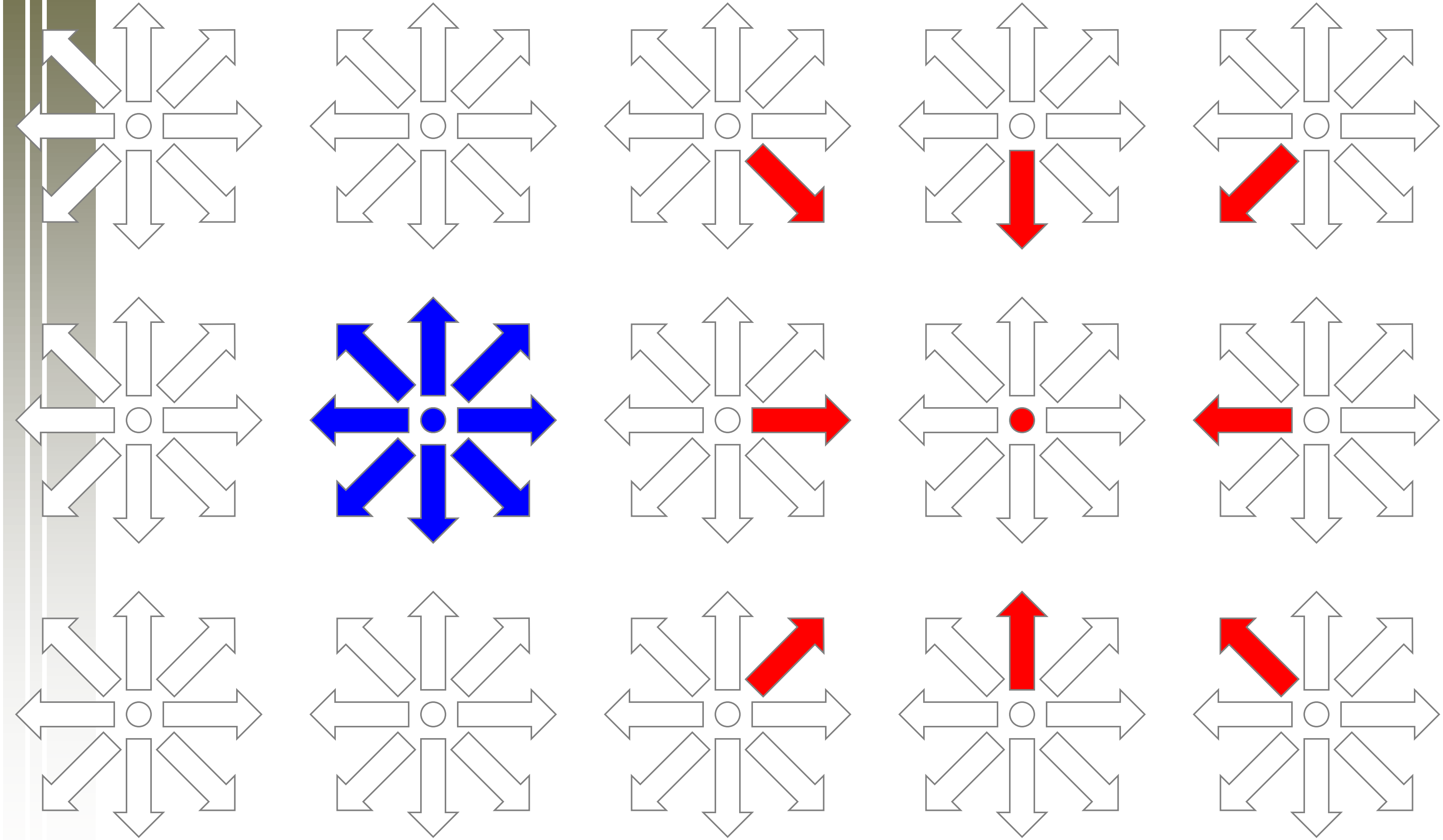
Macroscopic velocity
$$\mathbf{u} = \frac{1}{\rho}\sum_{a=0}^{8} f_a \mathbf{e}_a$$



D3Q19

Streaming

$$f_a(\mathbf{x}+\mathbf{e}_a\Delta t, t+\Delta t) = f_a(\mathbf{x}, t)$$

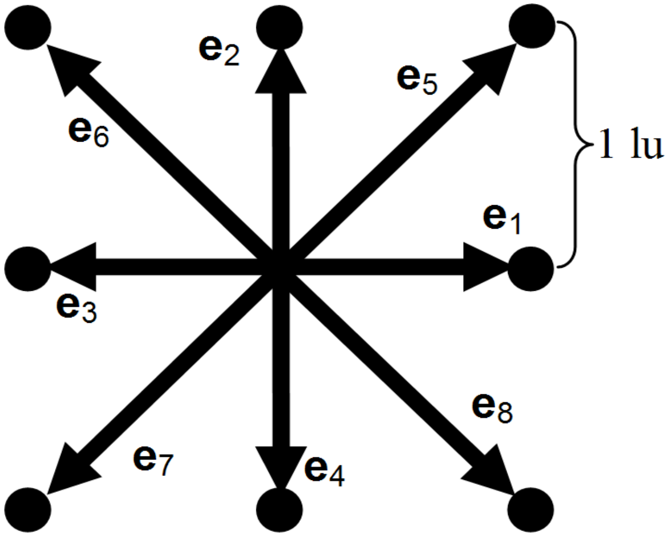


Single Relaxation Time BGK (Bhatnagar-Gross-Krook) Approximation

$$\underbrace{f_a\left(\mathbf{x}+\mathbf{e}_a\Delta t, t+\Delta t\right) = f_a\left(\mathbf{x},t\right) - \underbrace{\frac{\left[f_a\left(\mathbf{x},t\right)- f_a^{eq}\left(\mathbf{x},t\right)\right]}{\tau}}_{\text{Collision (i.e., relaxation towards equilibrium)}}}_{\text{Streaming}}$$

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

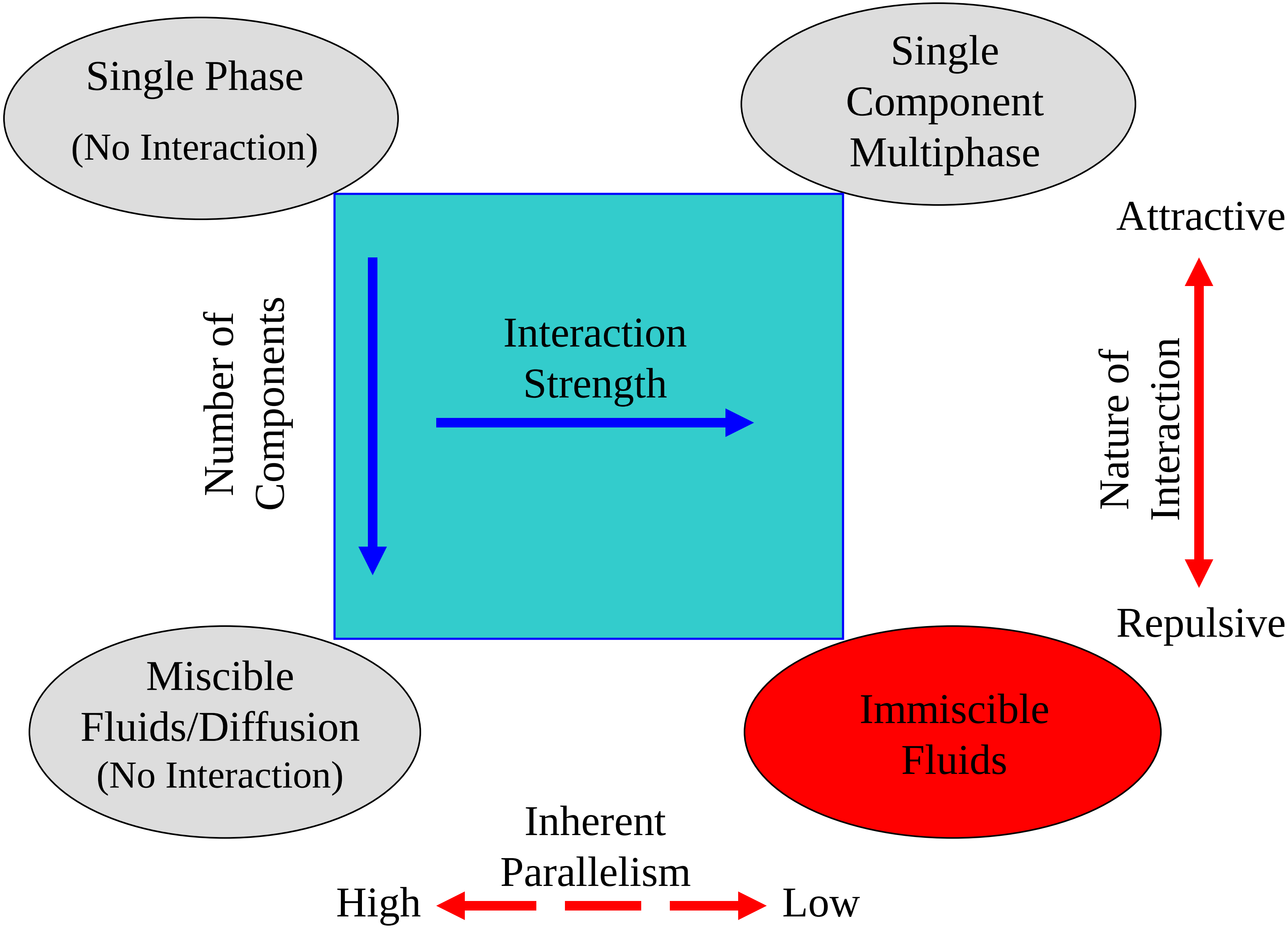
Collision and streaming steps must be separated if solid boundaries present (bounce back boundary is a separate collision)



- 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.

