School of Mechanical Engineering
FACULTY OF ENGINEERING

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Evaluation of a multiphase LB model for coating flows

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Schéma de Boltzmann sur réseau ; méthodes et applications, CEMAGRAF, Paris. Vendredi 05 décembre 2008

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What are coating flows?

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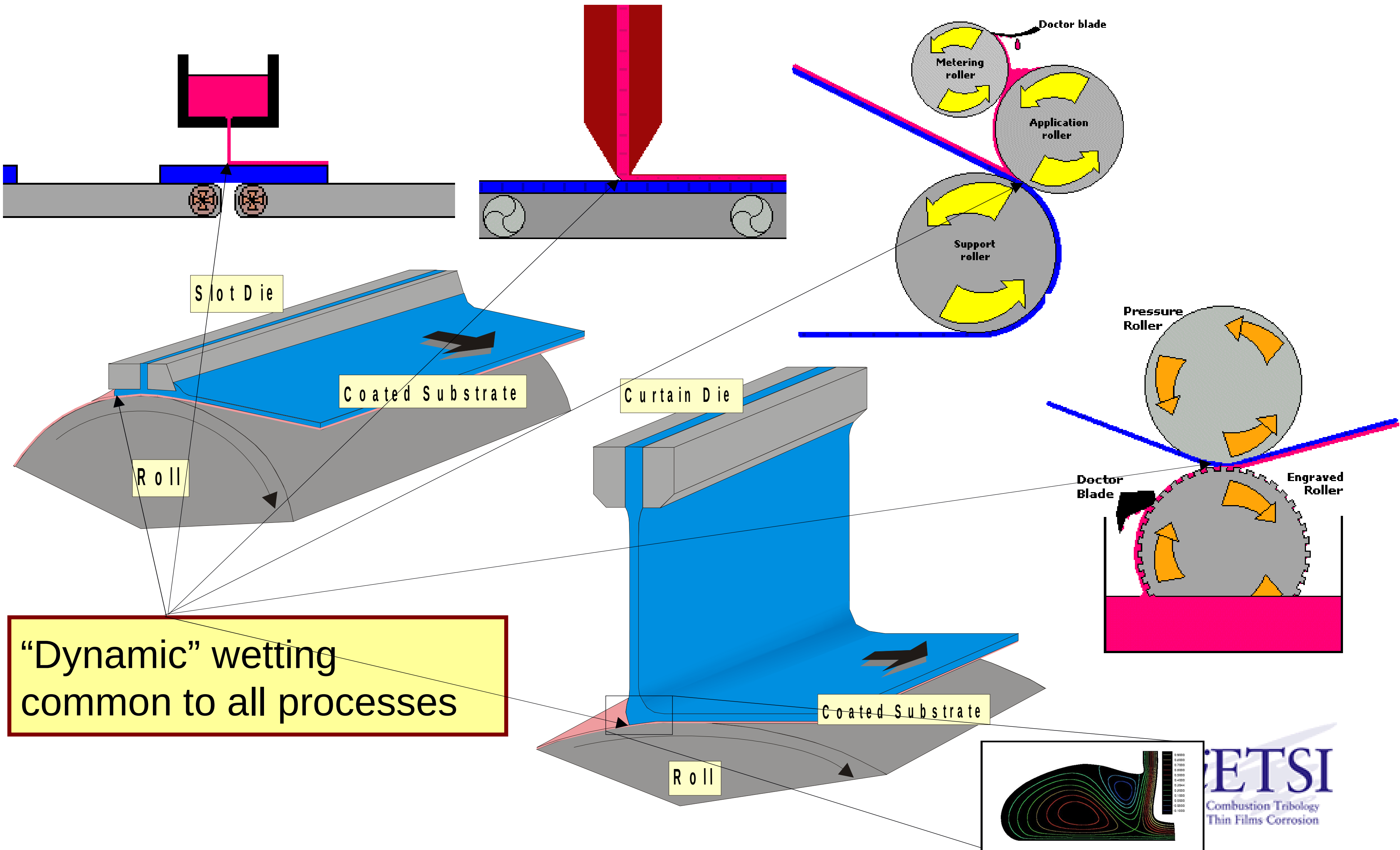

"Dynamic" wetting common to all processes

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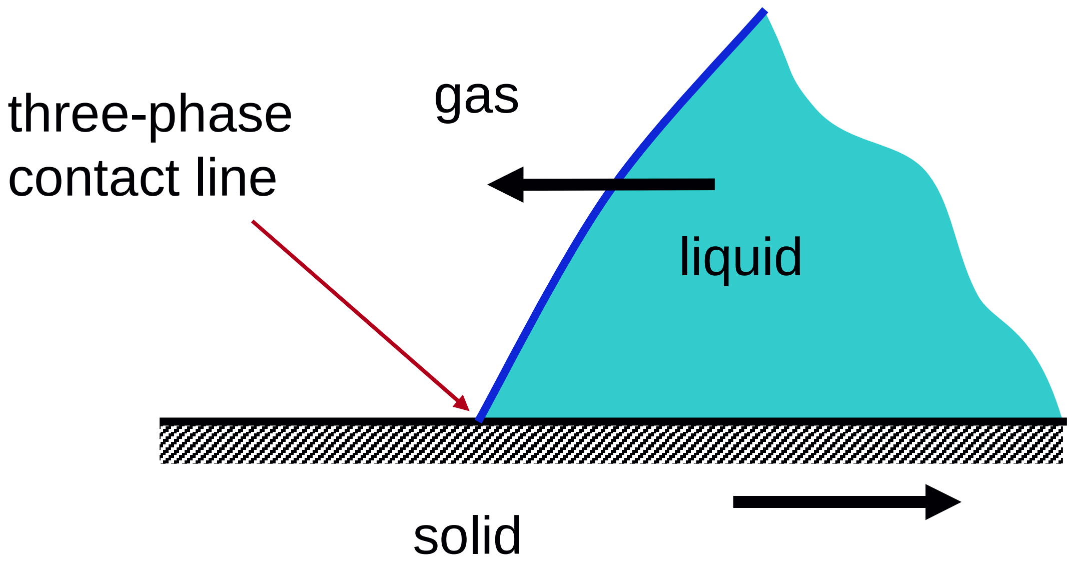
Wetting

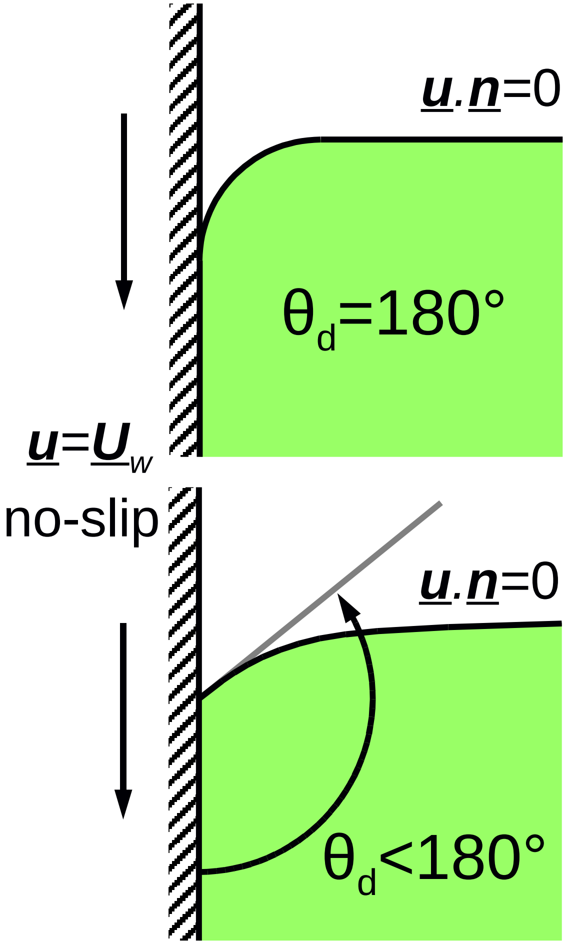
- Can categorize as either **natural wetting** or **forced wetting**
  - –Droplet spreading → natural wetting
  - –Coating flows → forced wetting
- Central to wetting is the problem of the **moving contact-line**



In first part of talk gas will be neglected – modelling only includes liquid

Problems with continuum modelling

- Presence of a finite contact angle causes problems
- Boundary conditions on liquid-gas and solid-liquid interfaces are in conflict at the contact line
- Contact line is stationary, but boundary is moving
- **Shear stress is infinite**
- Usually have to **prescribe contact angle and slip (relieve stress)**



Problems With Slip Models

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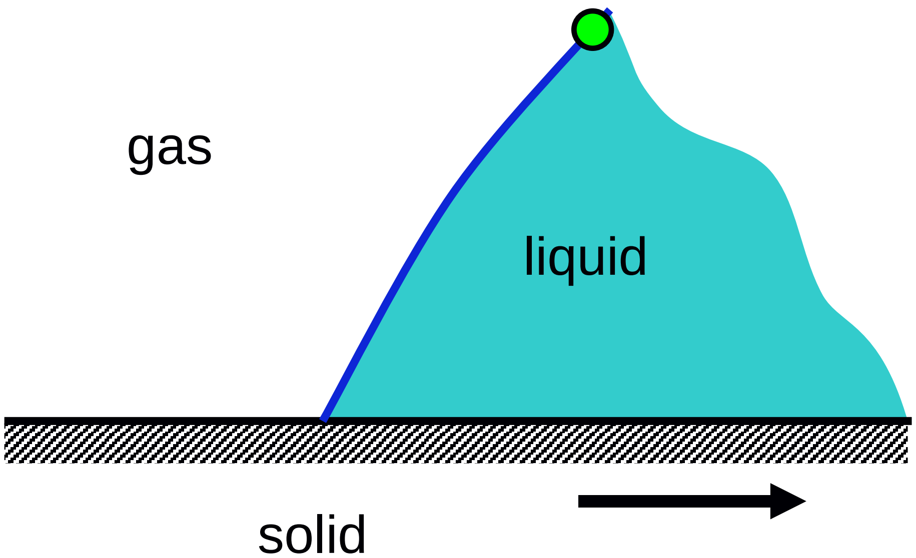

