A Contact Angle Model for the Parallel Free Surface Lattice Boltzmann Method in waLBerla

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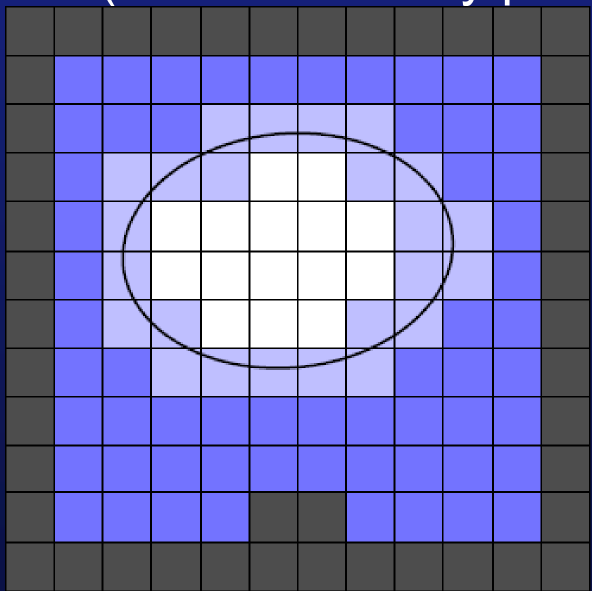
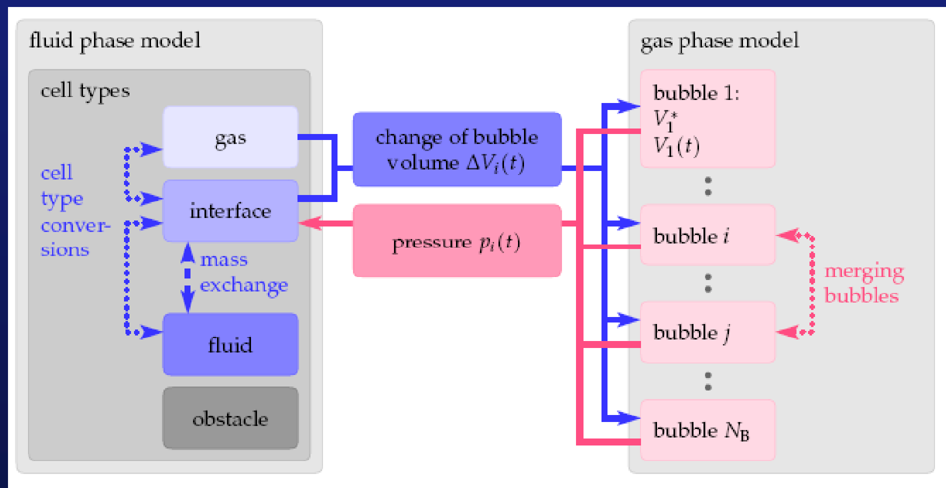
Outline

- Free-Surface LBM
  - Boundary condition
    - Gas volume pressure
    - Surface tension
  - Wetting model
    - Curvature computation for surface tension and contact angles
- Validation
  - Microdrops
  - Capillary
- Conclusion

Free-Surface LBM
Cell types and gas phase model

- „Free surface“ is „two phase“, however:
  - Compute only liquid phase
  - Model gas phase by ideal gas equation (no flow but only pressure is modeled)





T. Pohl, “High Performance Simulation of Free Surface Flows Using the Lattice Boltzmann Method”, PhD Thesis, 2008, http://www10.informatik.uni-erlangen.de/Publications/Dissertations/Diss_Pohl_2008.pdf

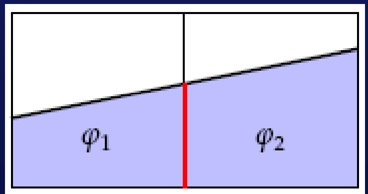
N. Thürey, “Physically based Animation of Free Surface Flows with the Lattice Boltzmann Method”, PhD Thesis, 2007, http://www10.informatik.uni-erlangen.de/Publications/Dissertations/Diss_Thuerey_070313.pdf

Free-Surface LBM
Fraction of fluid volume in Interface cells

- Interface cells store fluid fraction (similar to VoF)
- Fluid advection:
  - Mass transfer between interface and liquid cells
  - Mass is conserved

$$\Delta m_i(x,t) = \begin{cases} 0 & \text{for} \quad (x+c_i) \in \mathcal{C}^{\mathrm{G}} \\ F_{\bar{i}}(x+c_i,t) - F_i(x,t) & \text{for} \quad (x+c_i) \in \mathcal{C}^{\mathrm{F}} \\ \frac{1}{2}\left[\varphi(x,t) + \varphi(x+c_i,t)\right]\left[F_{\bar{i}}(x+c_i,t) - F_i(x,t)\right] & \text{for} \quad (x+c_i) \in \mathcal{C}^{\mathrm{I}} \end{cases}$$

  - For two interface cells a weighting factor depends on the fill levels



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Free-Surface LBM
Interface boundary condition

- Simplification of stress tensor at interface
  - Navier-Stokes for incompressible fluid

$$\rho\delta_t\vec{u} + \rho(\vec{u}\cdot\nabla)\vec{u} = \nabla\sigma$$

  - with stress tensor

$$\sigma_{ik} = -p_G(\vec{x},t)\delta_{ik} + \rho\nu(\delta_k u_i(\vec{x},t) + \delta_i u_k(\vec{x},t))$$

  - Treating gas as inert phase with vanishing density reduces stress to sole influence of pressure

$$p_G = p_V + p_\gamma$$

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Free-Surface LBM
Interface boundary condition: gas pressure

- Gas volume pressure
  - Initial state with initial gas volume
  - Tracking gas volume changes in all interface cells leads to current volume
  - Pressure is ratio of current volume to initial volume

$$p_V = \frac{V^{init}}{V(t)}$$

  - Remarks:
    - Tracking gas volume changes throughout a parallel simulation involves means of all-to-all communication
    - Gas pressure depends on accurate mass tracking in interface cells
    - Supports continuous inflation of bubbles

Free-Surface LBM
Interface boundary condition: surface tension

- Surface tension
  - Energy balance relates pressure to surface tension:

$$p_\gamma \cdot dV = \gamma \cdot dA$$

  - Young-Laplace equation (for 3 dimensions)

$$p_\gamma = 2\gamma\kappa(\vec{x}, t)$$

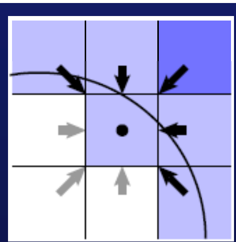
  - Takes only mean curvature into account, which is the mean value of the two principal curvatures