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

Multicomponent Multiphase LB Models



Single Phase

(No Interaction)

Single Component Multiphase

Attractive

Number of Components

Interaction Strength

Nature of Interaction

Repulsive

Miscible Fluids/Diffusion (No Interaction)

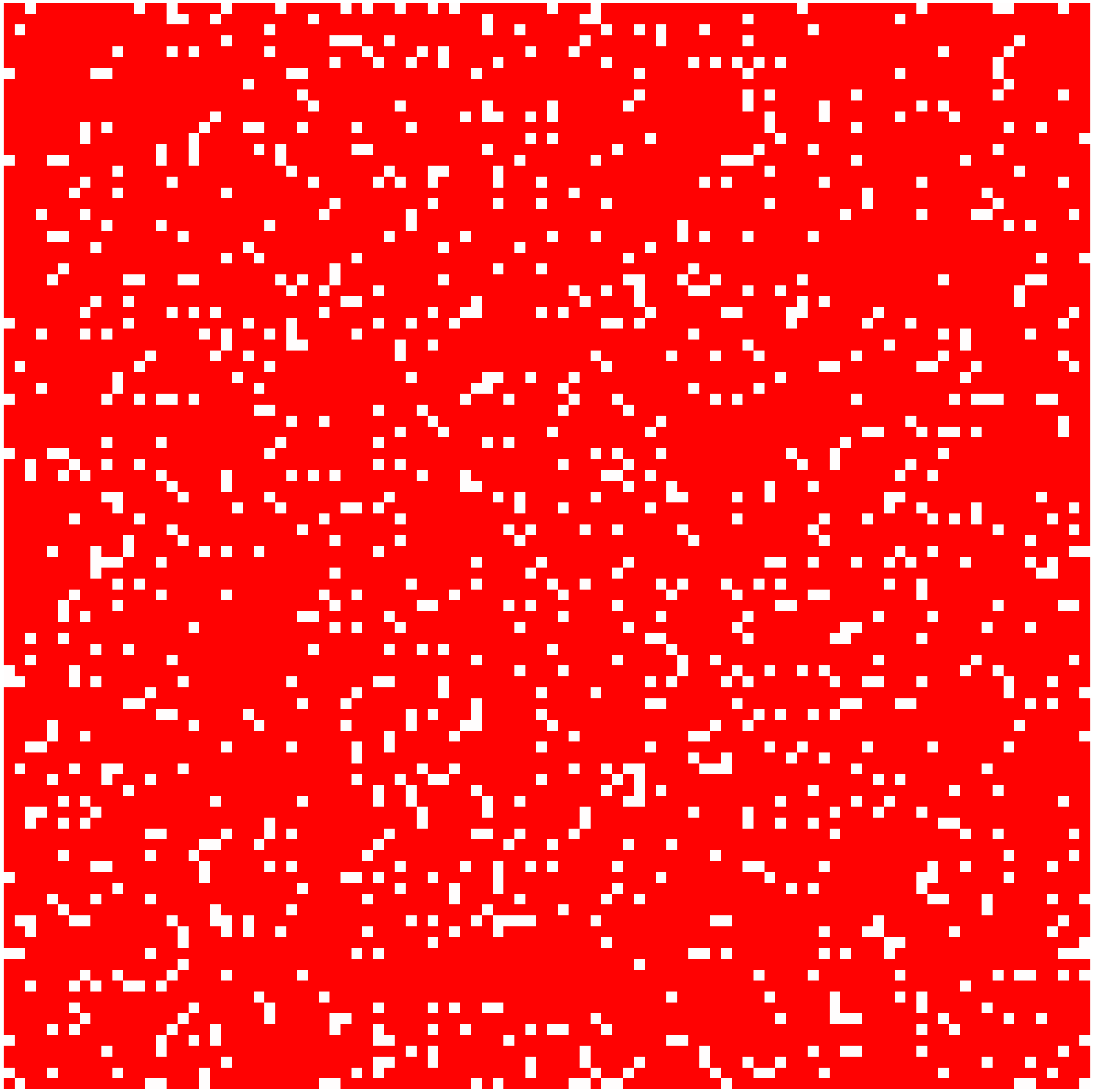
Immiscible Fluids

Inherent Parallelism

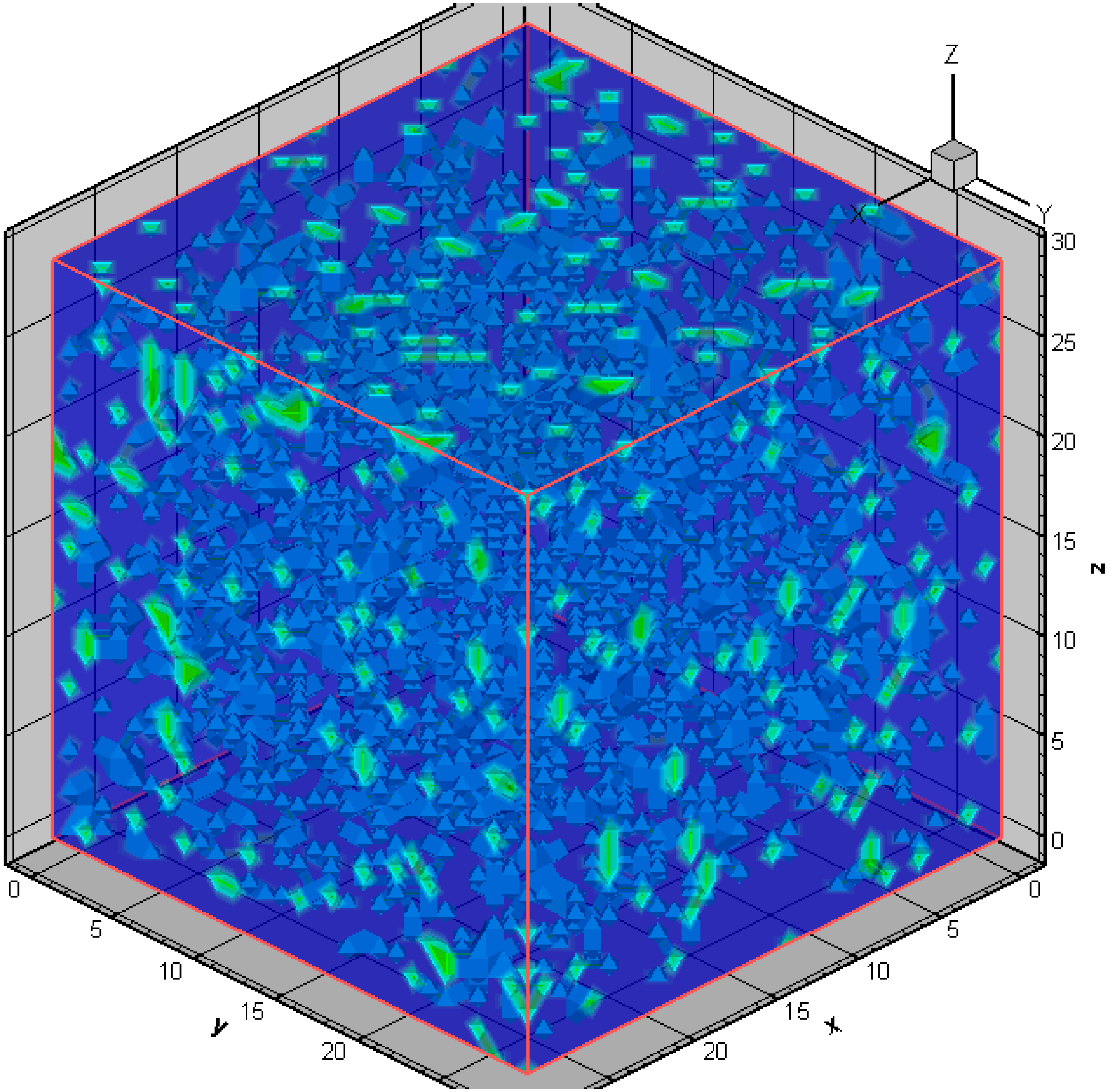
High

Low

Phase Separation

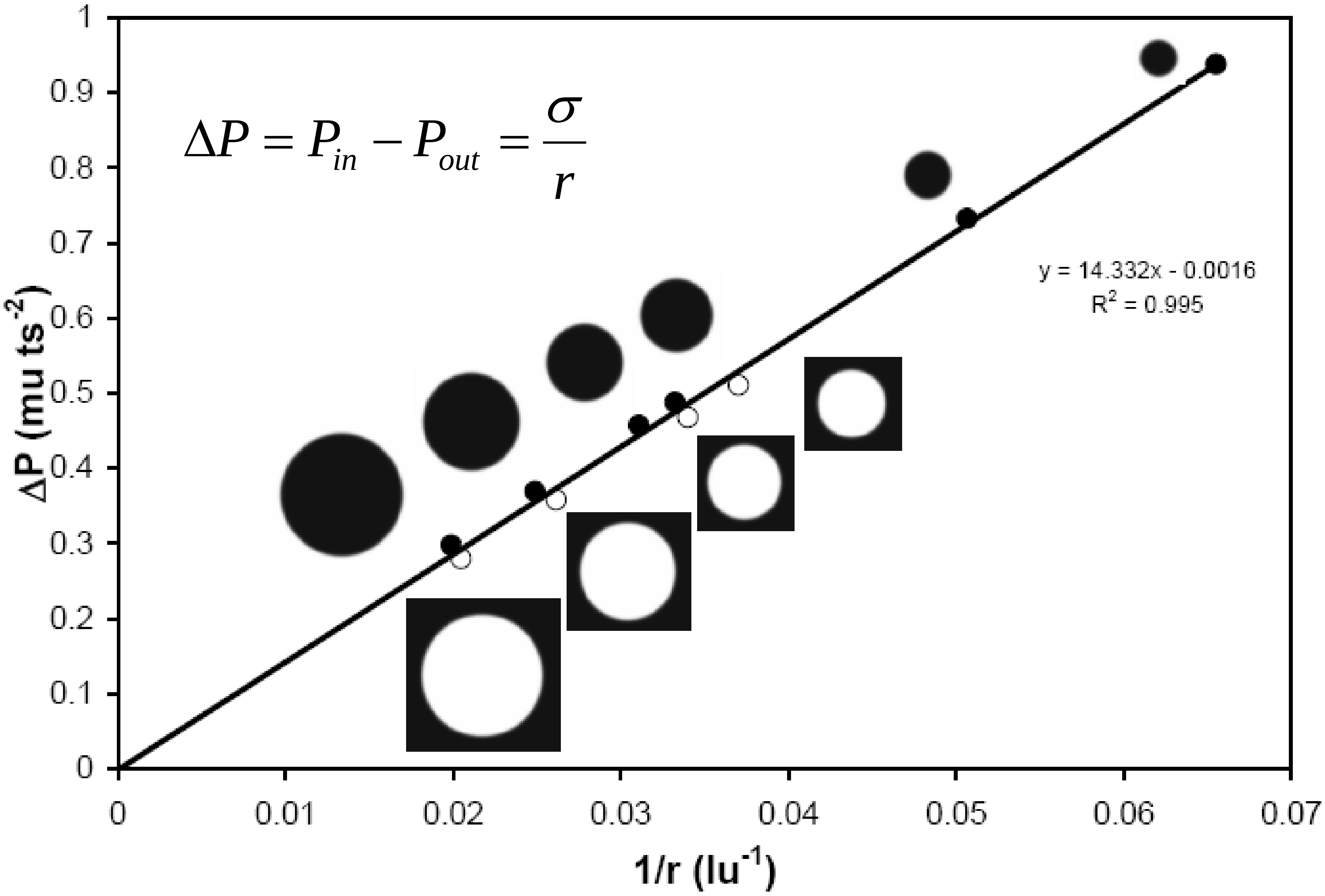


Phase Separation



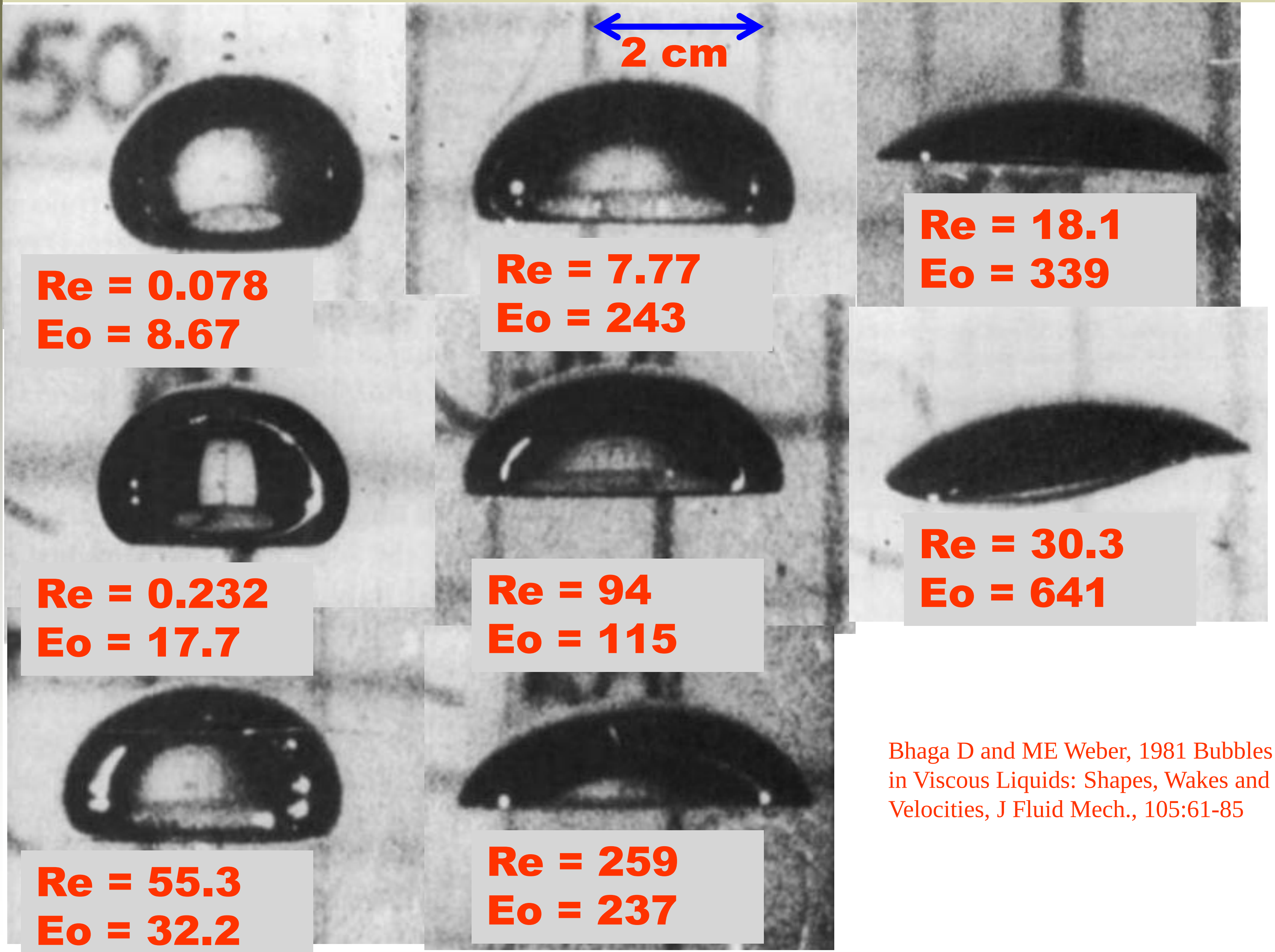
Interfacial Tension

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



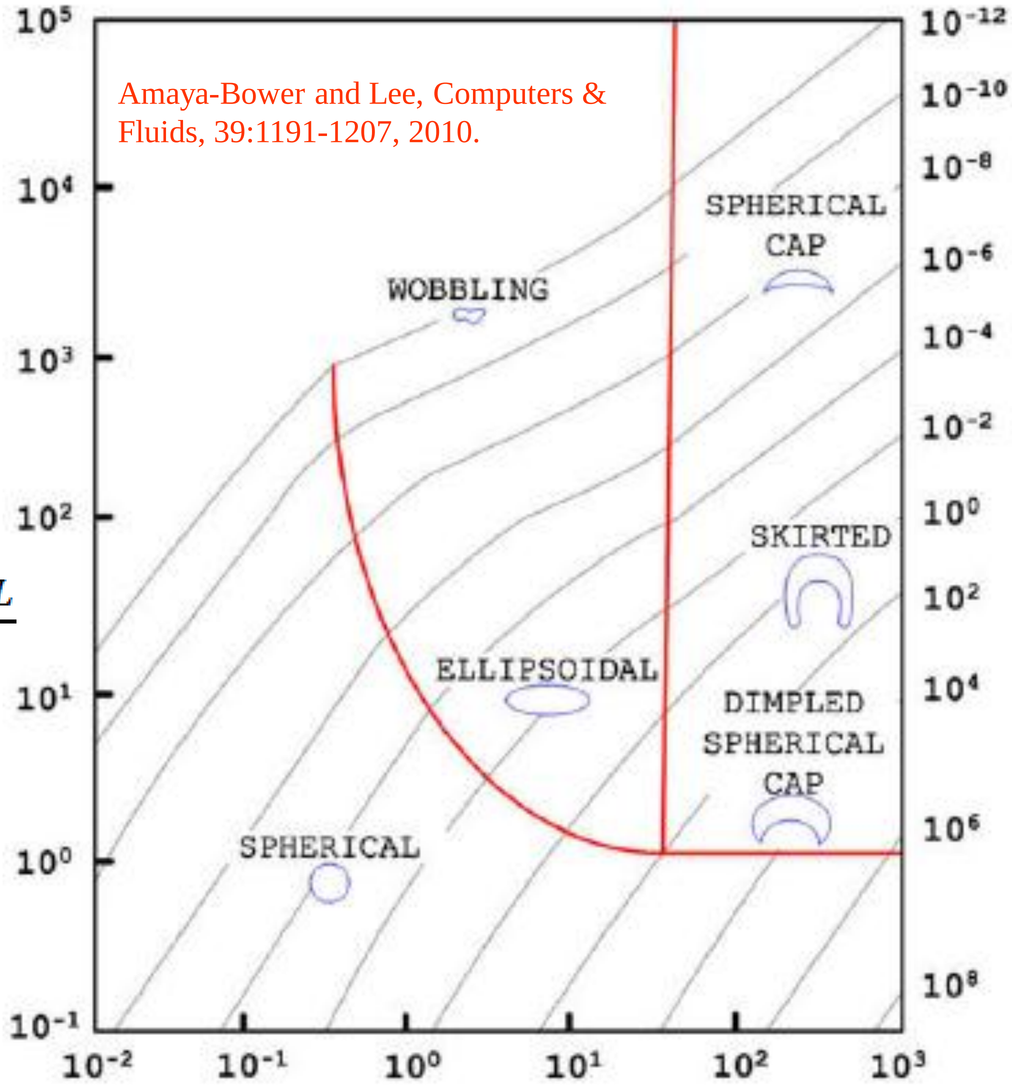
$$\Delta P = P_{in} - P_{out} = \frac{\sigma}{r}$$

Single Bubble Observations



Bhaga D and ME Weber, 1981 Bubbles in Viscous Liquids: Shapes, Wakes and Velocities, J Fluid Mech., 105:61-85