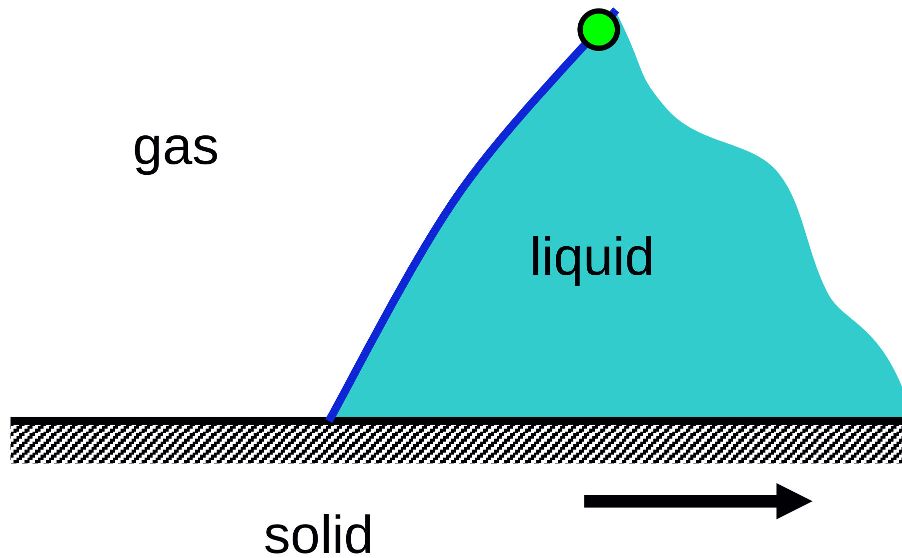

- ‘Rolling’ motion observed in experiments
- Particle on liquid-gas interface passes through contact line and onto solid-liquid interface

- ‘Sliding’ motion produced by most slip models
- Particle on liquid-gas interface never reaches contact line, because $u \rightarrow 0$

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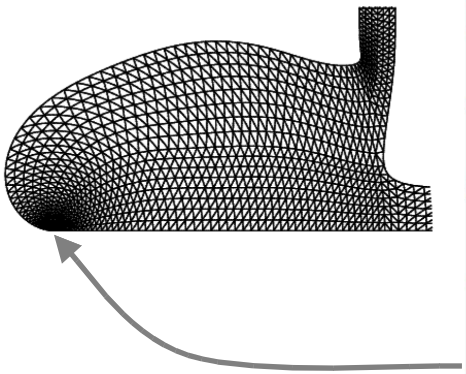
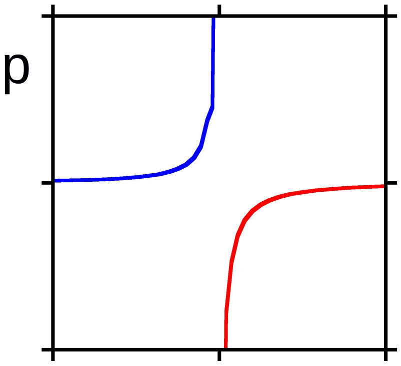
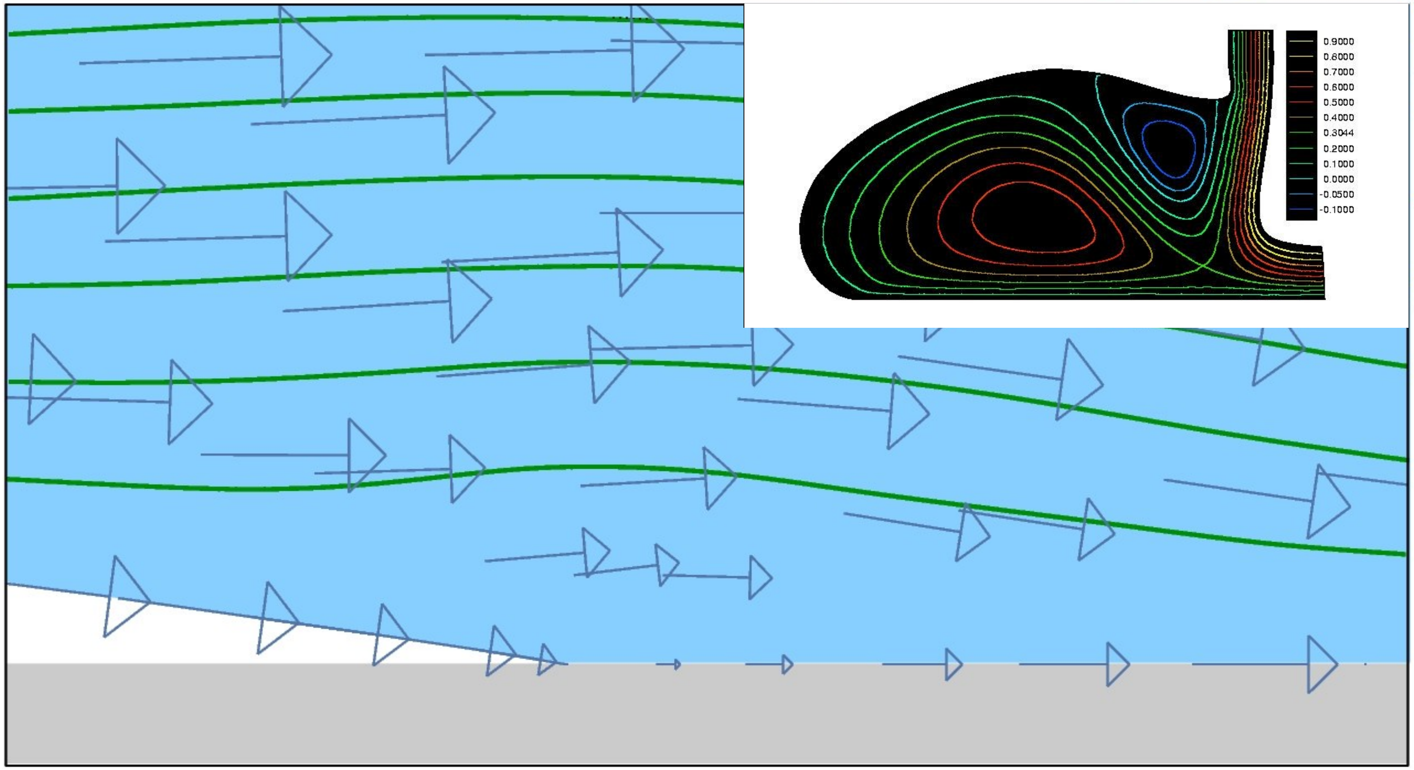
Problems With Slip Models







- Coating flows driven at high speed often have large θ_d
- Slip region produces **obstacle-type flow**
- Pressure is **singular**

`Interface Formation Model' of Shikhmurzaev

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- Based on idea of relaxation of surface tension
  - *–Interfacial tension changes smoothly from L-G to L-S*
  - *–Near contact line interfacial tensions deviate from equilibrium values*
  - *–Force balance at contact line gives contact angle as function of flow*
- The **usual** kinematic and impermeability conditions are replaced with equations describing fluxes between the bulk and the interfaces
- The stress conditions are modified to account for **variable interfacial tensions**
- Liquid velocity at the contact line is not zero – it is determined as part of the solution. Rolling motion preserved.
- Dynamic contact angle is obtained from solution

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`Interface Formation Model' of Shikhmurzaev

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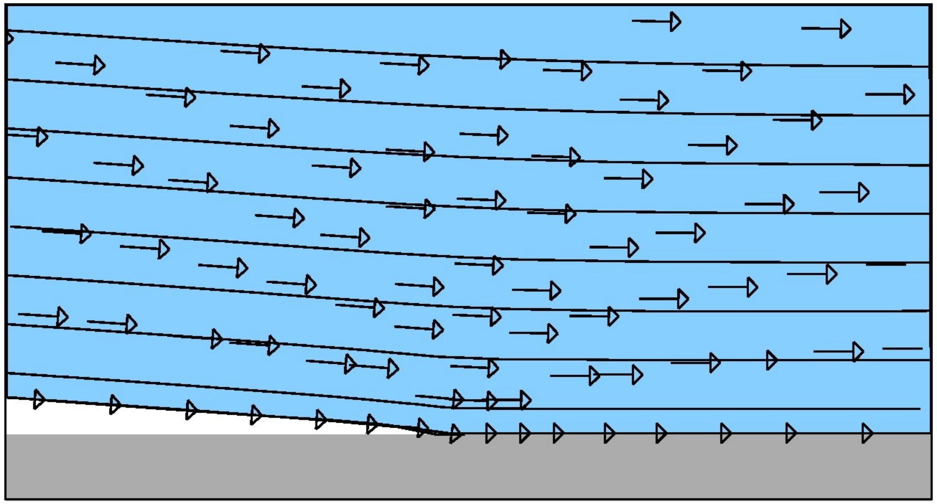
- Model has been used successfully for Stokes flows
  - –Lukyanov & Shikhmurzaev (2007) *Phys. Rev. E* **75**, 051604
  - –considered a microfluidic curtain coater
  - –observed variation of θ_d with a number of flow parameters
  - –used a combined finite element-boundary integral element method
- Navier-Stokes finite element solutions for the full-scale curtain coater are now possible.
- **But,** air-entrainment predictions are not possible.



Diffuse interface models

- Supported by molecular dynamics simulations, a diffuse interface for the **liquid-gas**, **solid-liquid** and **solid-gas** is more amenable to varying interfacial density.
- Diffuse interfaces can rupture and so could help to predict the important aspect of wetting failure, i.e. air-entrainment.
- Several multiphase lattice Boltzmann (LB) approaches exist.
- Wetting line tests for an LB method are:
  - 1. Forced wetting with failure
  - 2. Wetting line hysteresis
  - 3. Natural wetting (spreading/sticking) [agreement with experiments]

Multiphase Model

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Based on work of He, Chen & Zhang (1999)

Use mean-field approximation for intermolecular attractions, and include an exclusion volume effect to…

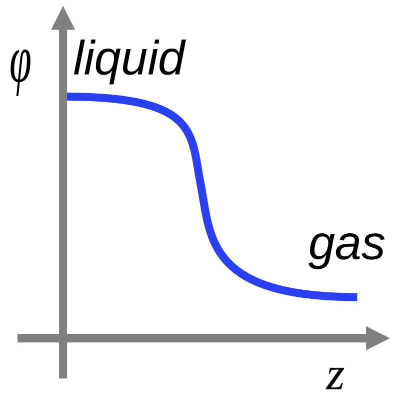
Rework force term in Boltzmann equation into a surface tension force

Use **non-ideal equation of state** to achieve phase separation

Introduce an **index function**, ϕ, to track the interface between two phases

Results in a **diffuse interface** model

- *index function, and fluid density, changes smoothly but rapidly between phases*



Finite-density Multiphase Lattice Boltzmann Equations

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- Following He, Chen and Zhang, two LB equations with forcing are derived for f_i and g_i, the moments of which give the macroscopic properties; mass and momentum densities, and pressure respectively as

$$\phi\left(x_\alpha, t\right) = \sum f_i\left(x_\alpha, t\right) \quad \left(\phi \text{ tracks density} = \text{index function}\right)$$

$$\rho u_\alpha\left(x_\alpha, t\right) = \frac{1}{RT}\sum e_{i\alpha} g_i\left(x_\alpha, t\right) + \frac{1}{2}\left[\kappa\rho\frac{\partial}{\partial x_\alpha}\left(\nabla^2\rho\right) + B_\alpha\right]\delta t$$

$$p\left(x_\alpha, t\right) = \sum g_i\left(x_\alpha, t\right) - \frac{1}{2}u_\alpha\frac{\partial\psi\left(\rho\right)}{\partial x_\alpha}\delta t$$