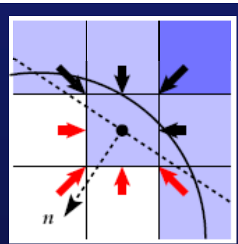
Free-Surface LBM

Interface boundary condition in LBM

- Reconstruction of distribution functions at interface
  - Simplified stress tensor means in LBM:
    - Velocity of liquid and gas phase have to be equal at interface
    - Force of the gas has to be balanced with force by fluid
  - Reconstruct distribution functions pointing in opposite direction of surface normal

$$F_i'(x - c_i, t) = F_i^0(\rho_G, v) + F_{\bar{i}}^0(\rho_G, v) - F_{\bar{i}}'(x, t) \quad , \quad x \in \mathcal{C}^{\mathrm{I}} \wedge \left[(x - c_i) \in \mathcal{C}^{\mathrm{G}} \vee c_i \cdot n(x,t) < 0\right]$$





  - Density of gas phase is computed from gas pressure

$$\rho_G = \frac{1}{c_s^2} \cdot p_G$$

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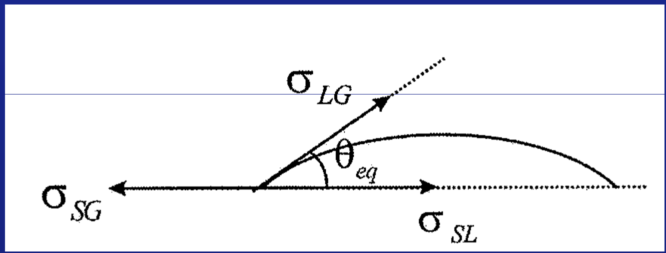
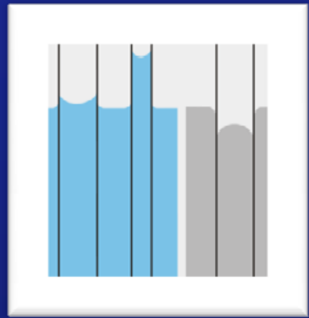
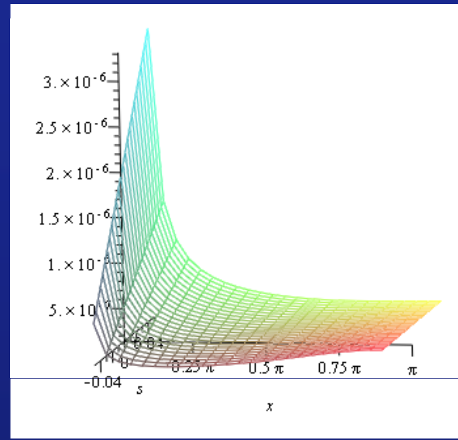
Free-Surface LBM

Wetting Phenomena Theory

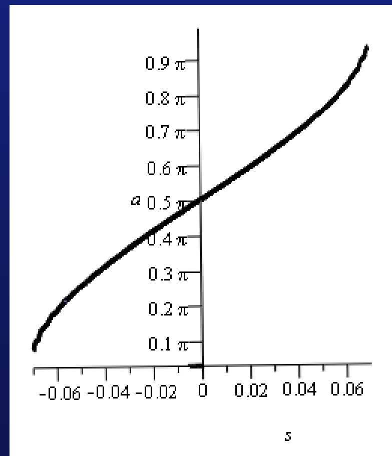






- Always tries to minimize overall energy

$$\min E = \sigma_{SL} A_{SL} + \sigma_{SG} A_{SG} + \sigma_{LG} A_{LG} + E_{pot}$$



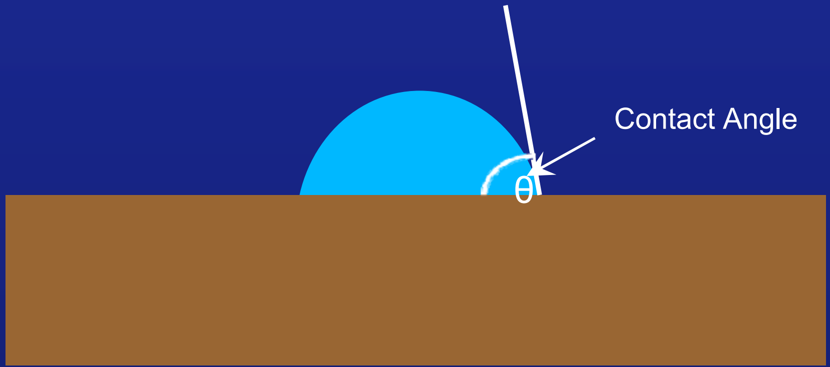
- Neglecting gravity, this leads ultimately to „Young‘s Law“:

$$\sigma_{SL} - \sigma_{SG} + \sigma_{LG} \cos\theta = 0$$

Free-Surface LBM

Capillary force and contact angles

- Different approaches:
  - Define additional “pressure” depending on contact angle
    $$p_G = p_V + p_\gamma + p_\theta$$



have been implemented:

  - Introduce additional force based on Young’s equation
    $$F_x = \sigma_{LG}\cos(\theta_d) - \sigma_{LG}\cos(\theta_{eq})$$
  - Enforce a curvature at triple line by manipulating curvature computation
    $$p_\gamma = 2\gamma\kappa(\vec{x}, t)$$
  - Introduce additional force depending on surface energies
    $$\vec{F} = (\sigma_{SG} - \sigma_{SL}) \int_C \vec{n} \times d\vec{s}$$

S. Donath, to be published 2010, http://www10.informatik.uni-erlangen.de/

Free-Surface LBM

Surface curvature computation

- Calculating the surface curvature
  - Needs information of a 5x5x5 neighborhood
  - For parallelization: Split in 3 parts:
    - Surface normal
    - Reconstruction of surface point
    - Surface curvature
  - Only one layer has to be communicated for parallelization

Free-Surface LBM

Surface curvature computation

- Calculating surface normal
  - Treat fluid fraction of cells as scalar field
  - Compute the gradient and its normal by Parker-Youngs approximation

$$n'_{x,y,z} = \sum_{dx,dy,dz \in [-1,0,+1]} -\omega_{dx,dy,dz}\ \varphi_{x+dx,y+dy,z+dz}\ \langle dx, dy, dz \rangle$$