Bubble Shape Regime Map



Amaya-Bower and Lee, Computers & Fluids, 39:1191-1207, 2010.

Reynolds number

$$R_e = \frac{V_b d_b \rho_L}{\mu_L}$$

Morton number

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

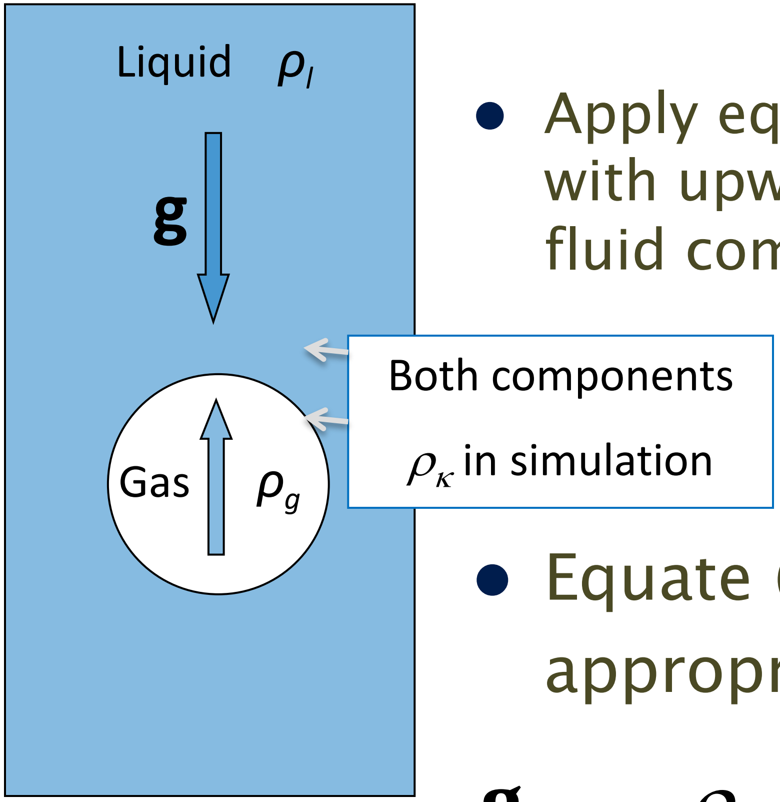
Eötvös number

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

Rising bubble dynamics: New effective buoyancy method

- Buoyant force per unit volume is

$$\mathbf{F}_B = \mathbf{g}\Delta\rho \qquad (1)$$



Both components ρ_κ in simulation

- Apply equivalent effective buoyant force with upward body force only on bubble fluid component κ of density ρ_κ:

$$\mathbf{F}_B = \mathbf{g}_{applied}\rho_\kappa \qquad (2)$$

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

$$\mathbf{g}_{applied}\rho_\kappa = \mathbf{g}\Delta\rho \Rightarrow \mathbf{g}_{applied} = \mathbf{g}\frac{\Delta\rho}{\rho_\kappa}$$