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Finite-density Multiphase Lattice Boltzmann Equations

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- Model is for a liquid and its gas. Values of the index function for liquid, φ_L, and gas, φ_G are obtained from the EoS and Maxwell's equal area construct.
- The liquid and gas values of φ can be used to account for the different fluid properties between the phases, that is

$$\rho(\phi) = \rho_G + \frac{\phi - \phi_G}{\phi_L - \phi_G}(\rho_L - \rho_G)$$

- The same is true for the viscosity, μ.
- Can be applied with MRT (see Premnath and Abraham (2007))

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Wetting

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Use the approach of Iwahara et al. (2003)

Define a **surface affinity** – a normalised surface density

$$\alpha_s = \frac{\phi - \bar{\phi}}{\phi_L - \bar{\phi}}, \quad \text{where } \{ \bar{\phi} = (\phi_L + \phi_G)/2 ¿$$

A **planar** interface has the profile (Rowlinson & Widom 1982)

$$\phi(z) = \bar{\phi} - \frac{1}{2}(\phi_L - \phi_G)\tanh\left(\frac{z - z_0}{\delta}\right)$$

The liquid-gas surface tension is therefore

$$\sigma_{LG} = \kappa \int_{-\infty}^{\infty} \left(\frac{\partial \phi}{\partial z}\right)^2 dz = \frac{\kappa (\phi_L - \phi_G)^2}{4\delta} \int_{-1}^{1} (1 - \alpha^2)\, d\alpha$$

$$¿ \frac{\kappa (\phi_L - \phi_G)^2}{3\delta}$$

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Wetting

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Similar expressions for the solid-liquid and solid-vapour surface tensions substituted into Young's equation give

$$\cos\theta_S = \alpha_S(3 - \alpha_S^2)/2$$

Static contact angle can be specified via the surface affinity

Index-function density at boundary given by

$$\varphi = \bar{\boldsymbol{\phi}} + (\boldsymbol{\phi}_L - \bar{\boldsymbol{\phi}})\alpha_S, \quad \{\bar{\boldsymbol{\phi}} = \frac{1}{2}(\boldsymbol{\phi}_L + \boldsymbol{\phi}_G), \quad -1 \le \alpha_S \le 1 \text{¿}$$

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Test Problem 1
(Forced wetting to failure)

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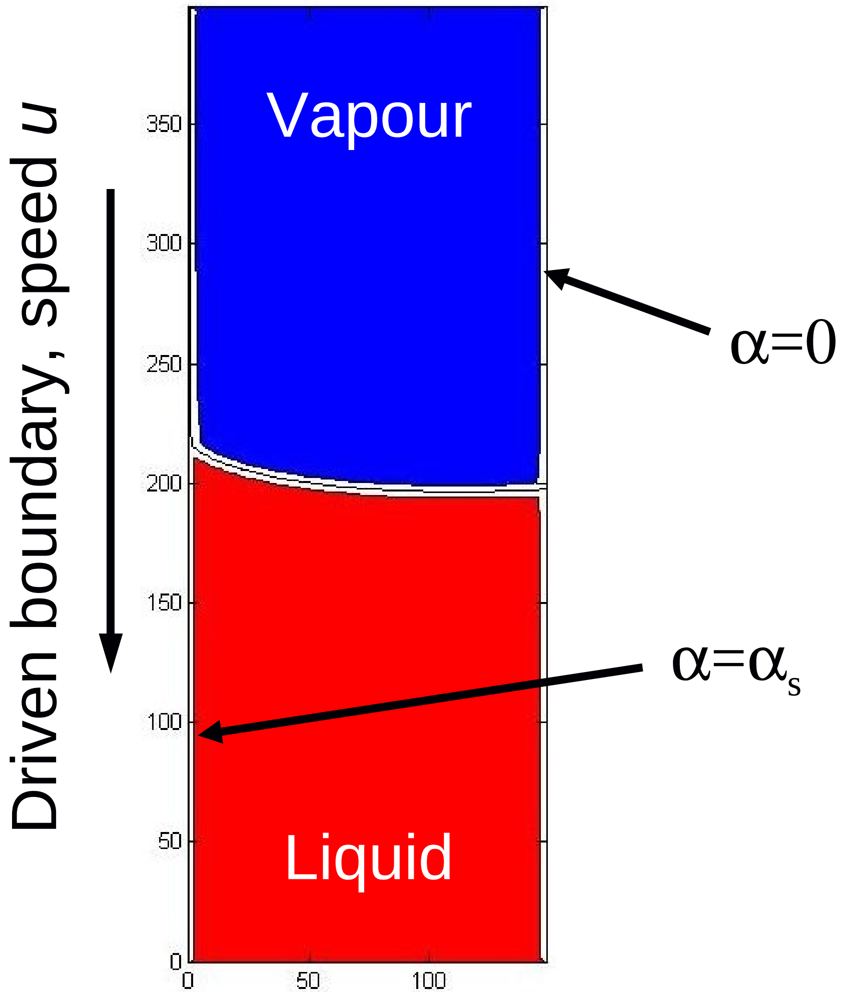
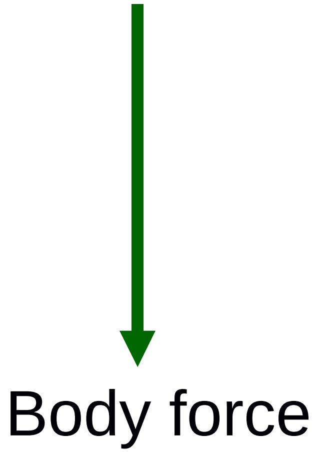


- Two-phase cavity
- Solid walls



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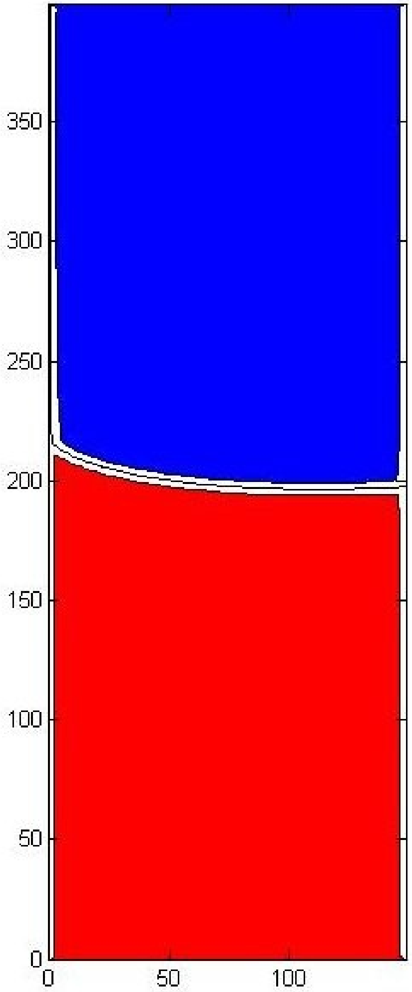
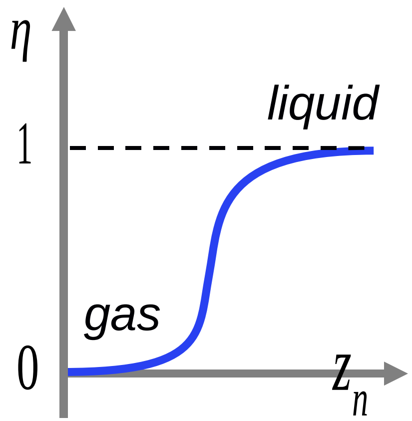
Static Case – Interface Shape

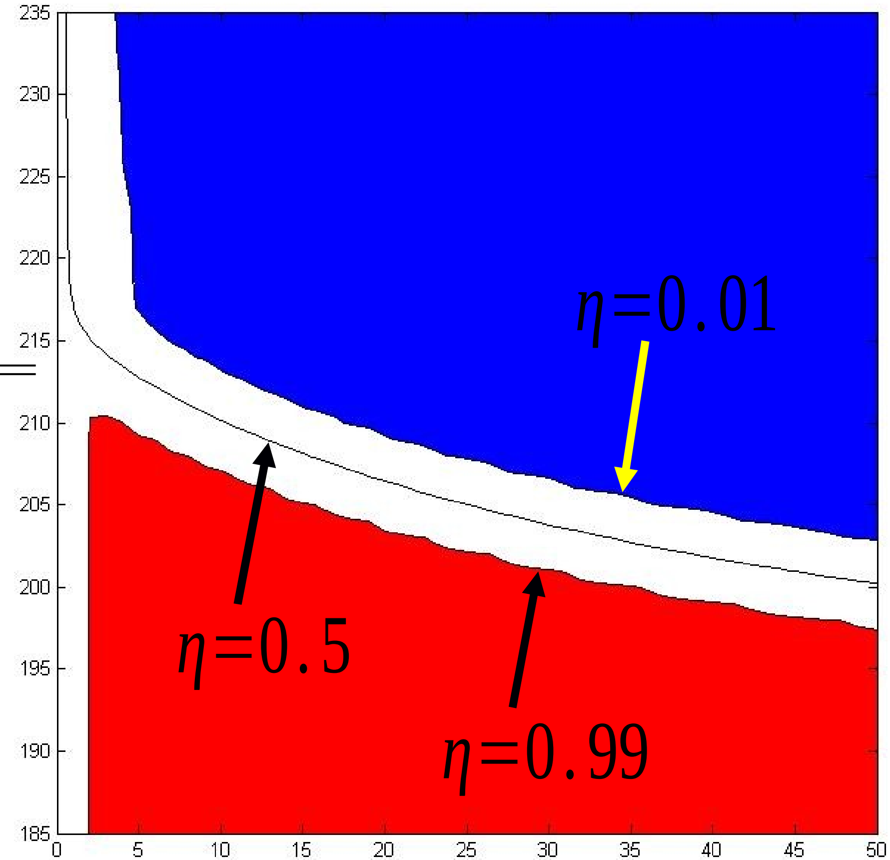


$$\alpha_S = 0.4$$

$$\Rightarrow \theta_S = 55°$$

$$\eta = \frac{\phi - \phi_G}{\phi_L - \phi_G}$$





Where is the contact 'line'?

Which is '*the*' contact angle?