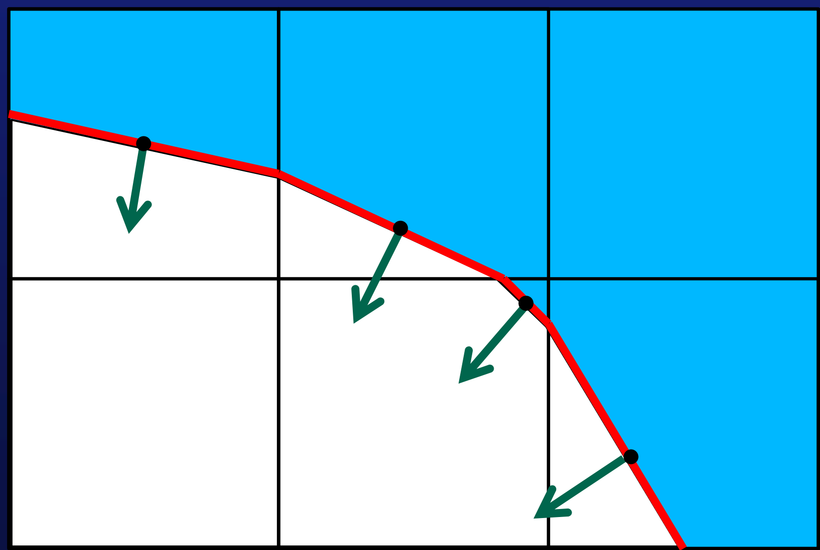
$$n_{x,y,z} = \frac{n'_{x,y,z}}{\left\| n'_{x,y,z} \right\|}$$

$$\omega_{dx,dy,dz} = \begin{cases} 1 & \text{for} \quad \|\langle dx, dy, dz \rangle\| = 1 \\ 2 & \text{for} \quad \|\langle dx, dy, dz \rangle\| = \sqrt{2} \\ 4 & \text{for} \quad \|\langle dx, dy, dz \rangle\| = \sqrt{3} \end{cases} .$$

  - Similar to Center-of-Mass method as used in VoF, but with coefficients different from 1

Free-Surface LBM
Surface curvature computation

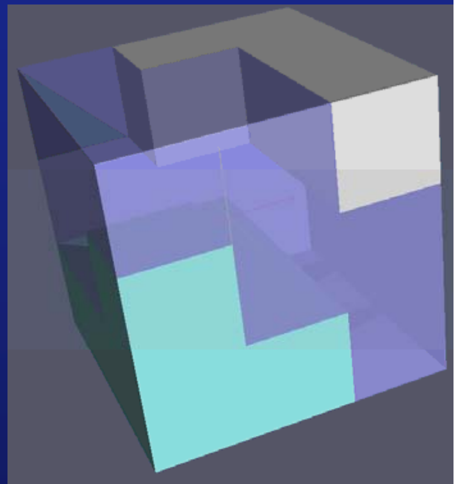
- Calculating the surface point
  - For simplification: Surface fraction in a cell is assumed to be planar, fulfilling two requirements:
    - Plane's normal is equal to surface normal
    - Plane bisects cell into two volumes corresponding to fluid fraction of cell

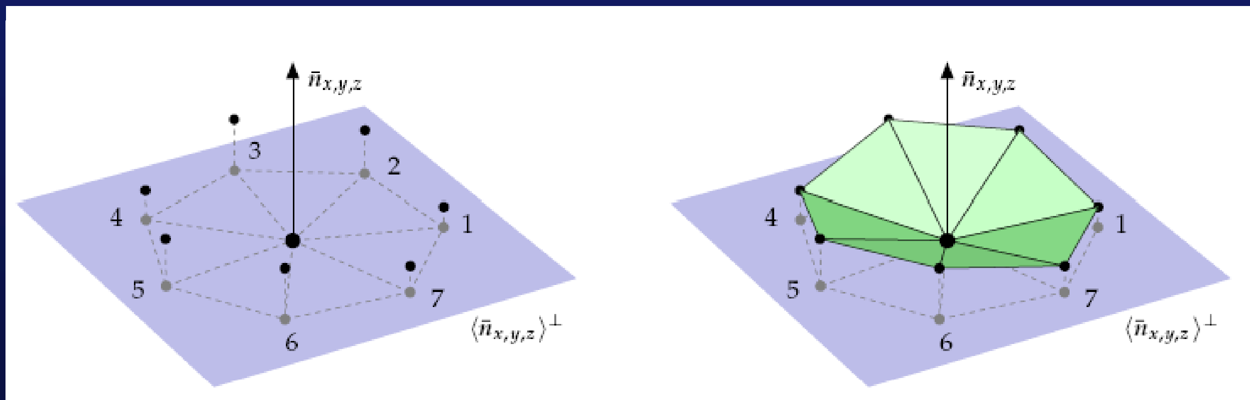


Free-Surface LBM
Surface curvature computation

- Calculating the surface curvature (of 3x3x3 neighborhood's interface cells)
  - Select appropriate subset of neighboring surface points (to avoid degenerated triangles)
  - Local triangulation of chosen surface points and calculation of surface curvature

(similar algorithm as described in: G. Taubin. *Estimating the Tensor of Curvature of a Surface from a Polyhedral Approximation*. In Proceedings of the Fifth International Conference on Computer Vision, pages 902–905, 1995)