- $\mathbf{g}_{applied}\rho_\kappa$ controls buoyancy and used in Eo and M

Air-Water Bubble During Rise

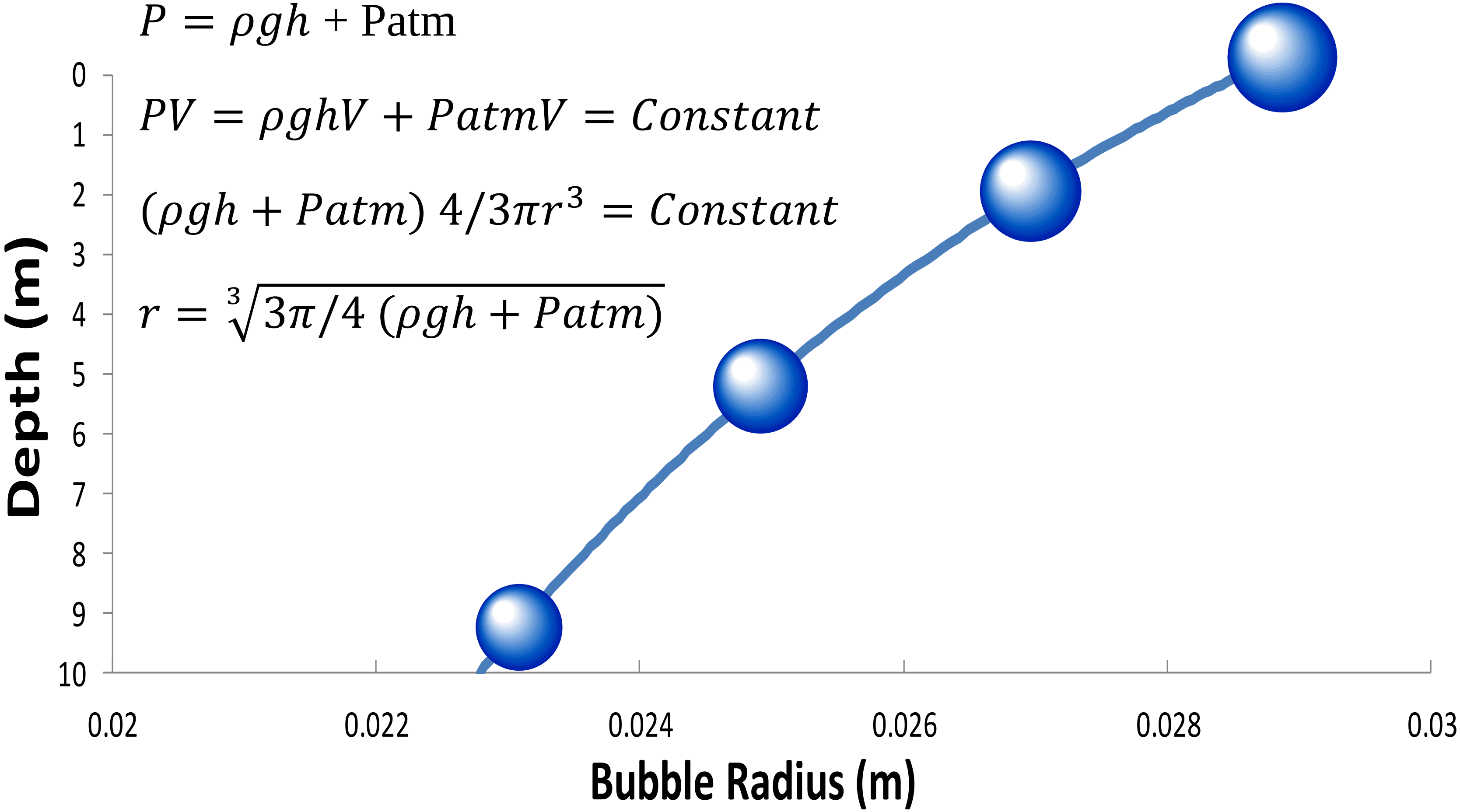
$$PV = n\mathrm{RT} = \mathrm{Constant}$$

$$P = \rho g h + \mathrm{Patm}$$

$$PV = \rho g h V + PatmV = Constant$$

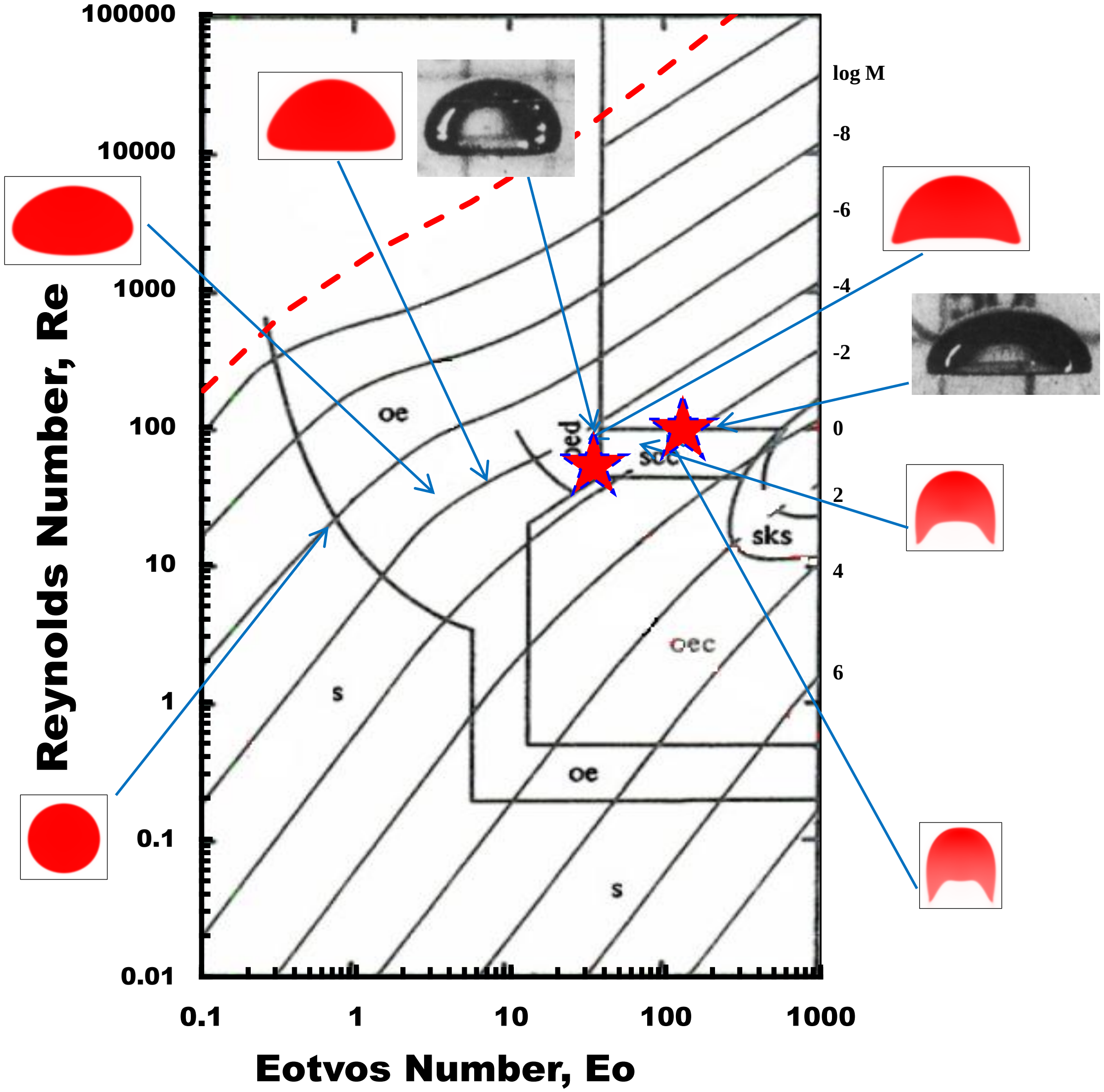
$$(\rho g h + Patm)\ 4/3\pi r^3 = Constant$$

$$r = \sqrt[3]{3\pi/4\ (\rho g h + Patm)}$$



Simulations

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



Bhaga D and ME Weber, 1981 Bubbles in Viscous Liquids: Shapes, Wakes and Velocities, J Fluid Mech., 105:61-85

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**

$$F^{\kappa}_{ads}(\mathbf{r},t) = -G^{\kappa}_{ads}\,\rho^{\kappa}(\mathbf{r},t)\sum_{a} \omega_a\, s(\mathbf{r}+\mathbf{e}_a\delta t)\,\mathbf{e}_a$$