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(Forced wetting to failure)

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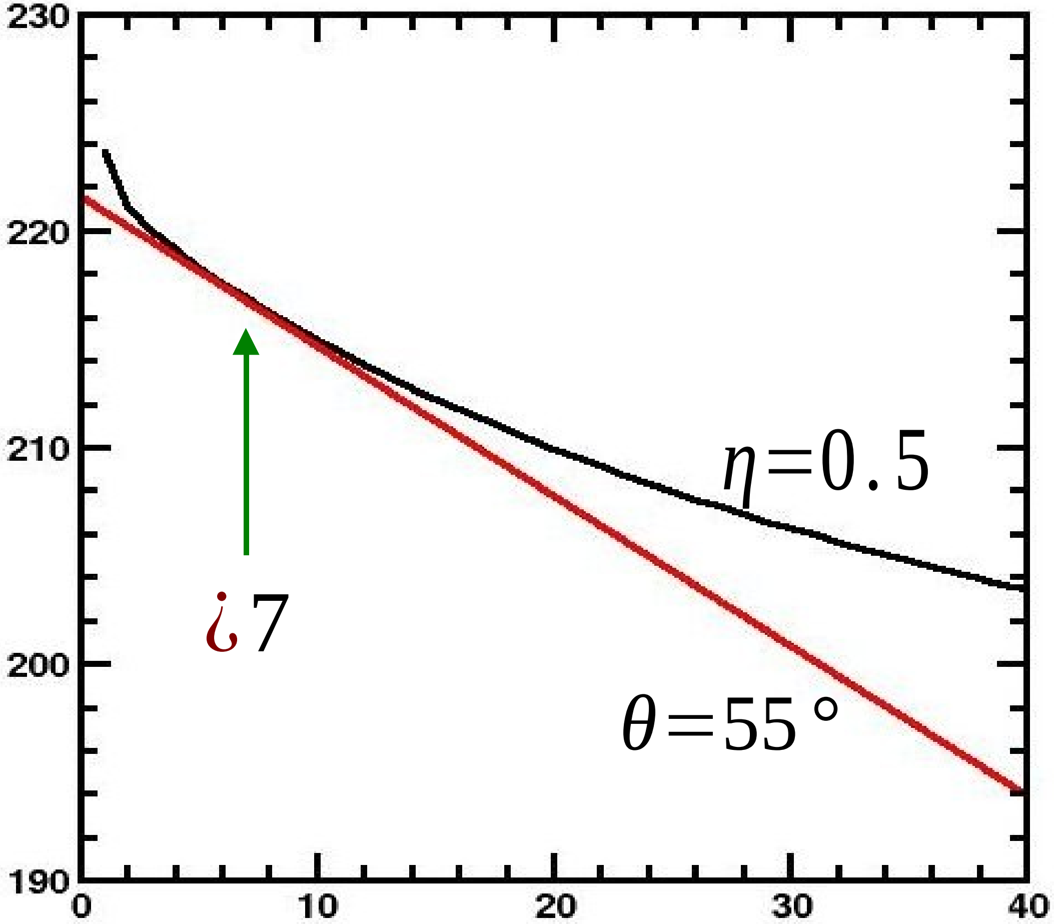
Static Case – Contact Angle



Angle of interface matches imposed angle at roughly 7 lattice units away from the boundary

Just outside the diffuse three-phase contact region

Use this as the point to measure variation in contact angle

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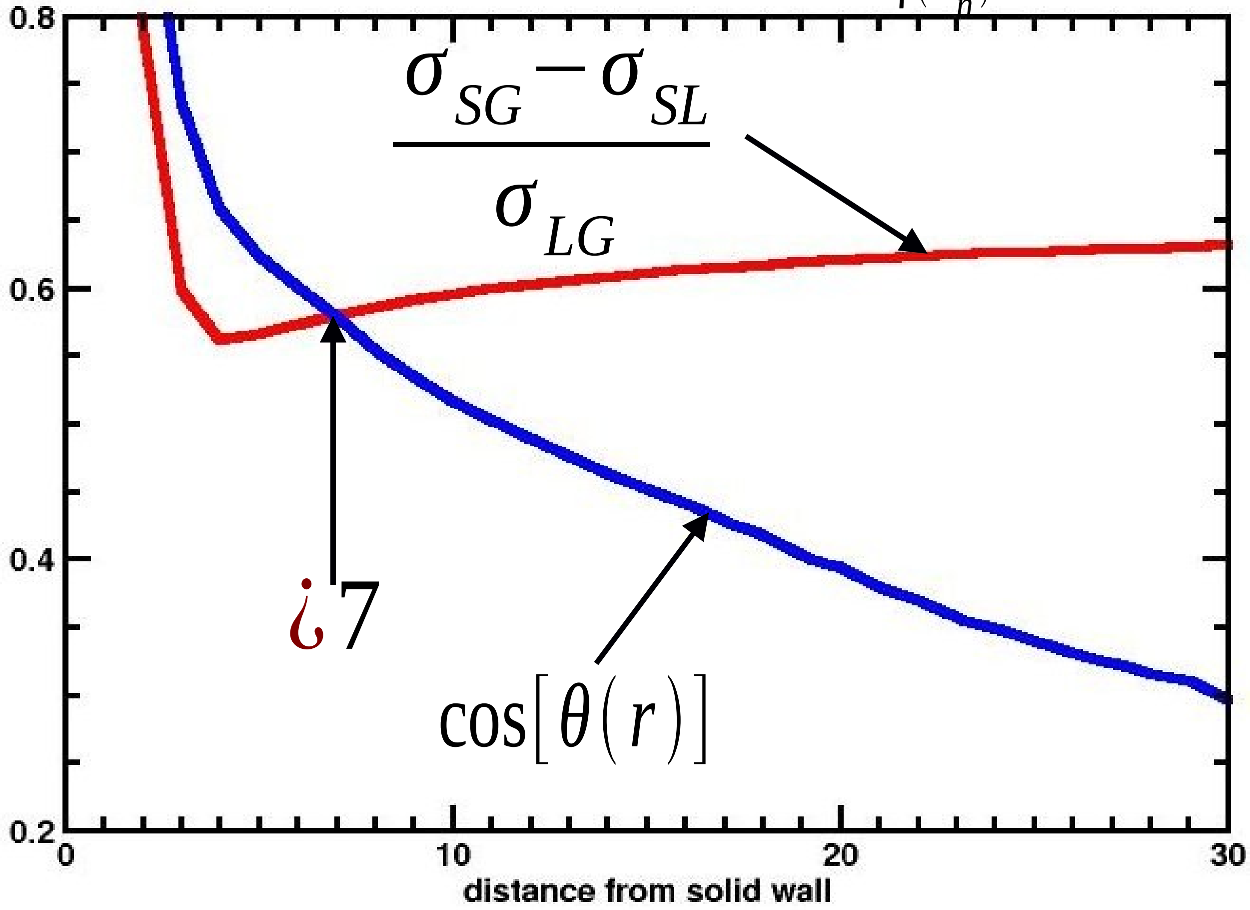
Static Case – Young equation

$$\sigma = \kappa \int_{\eta(z_n)=0.01}^{\eta(z_n)=0.99} [\nabla \phi]^2 dz_n$$



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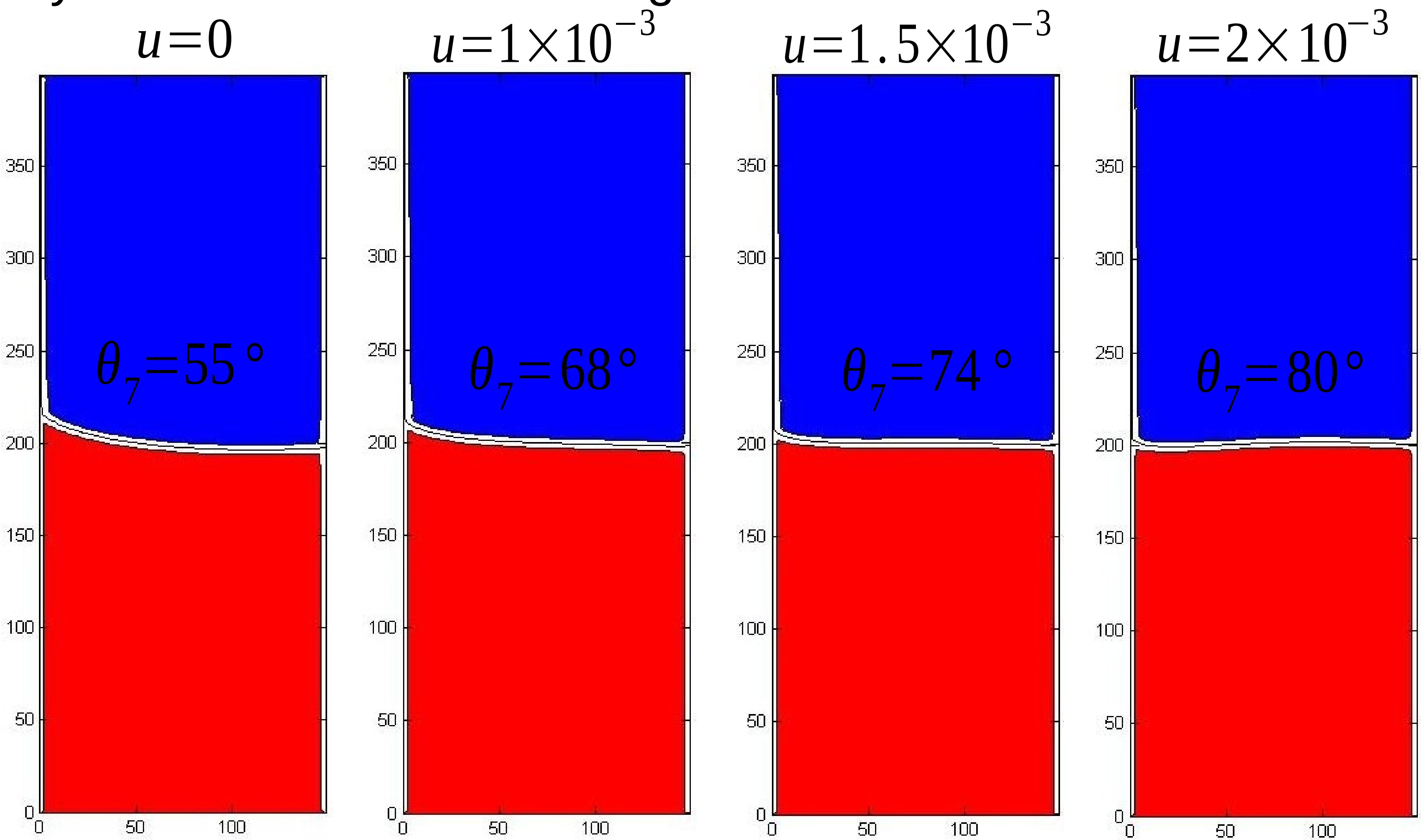
Dynamic Case – Contact Angle



Test Problem 1
(Forced wetting to failure)