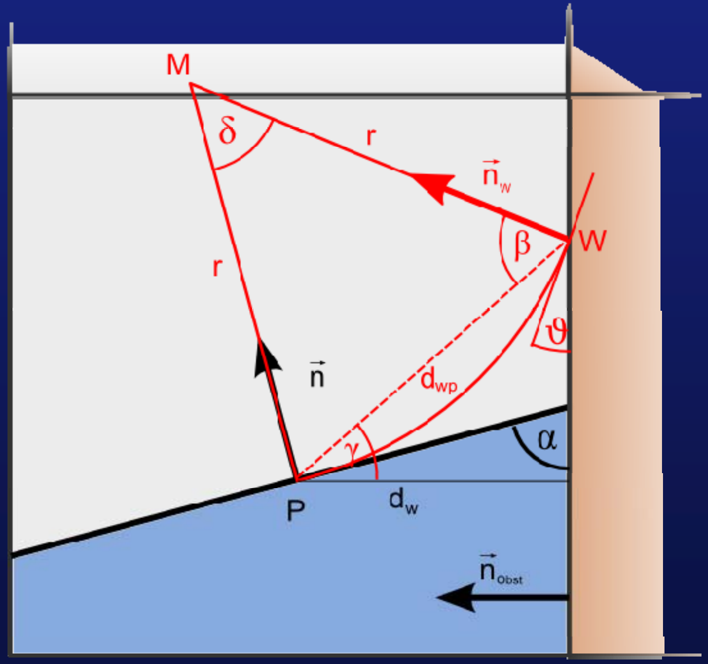


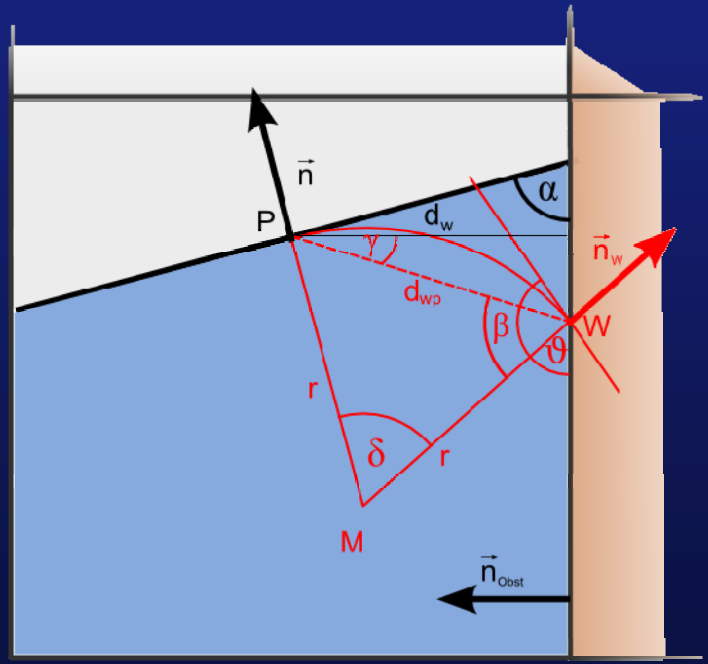


Free-Surface LBM

Curvature manipulation for contact angles

- Create virtual wall points and normals to reproduce desired curvature by constructing circular surface fulfilling the requirements
  - Same incline at surface point
  - Targeted contact angle at wall





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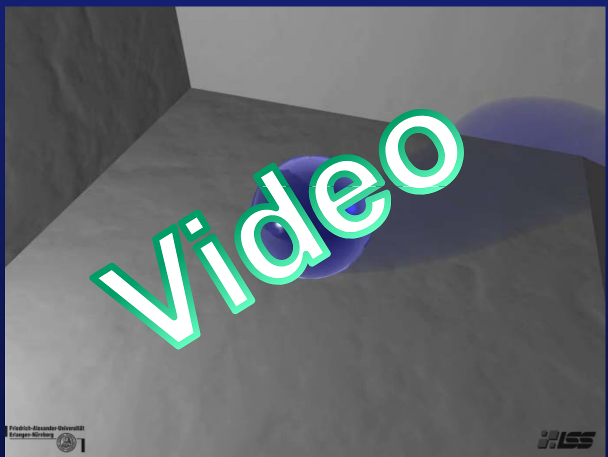
Validation

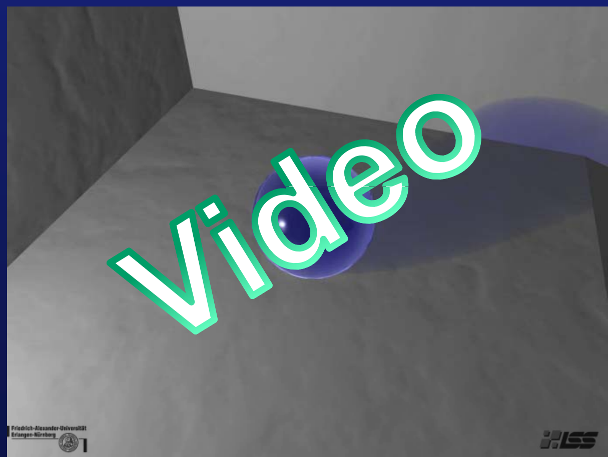
Microdrop on plate

- Drop on Plate
  - Defined volume, prescribed contact angle, measure height

$$h = \sqrt[3]{\left(\frac{1}{1-\cos\theta} - \frac{1}{3}\right)^{-1} \frac{V}{\pi}}$$



Θ=30°, h_{ideal}=6.86, h=7.05 (3%)