- 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

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

ρ_A main equilibrium density = 1

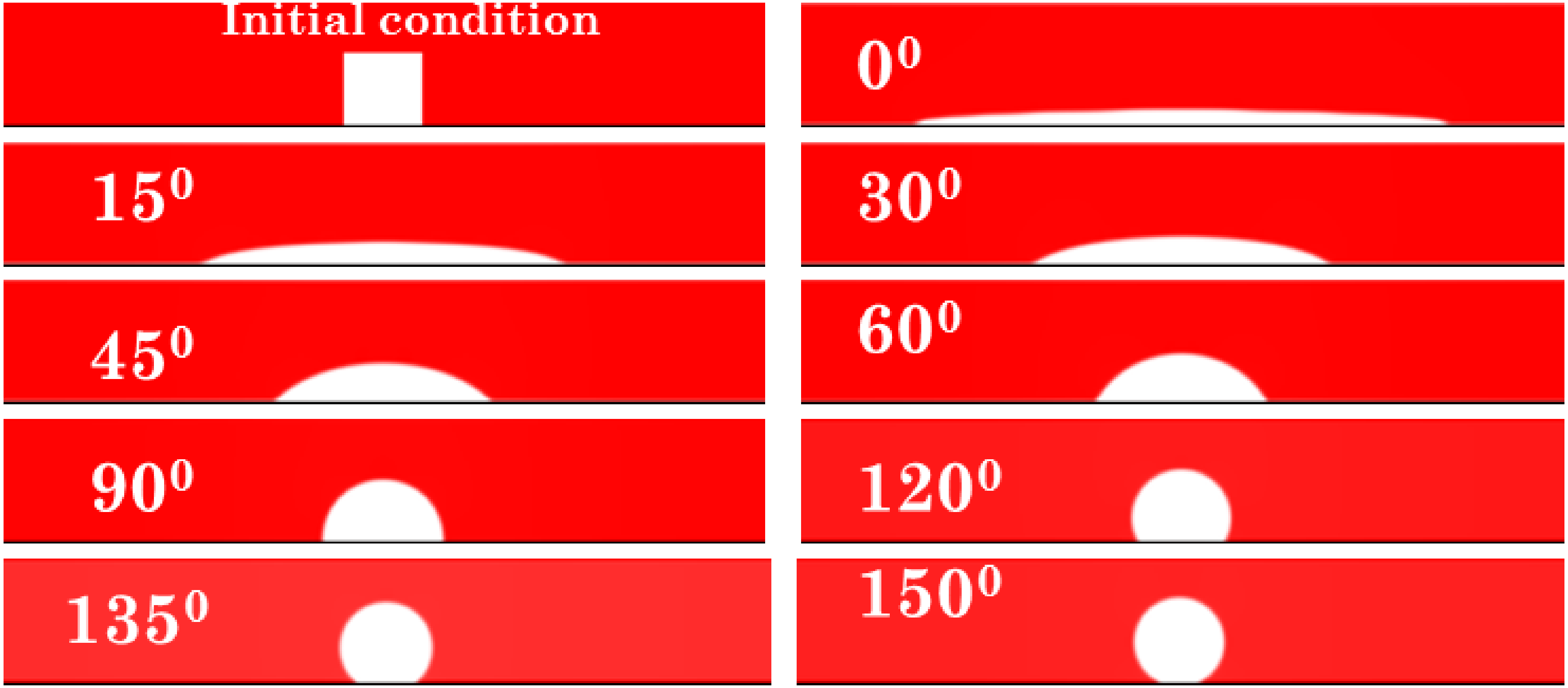
ρ_B dissolved equilibrium density ~10^{-3}

Martys NS, Chen H (1996) Simulation of multicomponent fluids in complex three-dimensional geometries by the lattice Boltzmann method. Phys Rev E 53:743-750

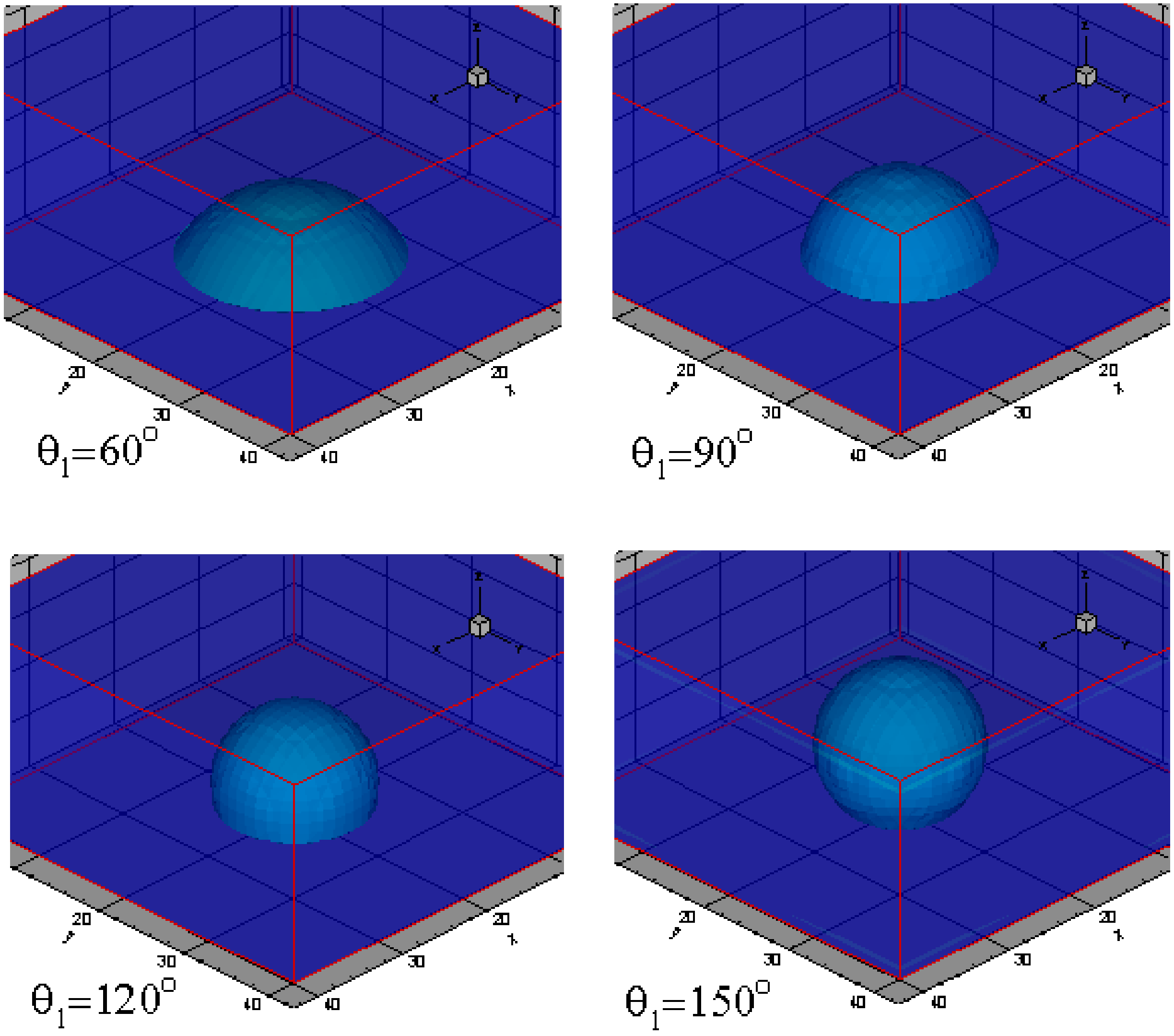
Sukop, M. C. & Thorne, D. T. Lattice Boltzmann Modeling: An Introduction for Geoscientists and Engineers (Springer, Heidelberg-Berlin-New York, 2006).

Huang, H., D.T. Thorne, Jr., M.G. Schaap, and M.C. Sukop (2007). Proposed approximation for contact angles in Shan-and-Chen-type multicomponent multiphase lattice Boltzmann models. Phys. Rev. E 76, 066701

Fluid/Solid Interaction (Wetting)



MCMP LBM with Surfaces

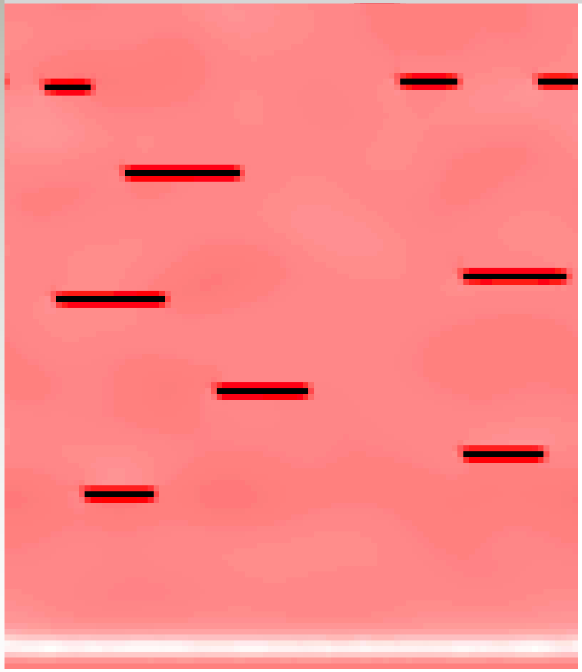


Huang, H., D.T. Thorne, Jr., M.G. Schaap, and M.C. Sukop. Proposed approximation for contact angles in Shan-and-Chen-type multicomponent multiphase lattice Boltzmann models. Phys. Rev. E 76, 066701 (2007)

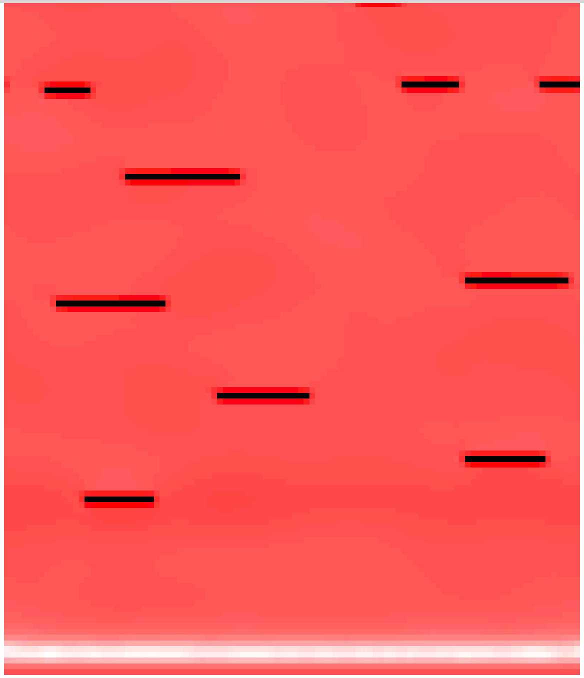
Peat bubbles: Reduced-complexity inverted sand pile model

Coulthard, T., A. J. Baird, J. Ramirez, and J. M. Waddington, Methane dynamics in peat: the importance of shallow peats and a novel reduced-complexity approach for modeling ebullition. in Carbon Cycling in Northern Peatlands (eds. Baird, A. J., Belyea, L. R., Comas, X., Reeve, A. S. & Slater, L.) (AGU, 2009).