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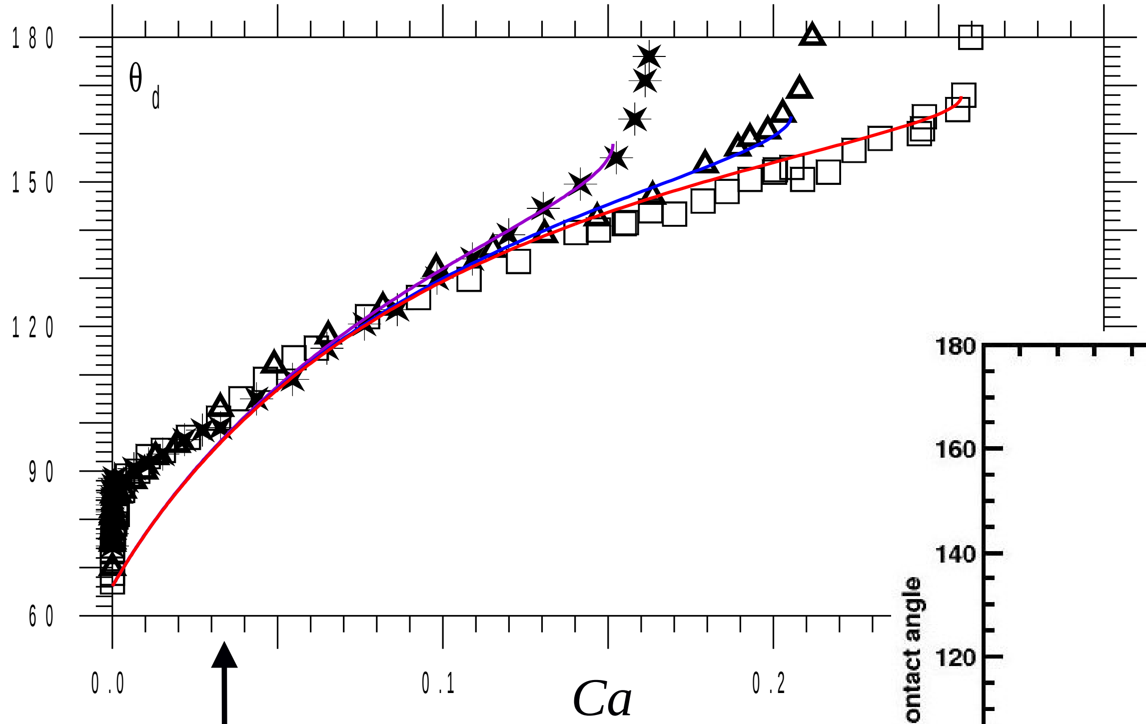
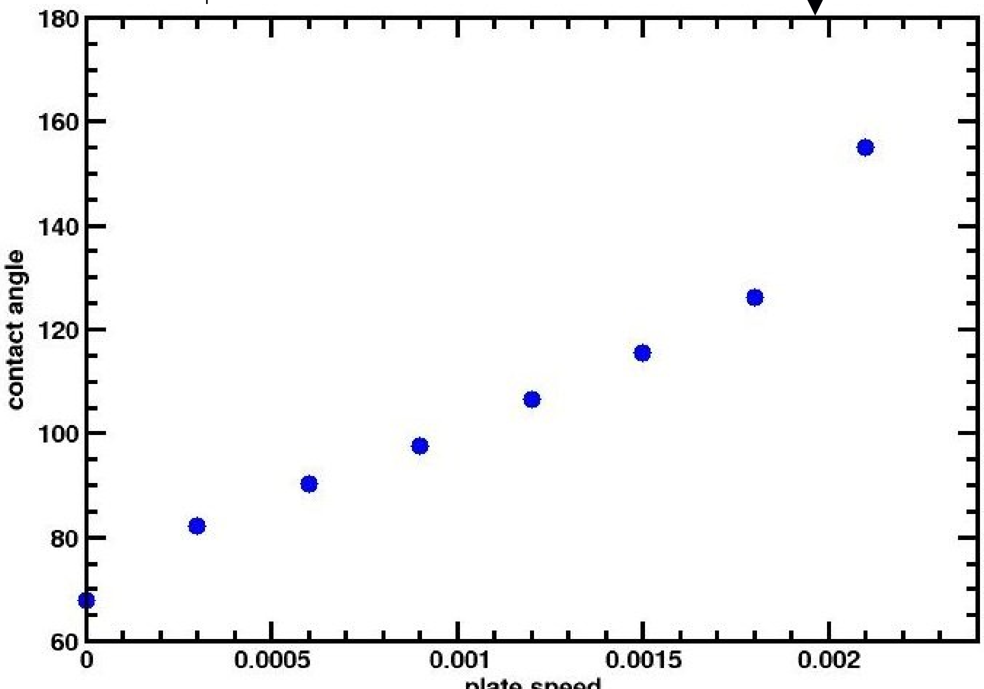
Contact Angle Versus Speed



Experiments of Blake *et al.*

J. Colloid Interf. Sci. **253,**196 (2002)

Lattice Boltzmann results



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(Forced wetting to failure)

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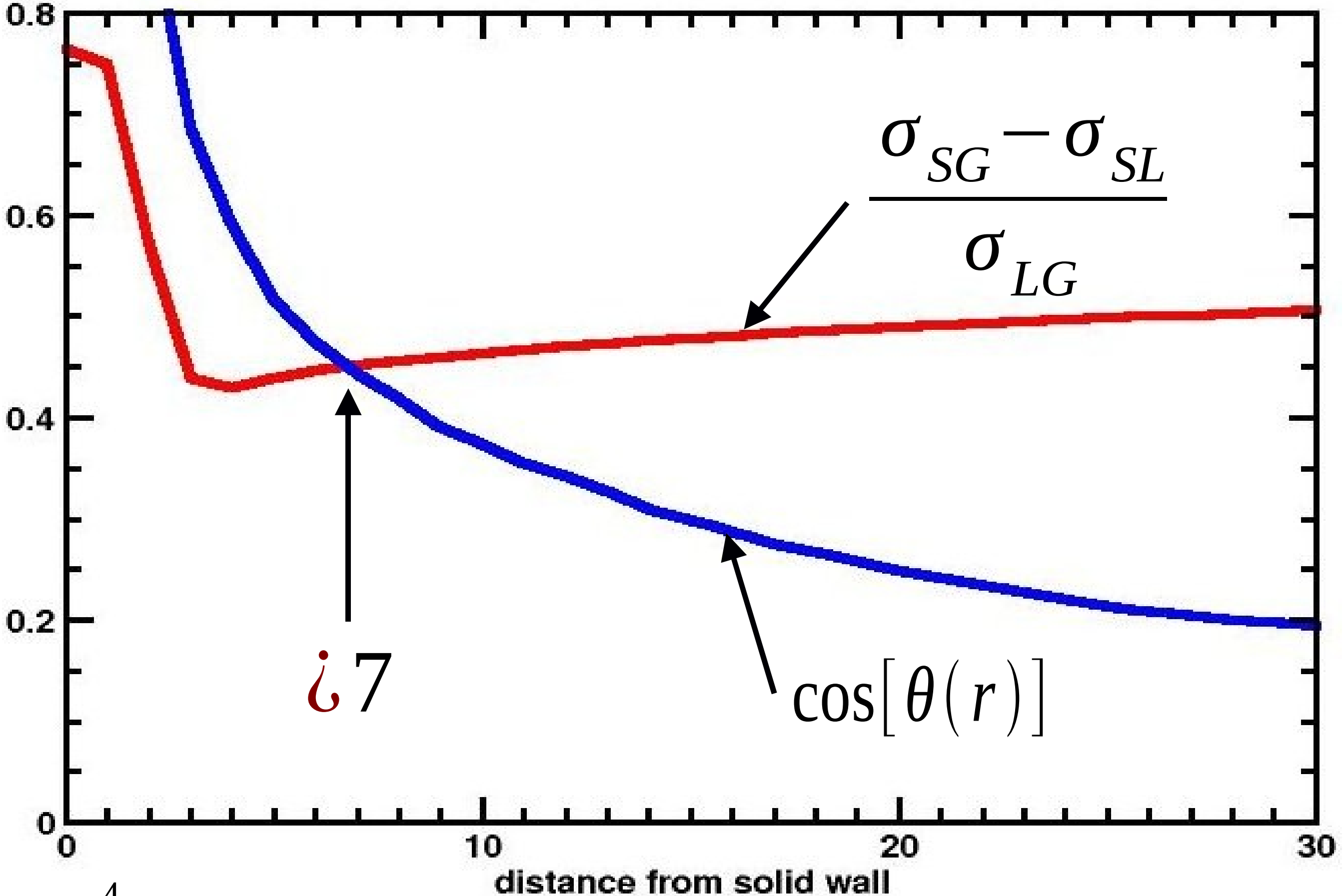
Dynamic Case – Young Equation



$u=5\times10^{-4}$

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Test Problem 1
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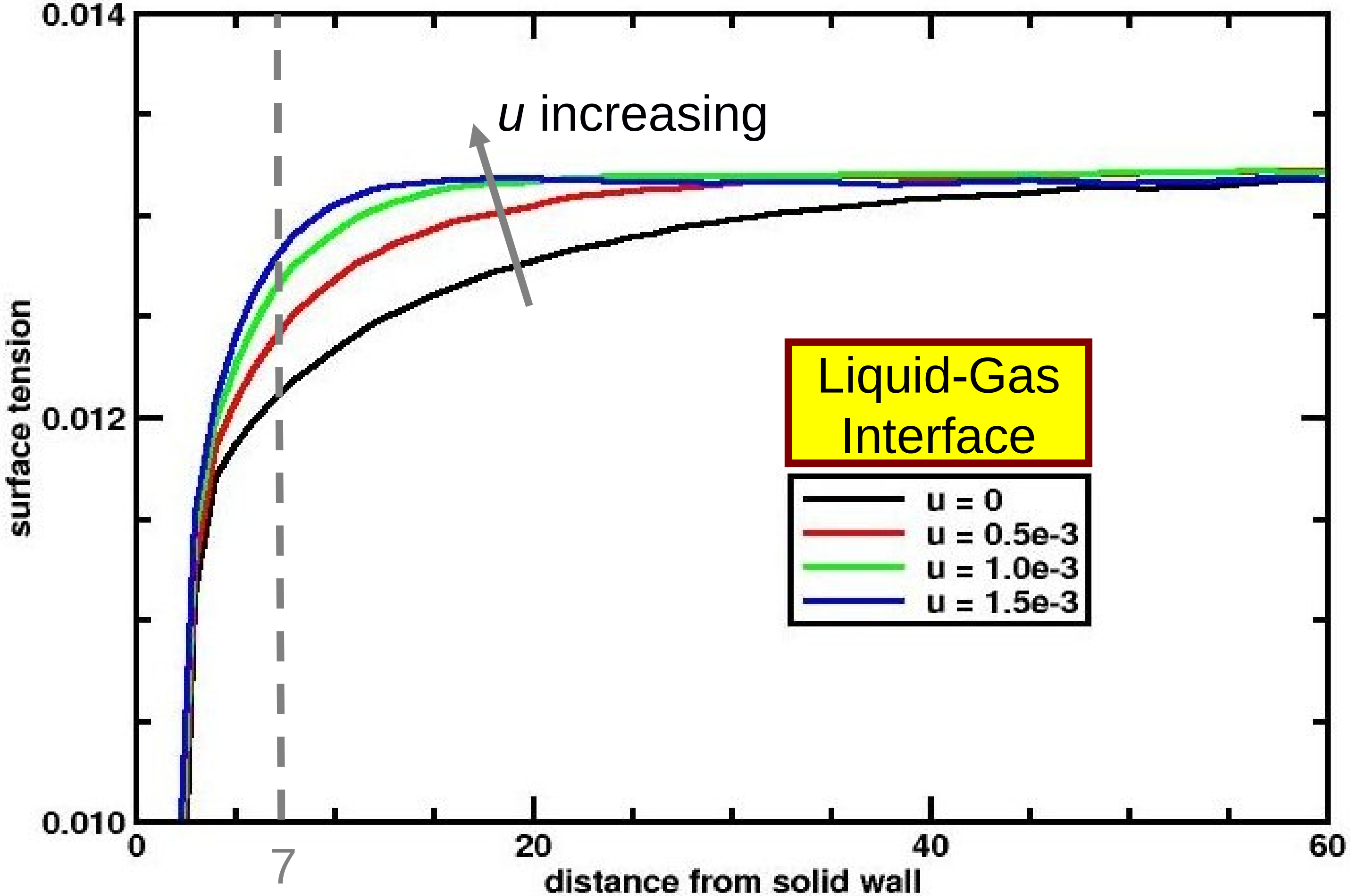
Dynamic Case – Surface Tension