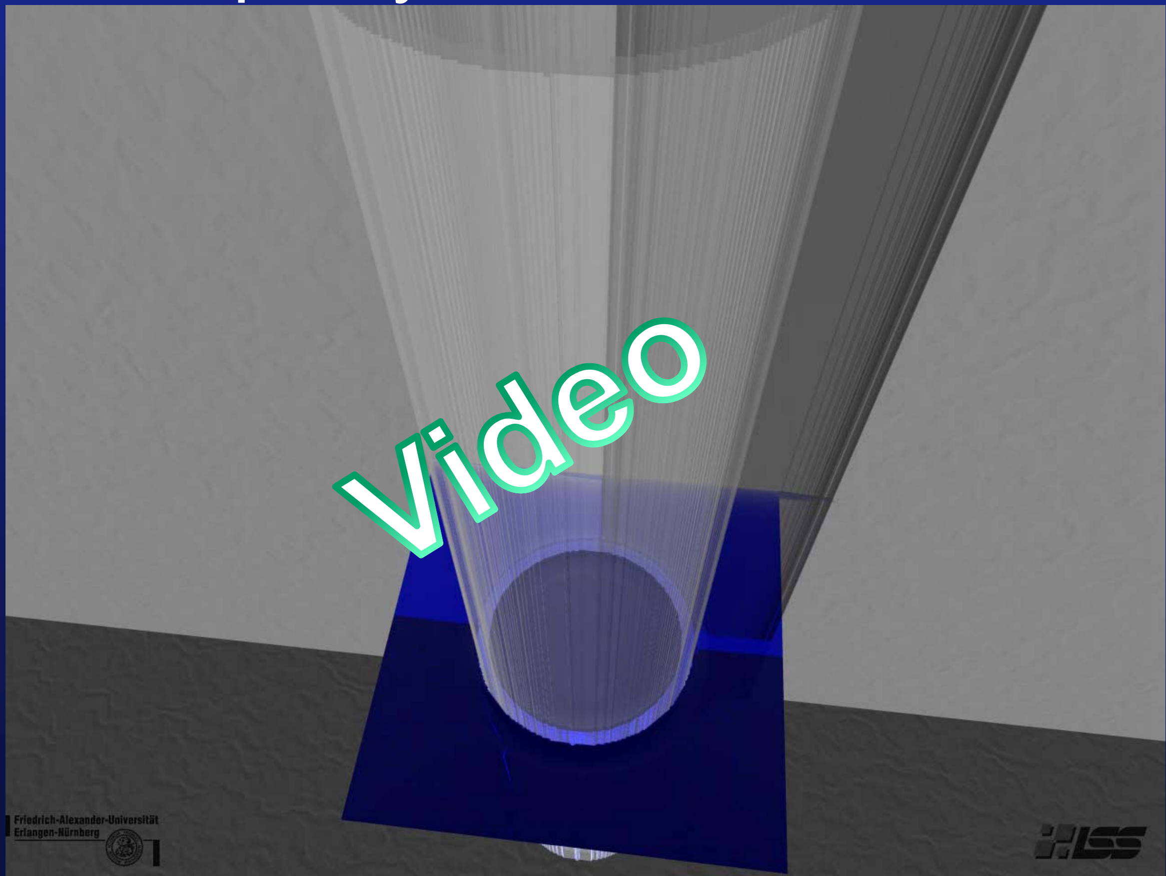


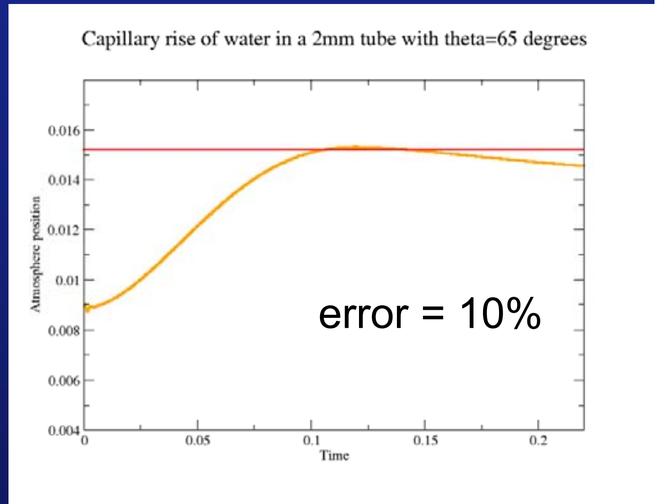
Θ=90°, h_{ideal}=15.12, h=15.04 (1%)

Θ=150°, h_{ideal}=22.49, h=21.72 (3%)