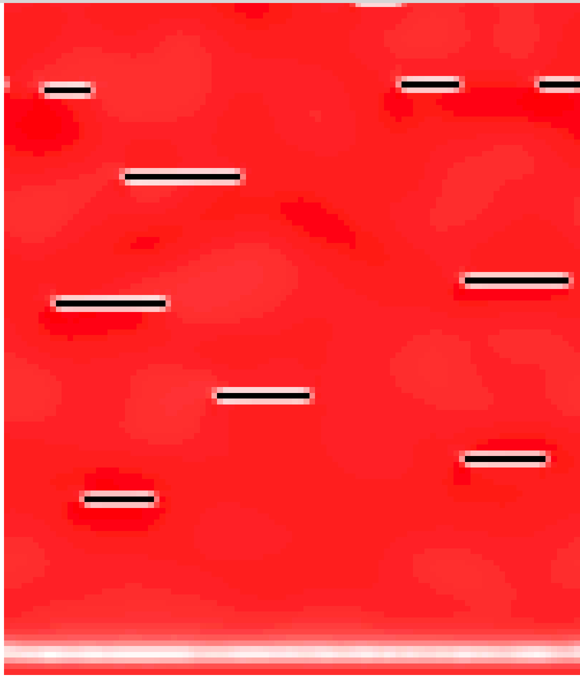
LBM Model



180^0

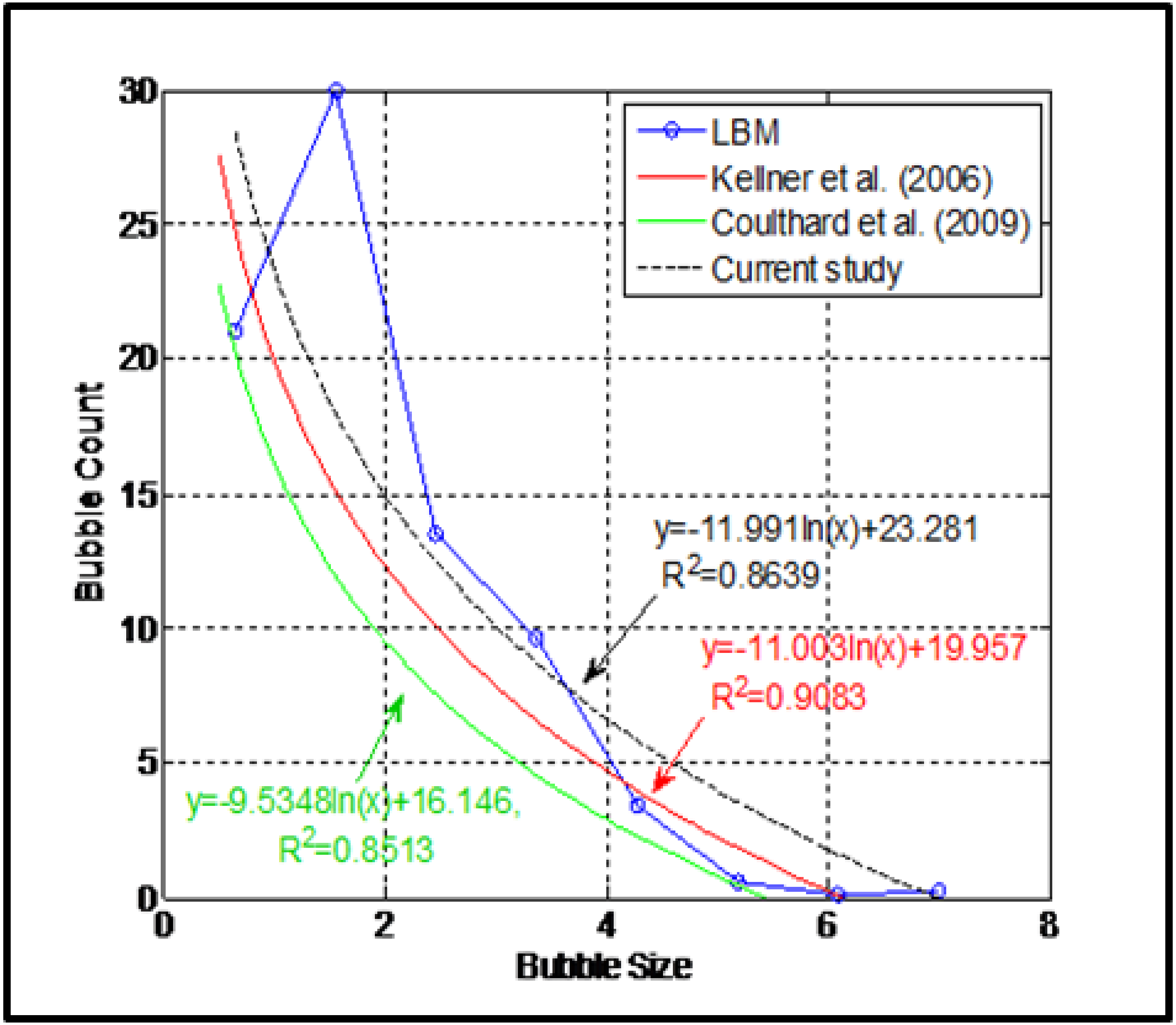


120^0



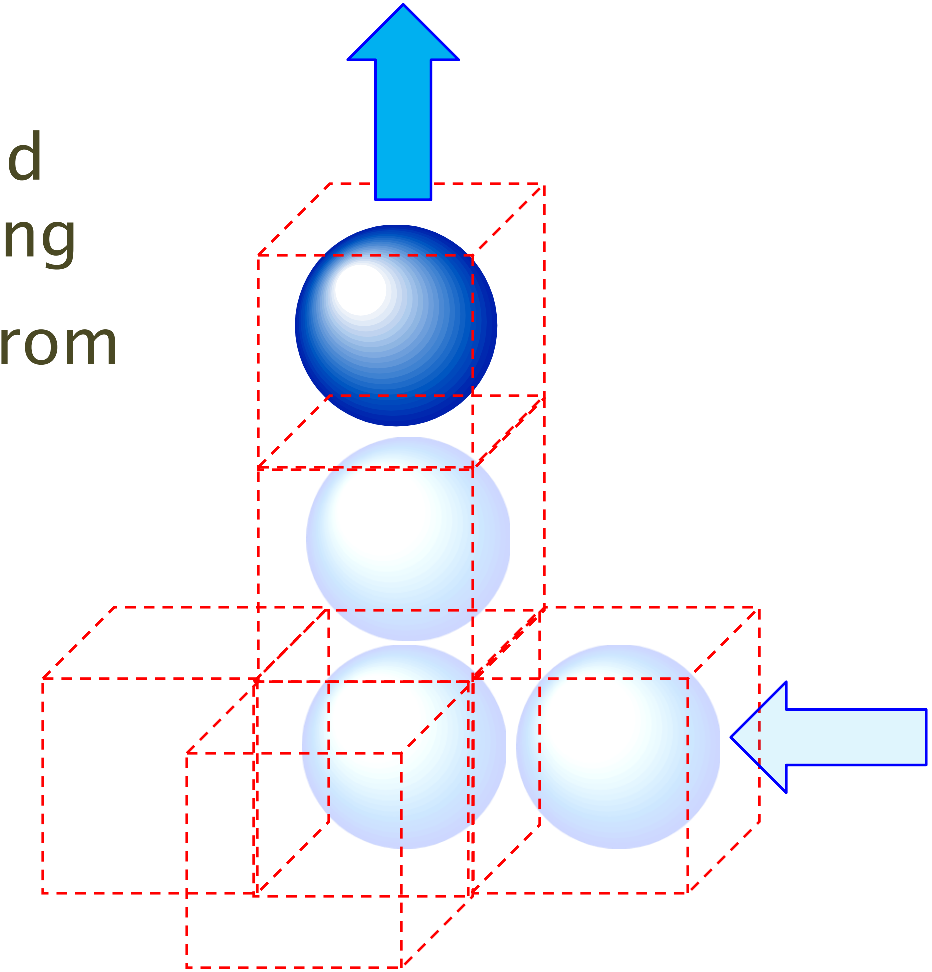
15^0

Bubble Frequency Distributions



Rule-based model

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



Kettridge, N., and A. Binley (2011), Characterization of peat structure using X-ray computed tomography and its control on the ebullition of biogenic gas bubbles, J. Geophys. Res., 116, G01024, doi:10.1029/2010JG001478.

Computed Tomography of Peats

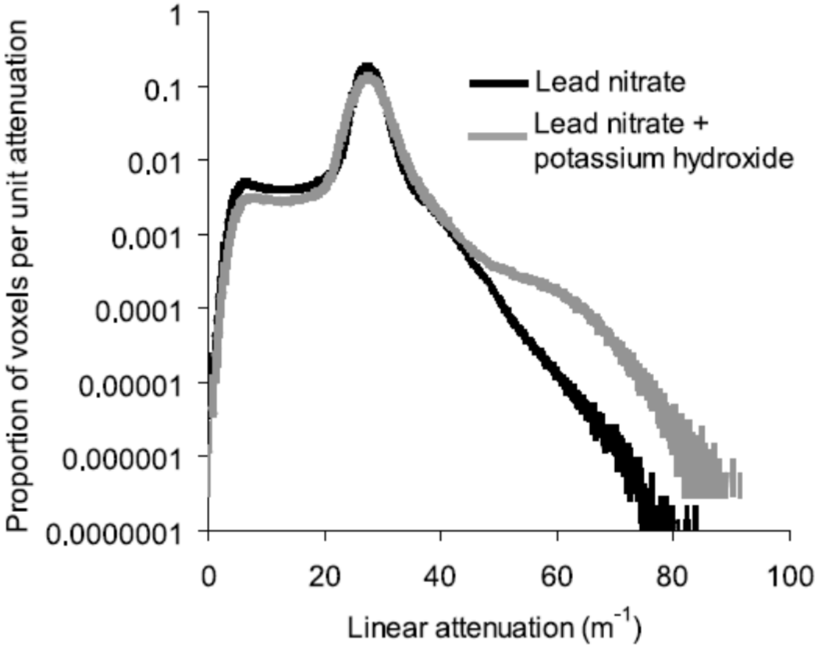
- Low density makes CT difficult
- Contrast agents: adsorbed Pb
- X-ray intensity ***I***