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Test Problem 1
(Forced wetting to failure)

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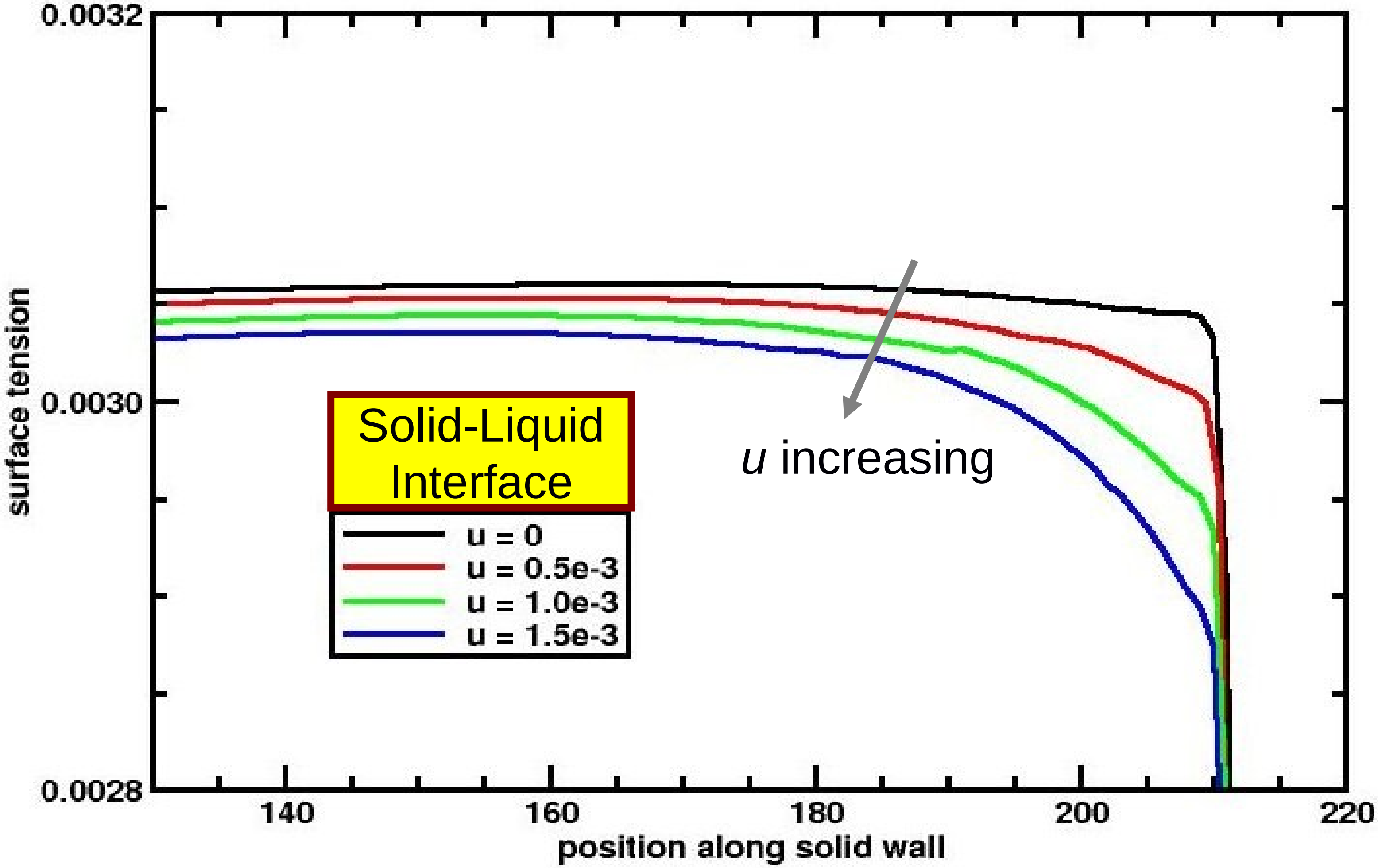
Dynamic Case – Surface Energy



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Test Problem 1
(Forced wetting to failure)

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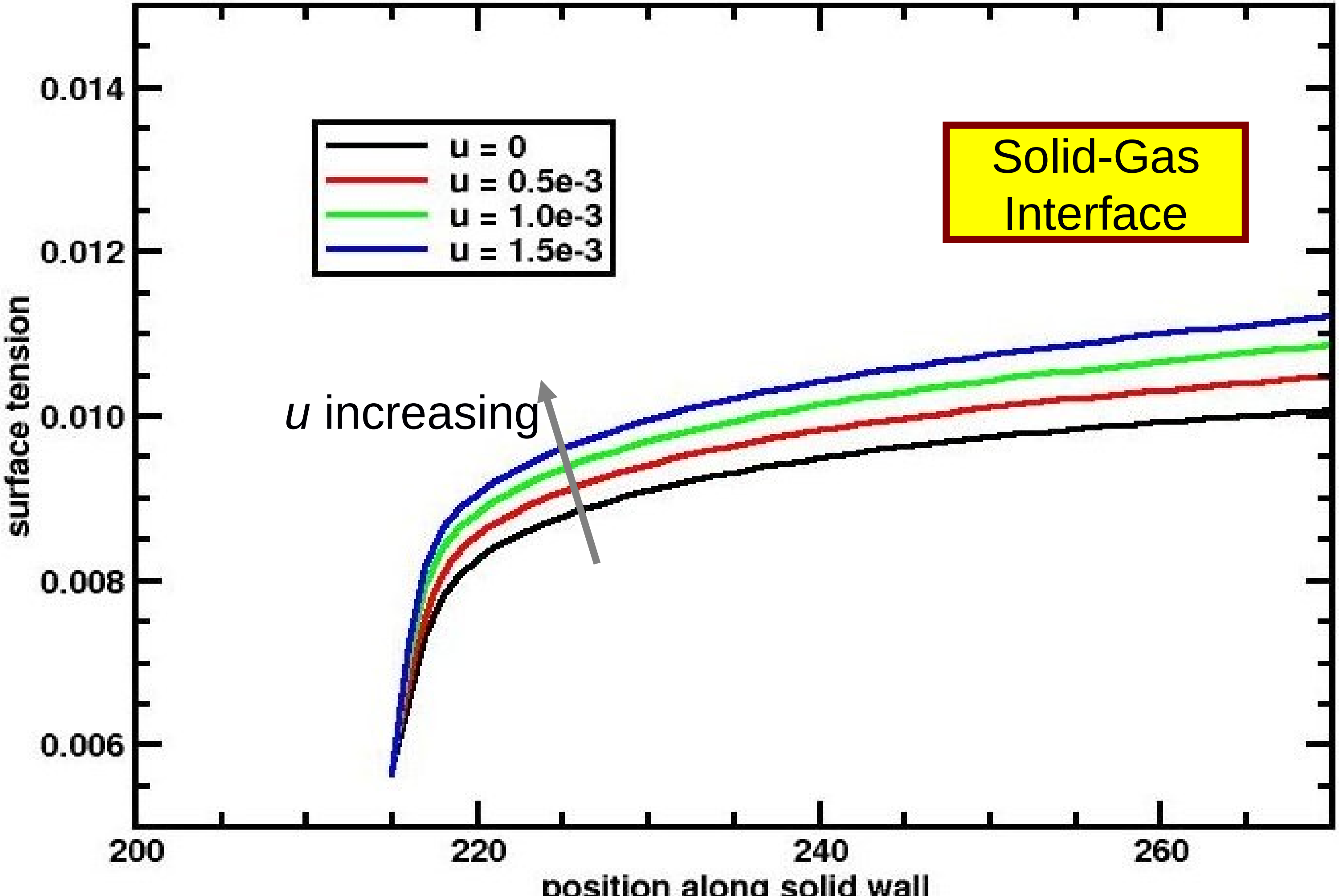
Dynamic Case – Surface Energy



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Test Problem 1
(Forced wetting to failure)

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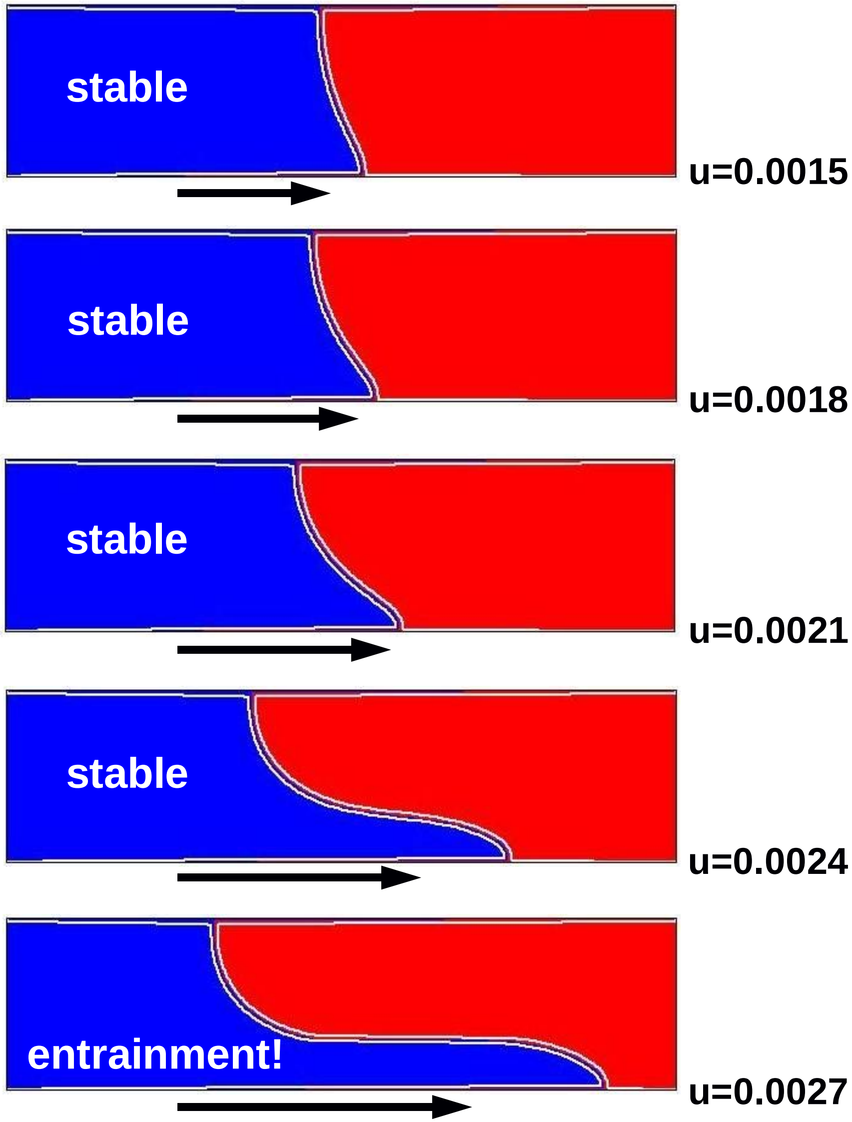