Validation
Capillary rise and depression

- Capillary rise of water with 65°

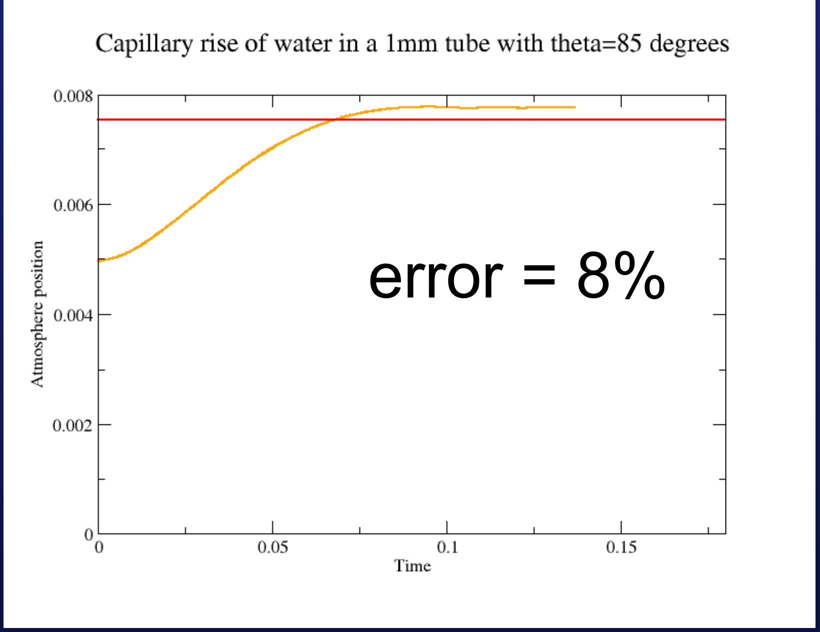


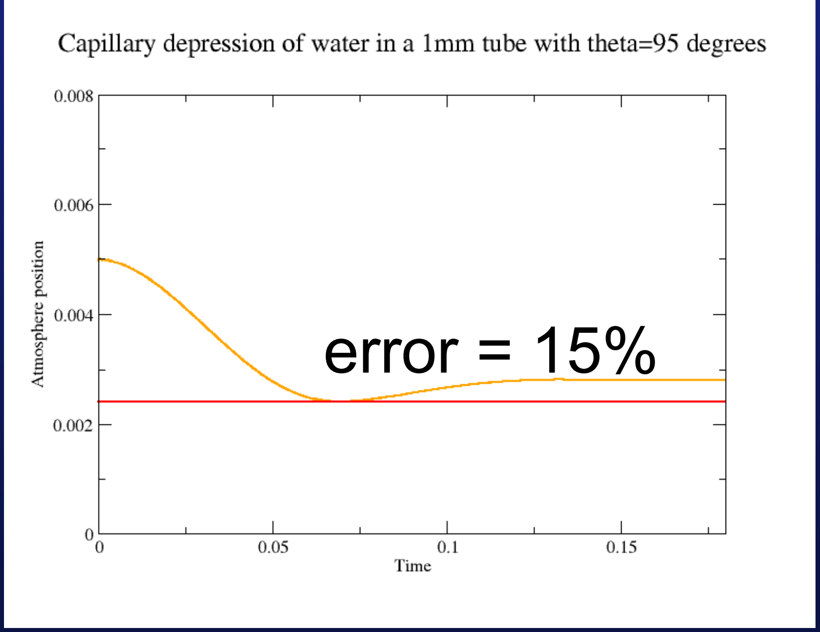


Validation

Capillary rise and depression

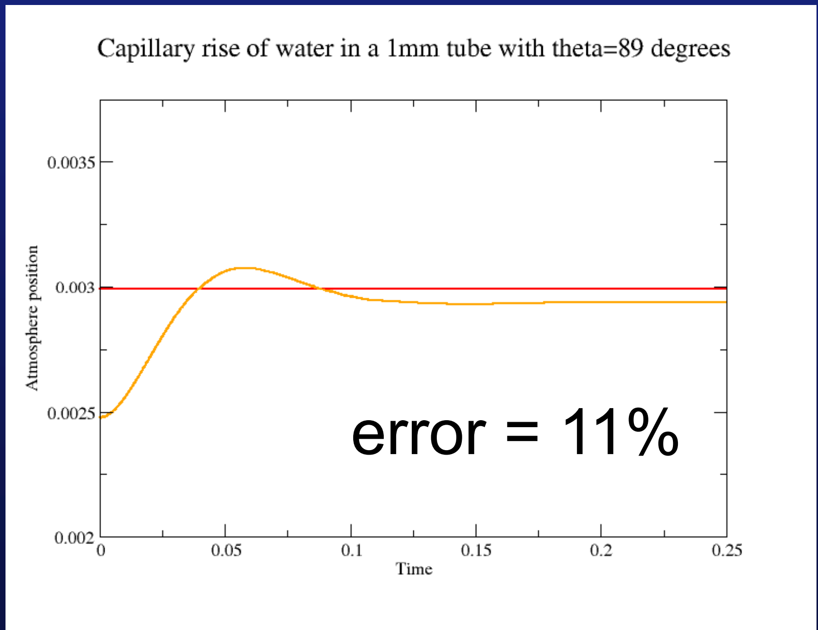
- Capillary rise and depression under influence of gravity: $$h = \frac{2\sigma_{LG}\cos\theta}{\rho g r}$$

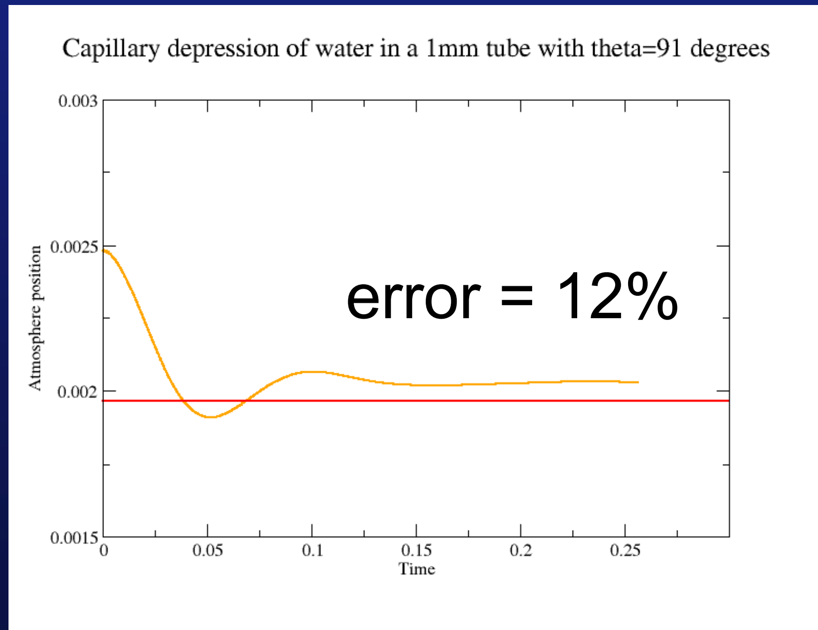




Validation
Capillary rise and depression

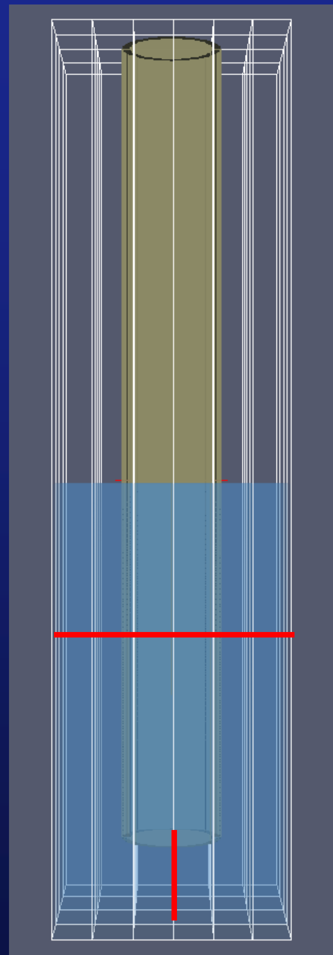
- Capillary rise and depression under influence of gravity: $h = \frac{2\sigma_{LG}\cos\theta}{\rho g r}$





Validation
Possible error sources

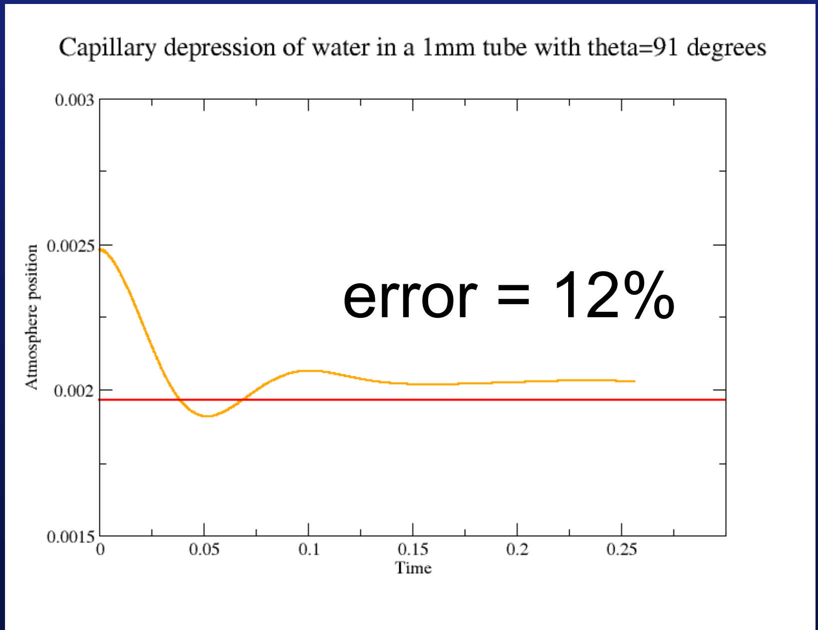
- Number of points taken into account in curvature computation
  - Direct influence on accuracy
- Influence of collision model
  - Up to now only SRT, have to use small T
- Influence of domain/boundary
  - Width of domain restricts volume of available water, thus forces outside of capillary influence rise behavior
  - Distance of capillary to tub ground limits amount of water that can flow in/out
  - Capillary has same wetting behavior on outside wall, forcing water against the flow