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

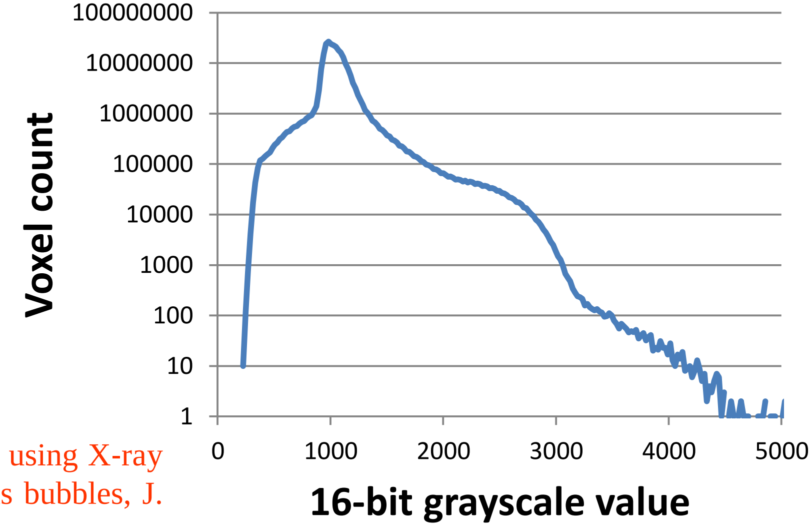
μ Linear attenuation coefficient

I_0 Original beam intensity

x Path length through sample



- Related to voxel gray scale distribution



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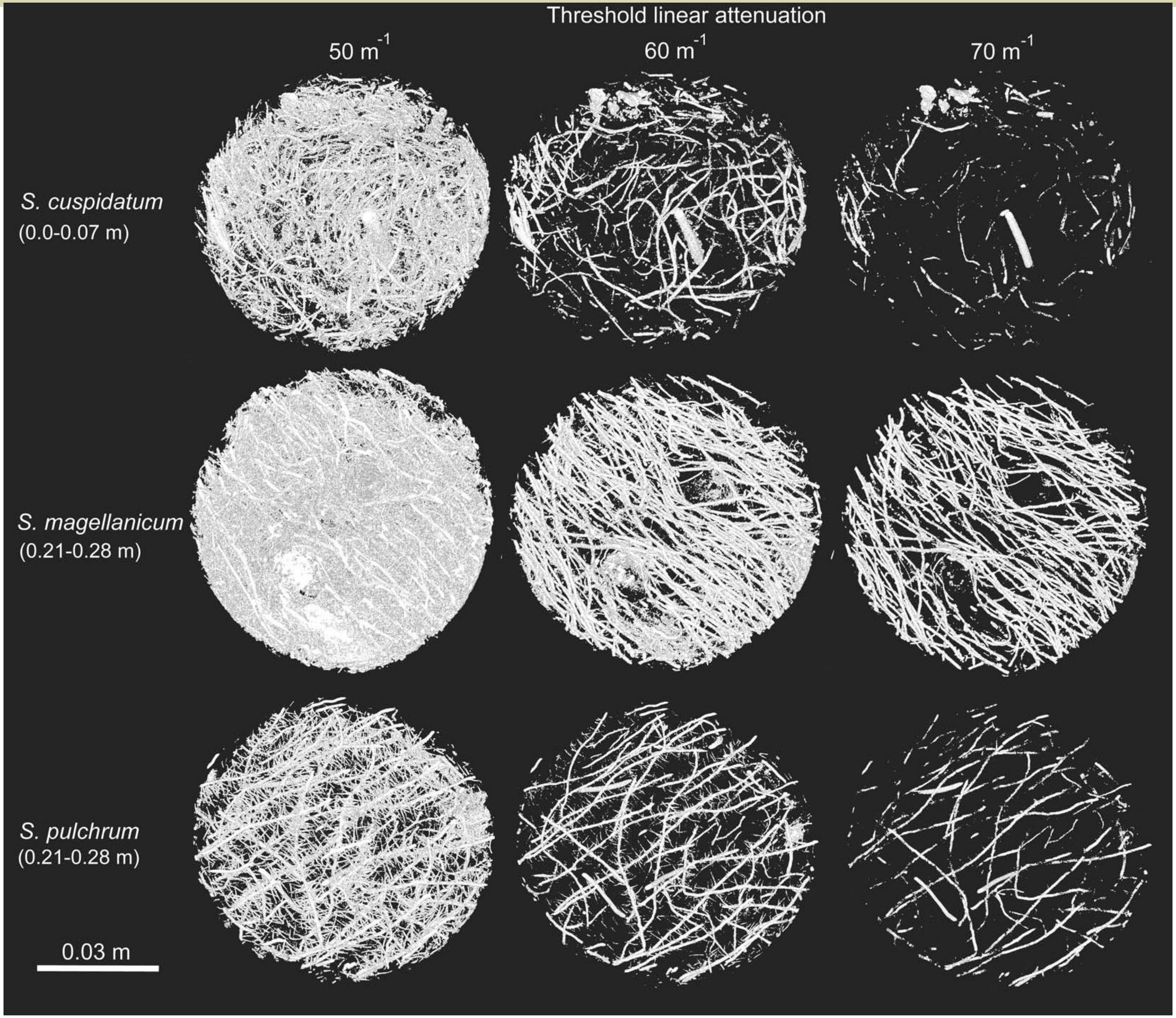
Computed Tomography of Peats

- 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?



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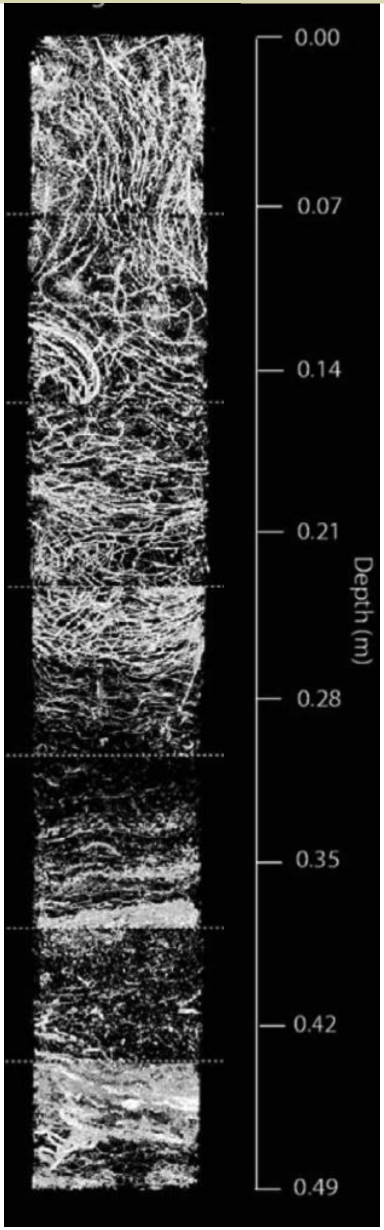
Computed Tomography of Peats

- S. magellanicum



Organic structures not clearly visible

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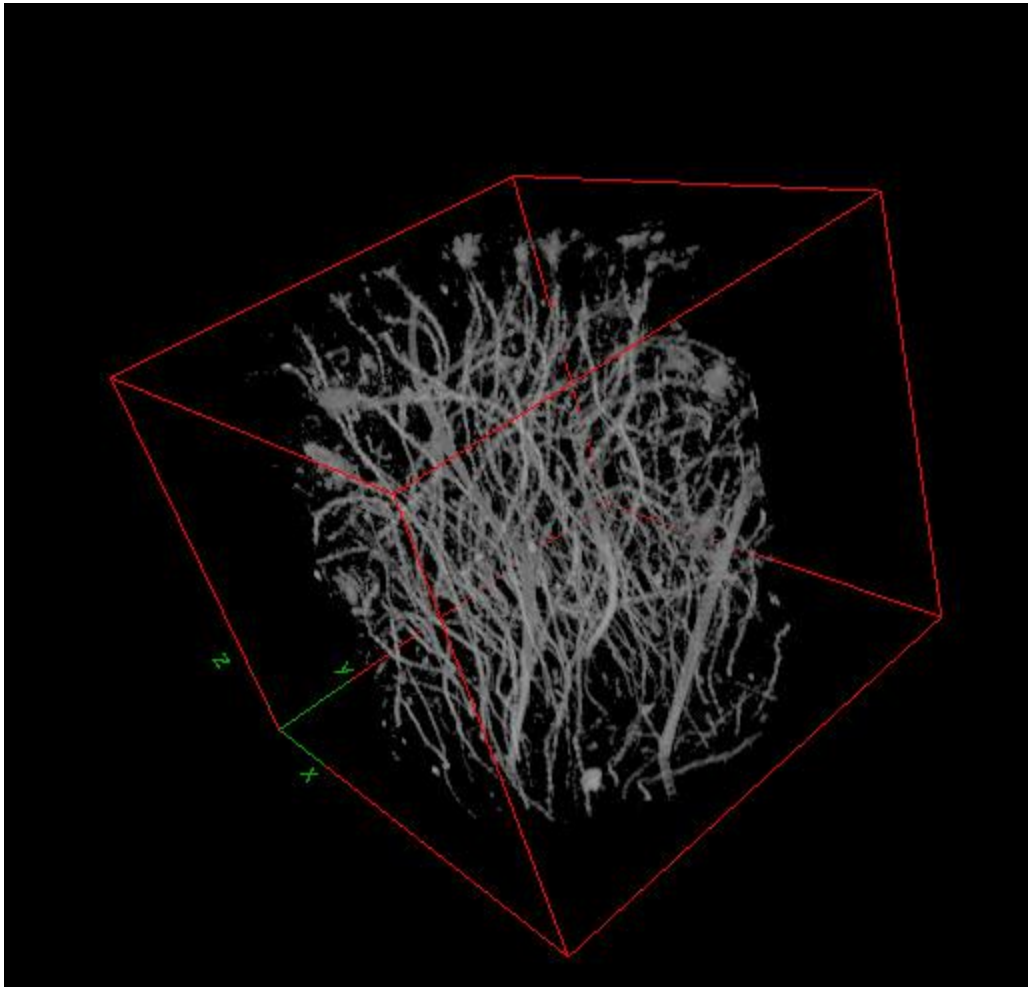
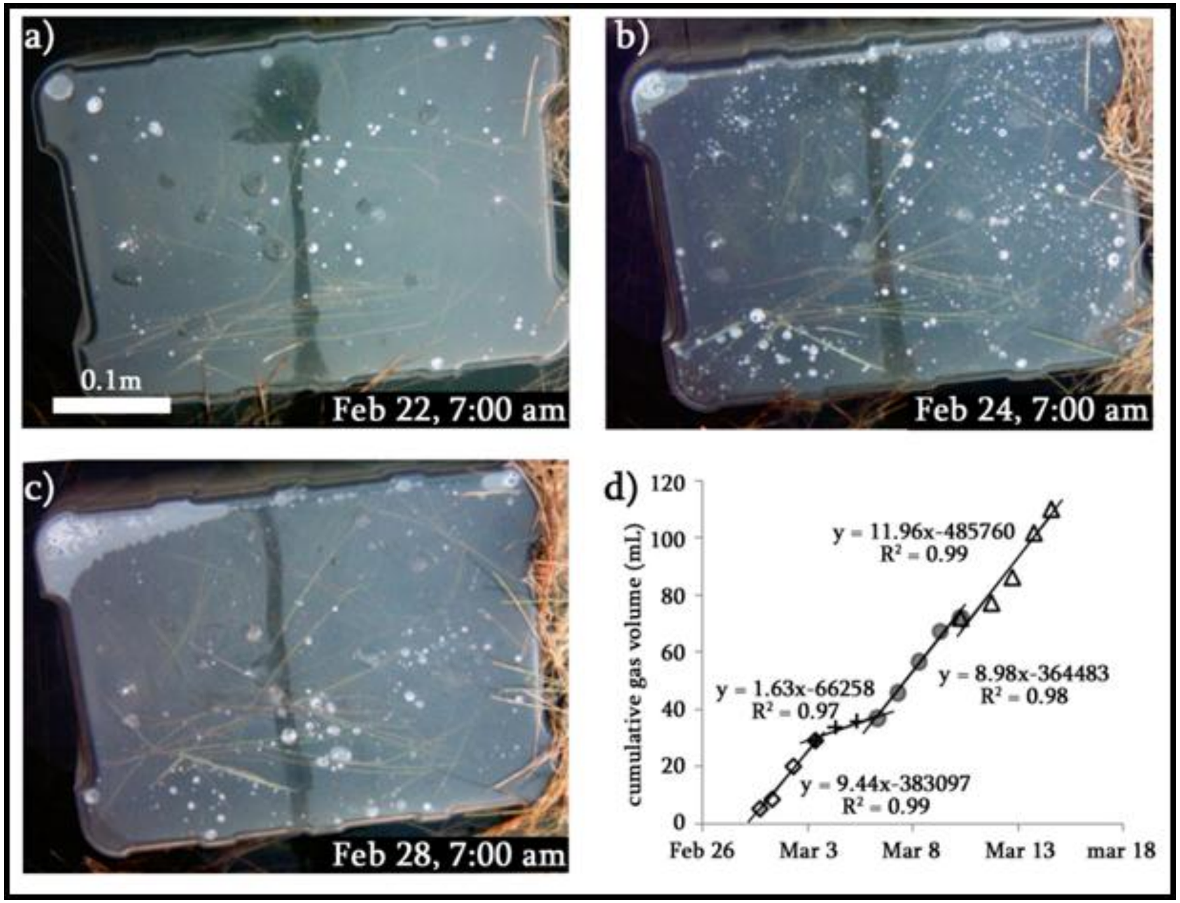
Application to Peat and other Porous Media