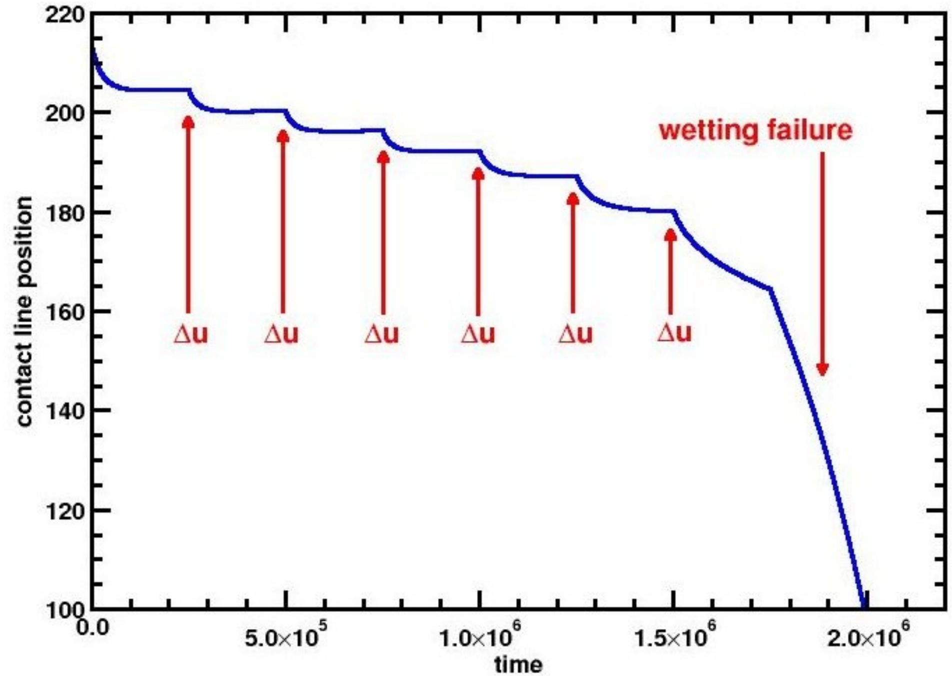

light phase

dense phase

body force (gravity)

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Test Problem 2
(Wetting line hysteresis)

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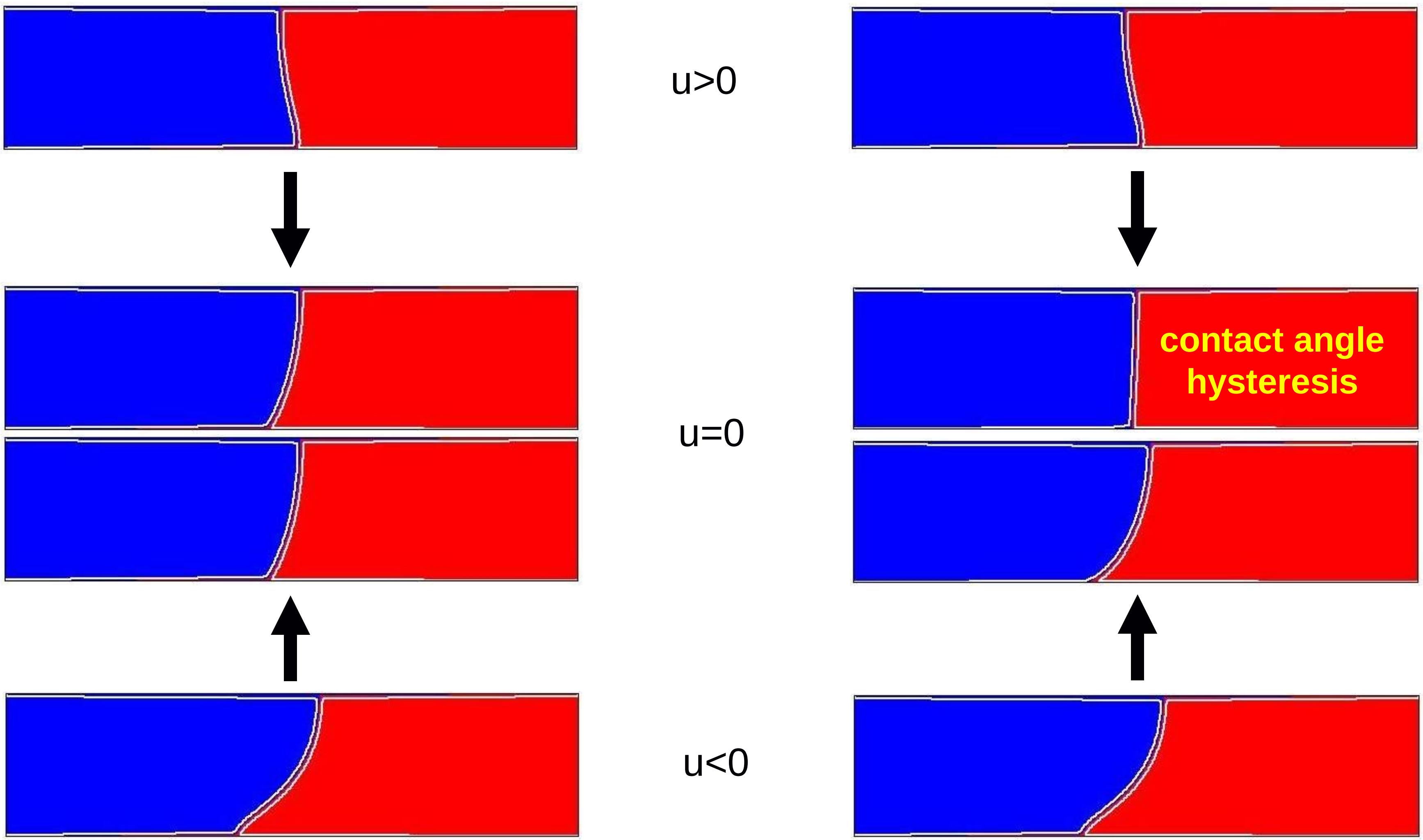
uniform wettability | sinusoidally varying wettability



Test Problem 2
(Wetting line hysteresis)

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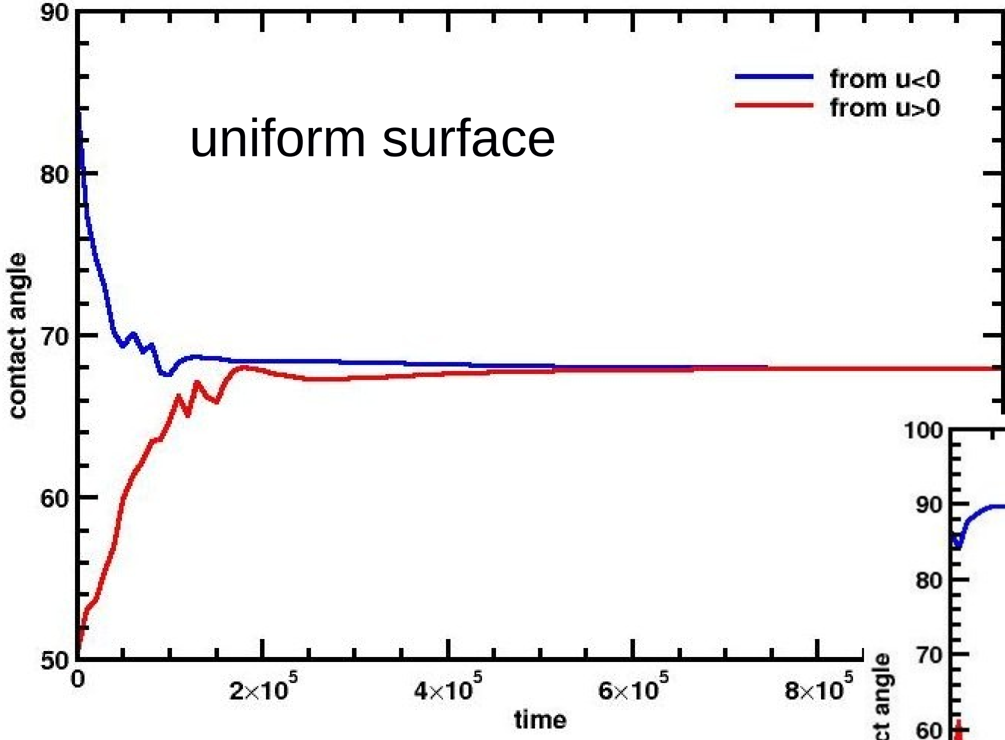