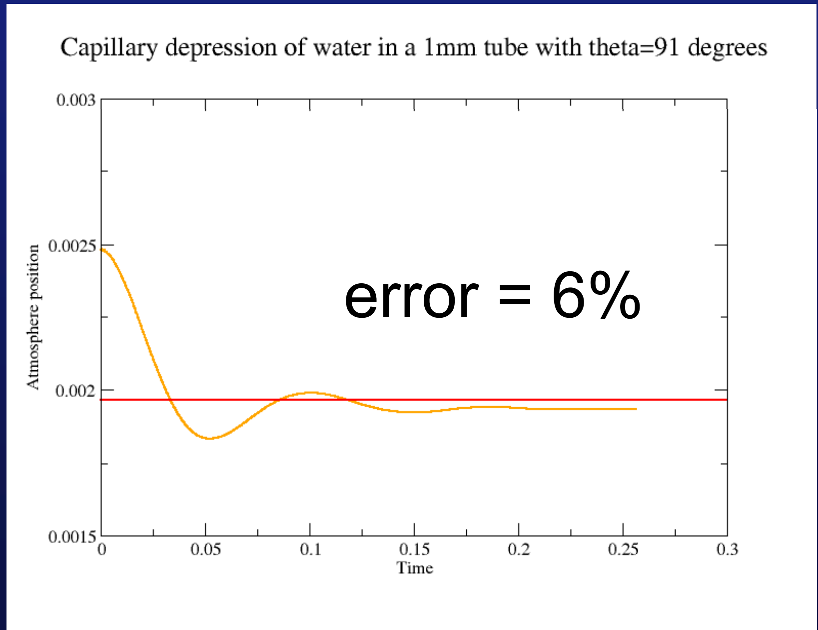
Validation
Possible error sources

- Influence of tub size

2% of tub volume 16.9mm³

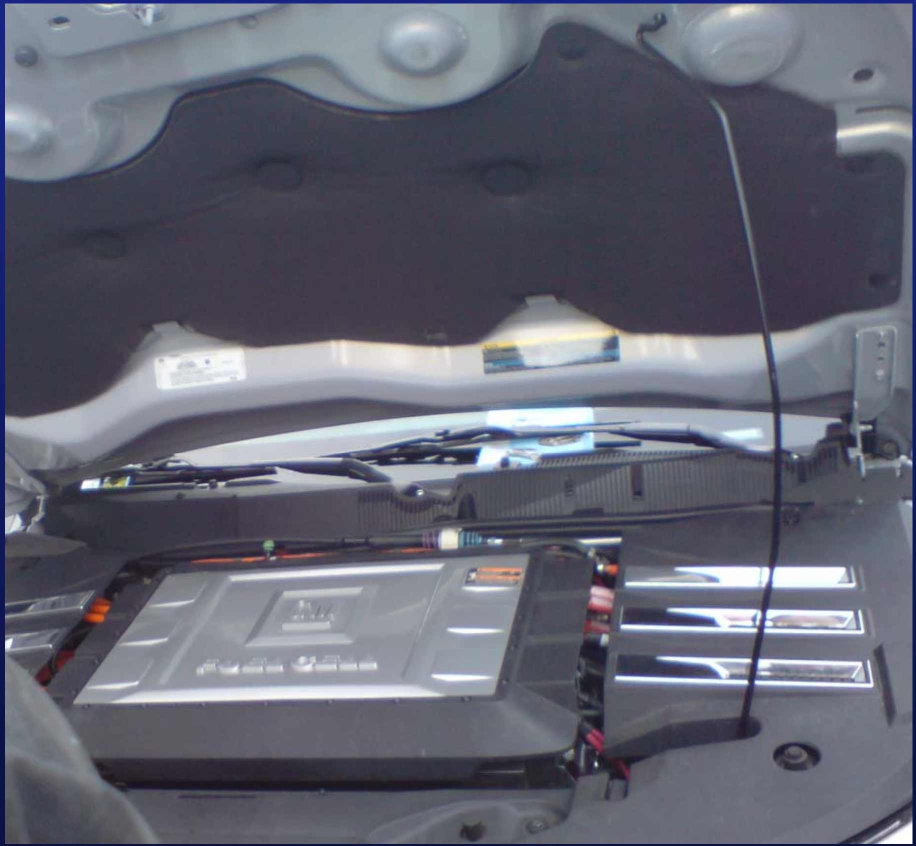


1% of tub volume 32.4mm³



Application

- Liquid Water Management in Fuel Cell
  (Derive input values for Darcy-like evaluations)