- Peat surface
- Living/minimally decomposed

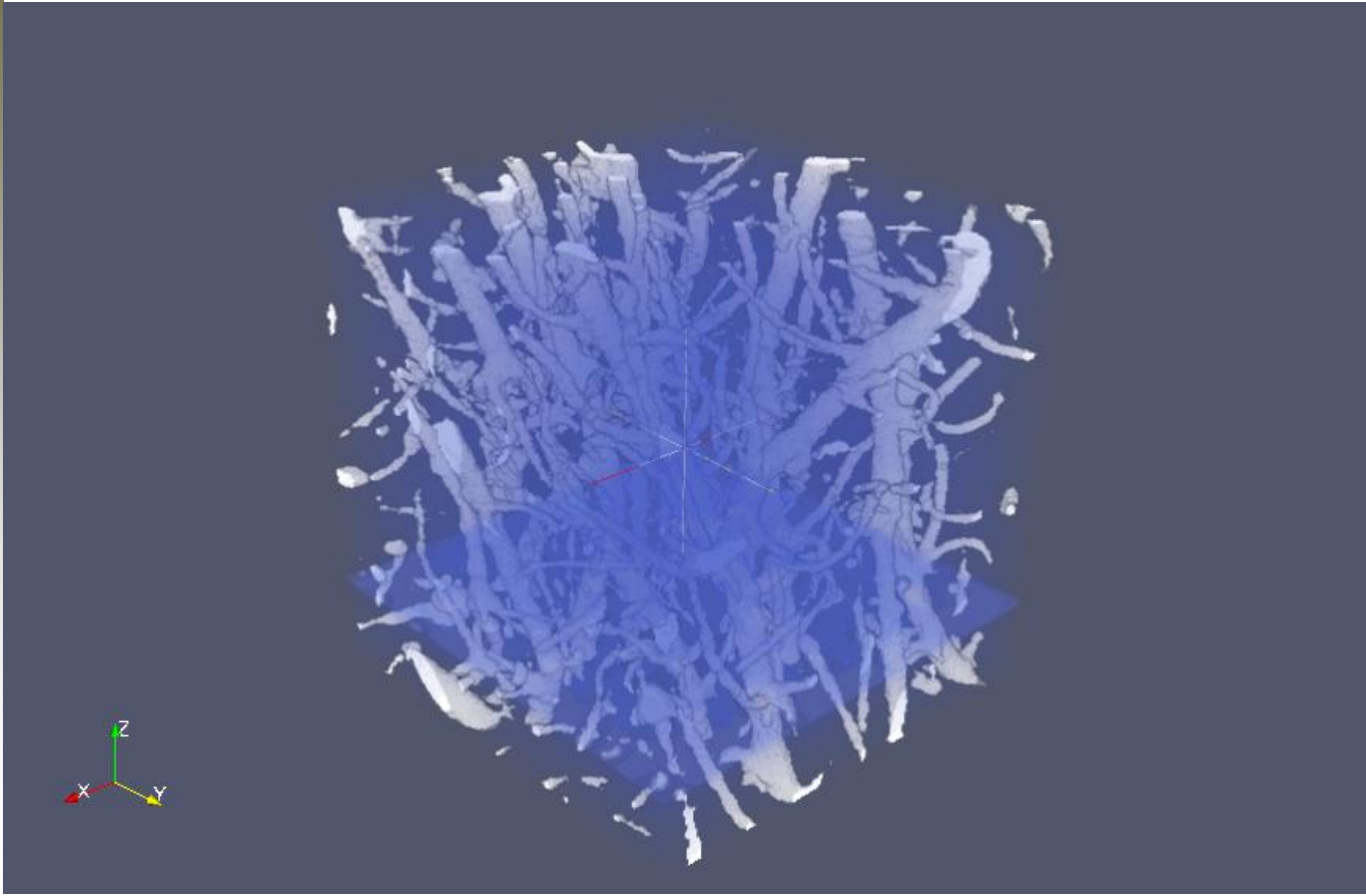


Where the bugs are: source terms for gas

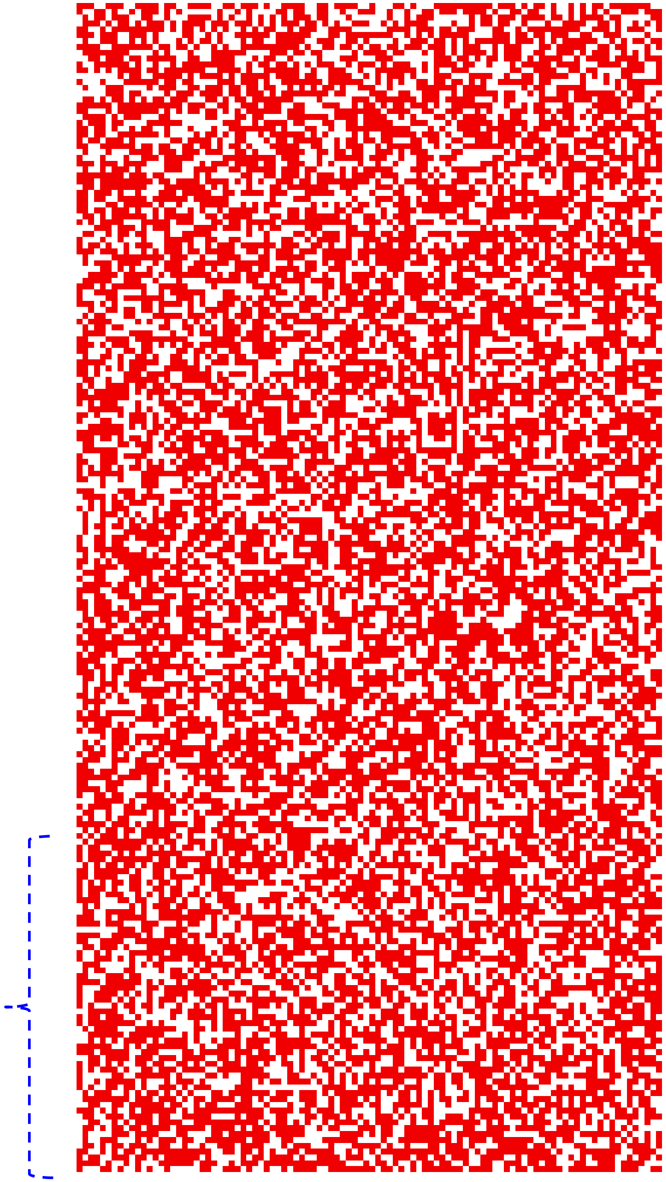
- Sensitive to Eh and other chemistry
- In micropores and/or on surfaces?
- First cuts:
  - Planar source
- Rates?



First 3D simulation



LBM Model (w/ porous medium)



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

Glaser, P. H., J. P. Chanton, P. Morin, D. O. Rosenberry, D. I. Siegel, O. Ruud, L. I. Chasar, and A. S. Reeve (2004), Surface deformations as indicators of deep ebullition fluxes in a large northern peatland, Global Biogeochem. Cycles, 18, GB1003, doi:10.1029/2003GB002069.

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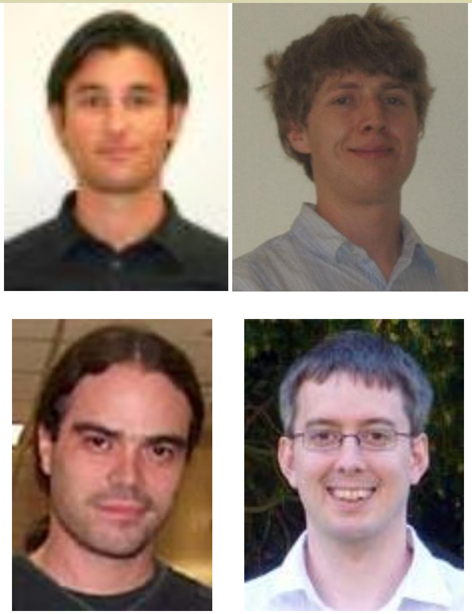
    - Jamie Mudrich



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