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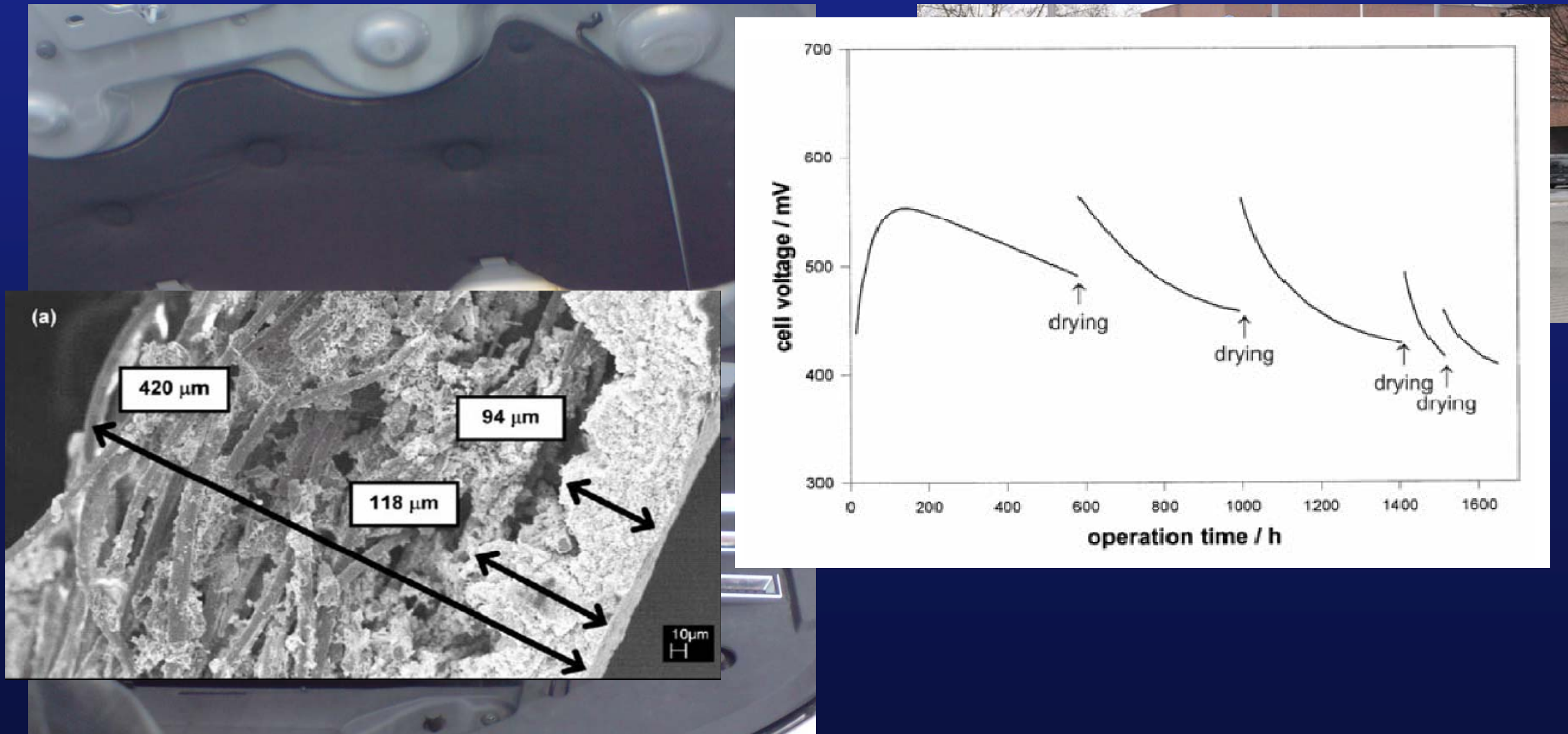

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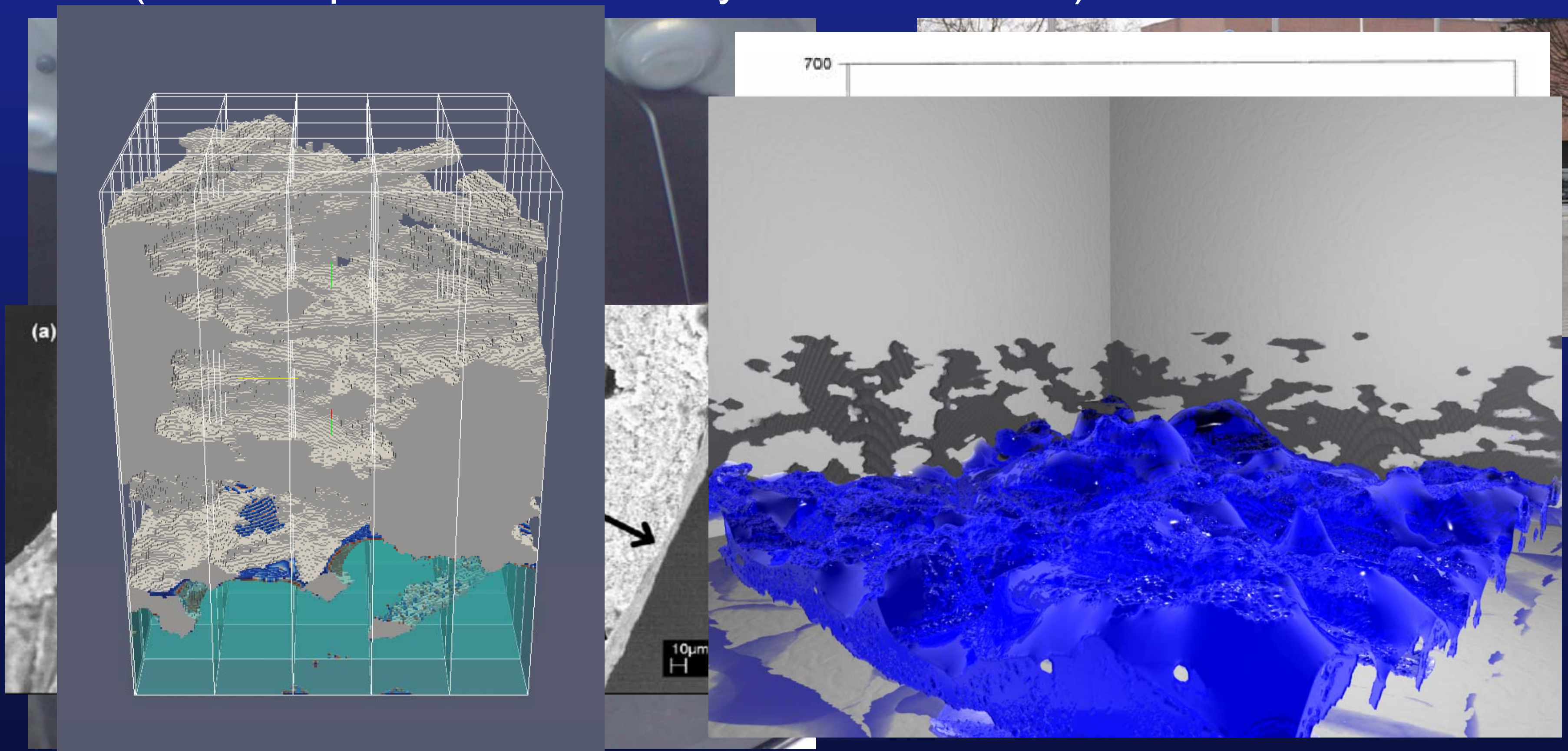

Conclusion

- Free-Surface Method
  - Parallel
  - Surface Tension
  - Capillary Effects
  - Satisfying accuracy
  - Enables large scale real-world applications
- Compared to other methods (like Shan-Chen)
  - Explicitly modeled to enable direct transition from real to lattice values
  - Viscosity, surface tension and contact angle configured separately

Outlook

- Further Validation
  - Study of dynamic behavior, compare to Washburn's equation (1921)
- Further models
  - Model based on wetting force (constant force depending on material properties)

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The End

Thank you for your attention!

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