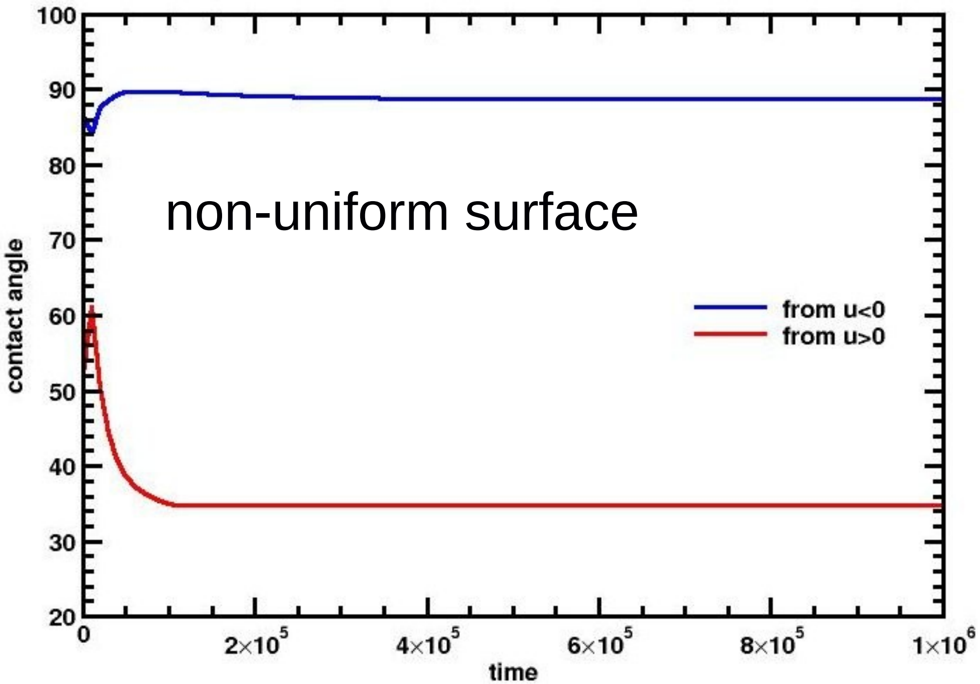

Test Problem 3
(Natural wetting spreading/sticking)

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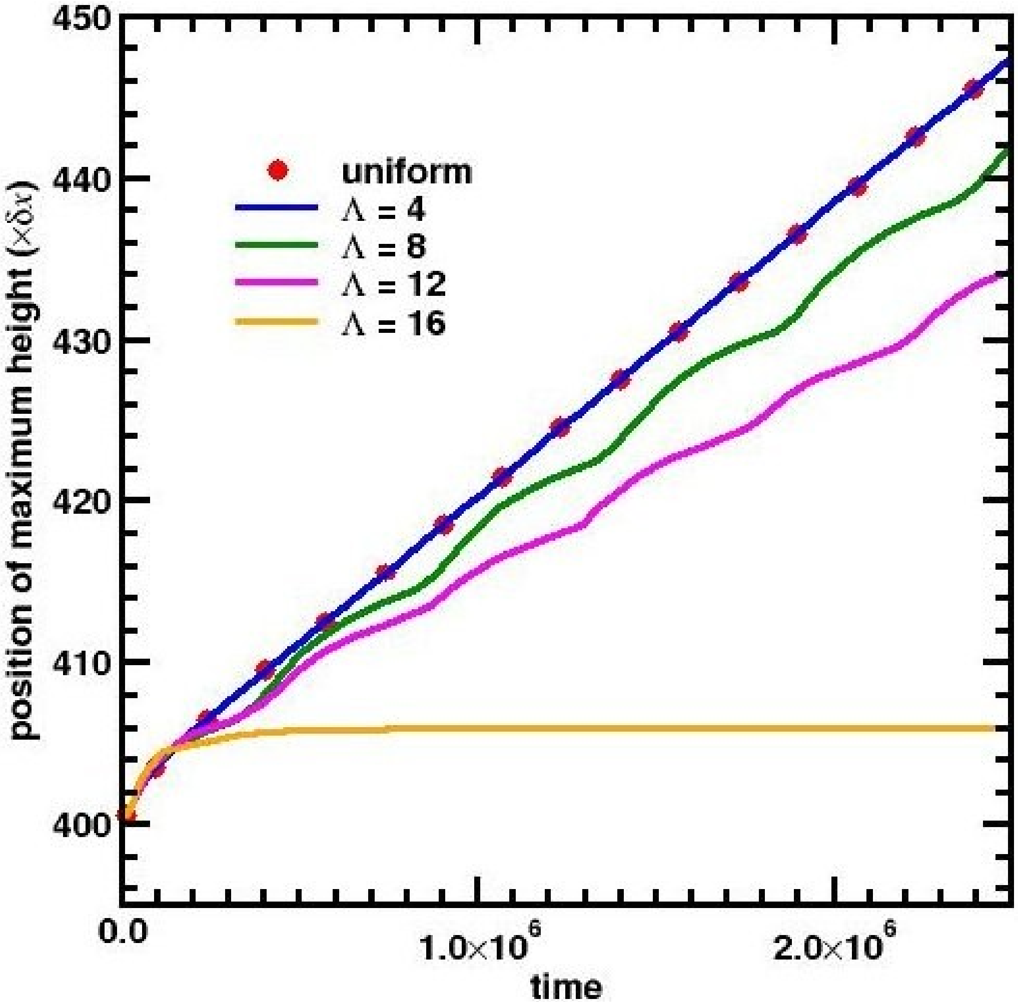
- Flow of a droplet down an incline with a sinusoidally varying wettability of wavelength Λ
- Varying Λ for fixed interface thickness
- Droplet is pinned for certain values

Davies, Summers & Wilson (2006)



A Tale of Two Length Scales

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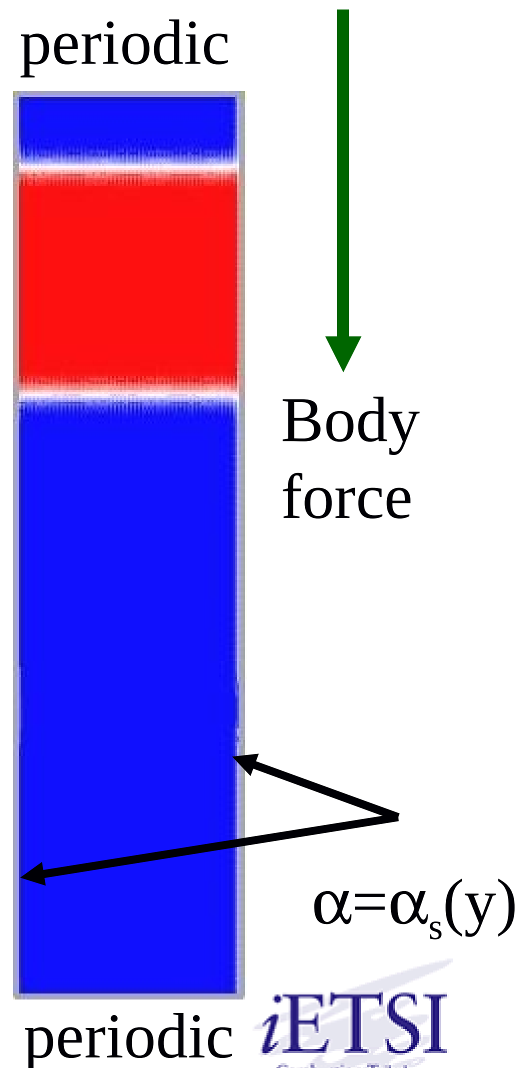
- What is the effect of interface thickness for wetting of non-uniform surfaces?
  - interface thickness versus characteristic size of non-uniformity
- Interface thickness is always ~4 or 5 lattice units…can scale up problem
- Use two lattices – one twice the size of the other (i.e. twice as dense)
  - need to adjust relaxation time and surface tension parameter to match physical scales on each lattice
- Use sinusoidal/alternating surface affinity



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Motion of slug centre

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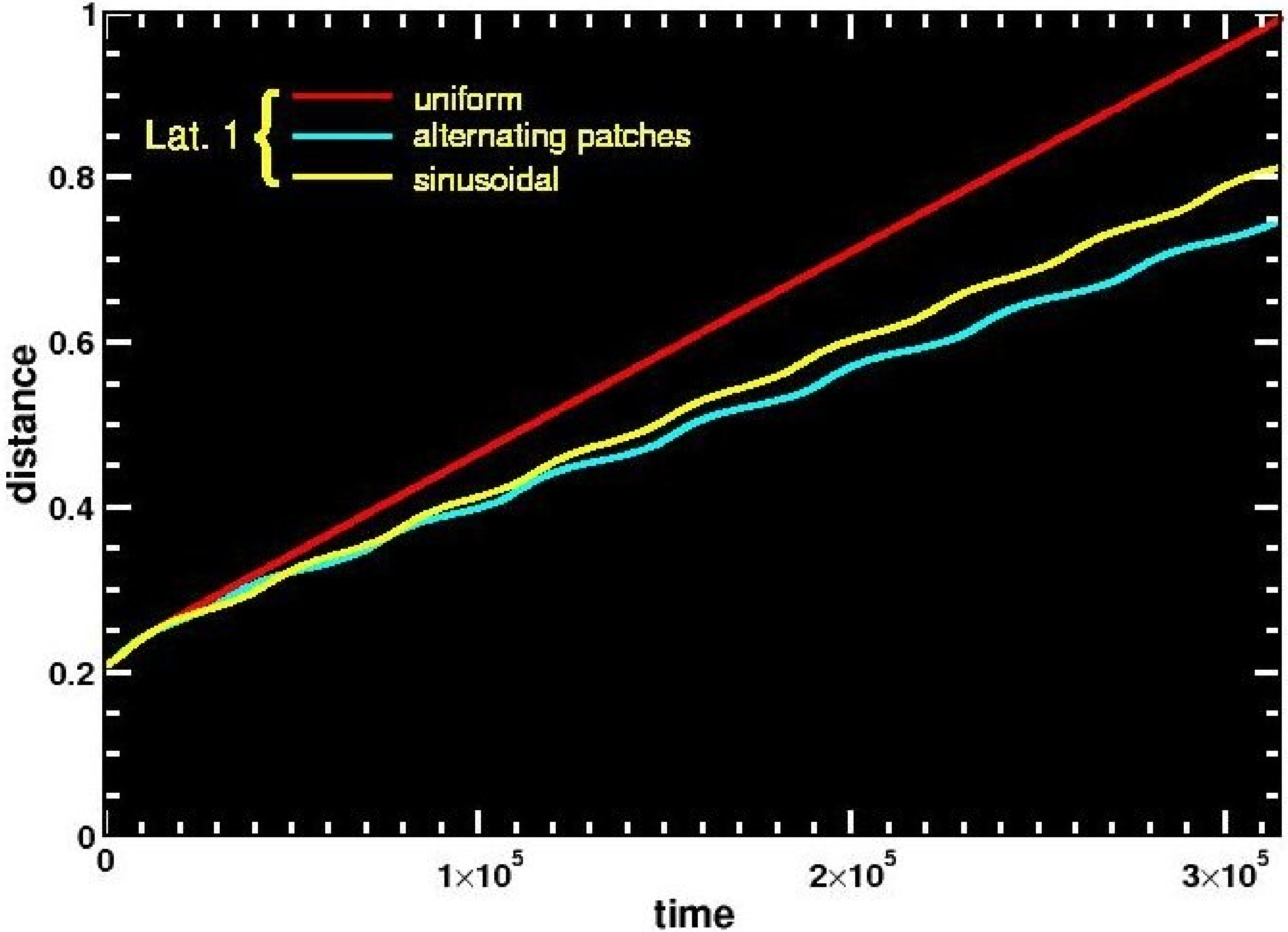

Motion of slug centre

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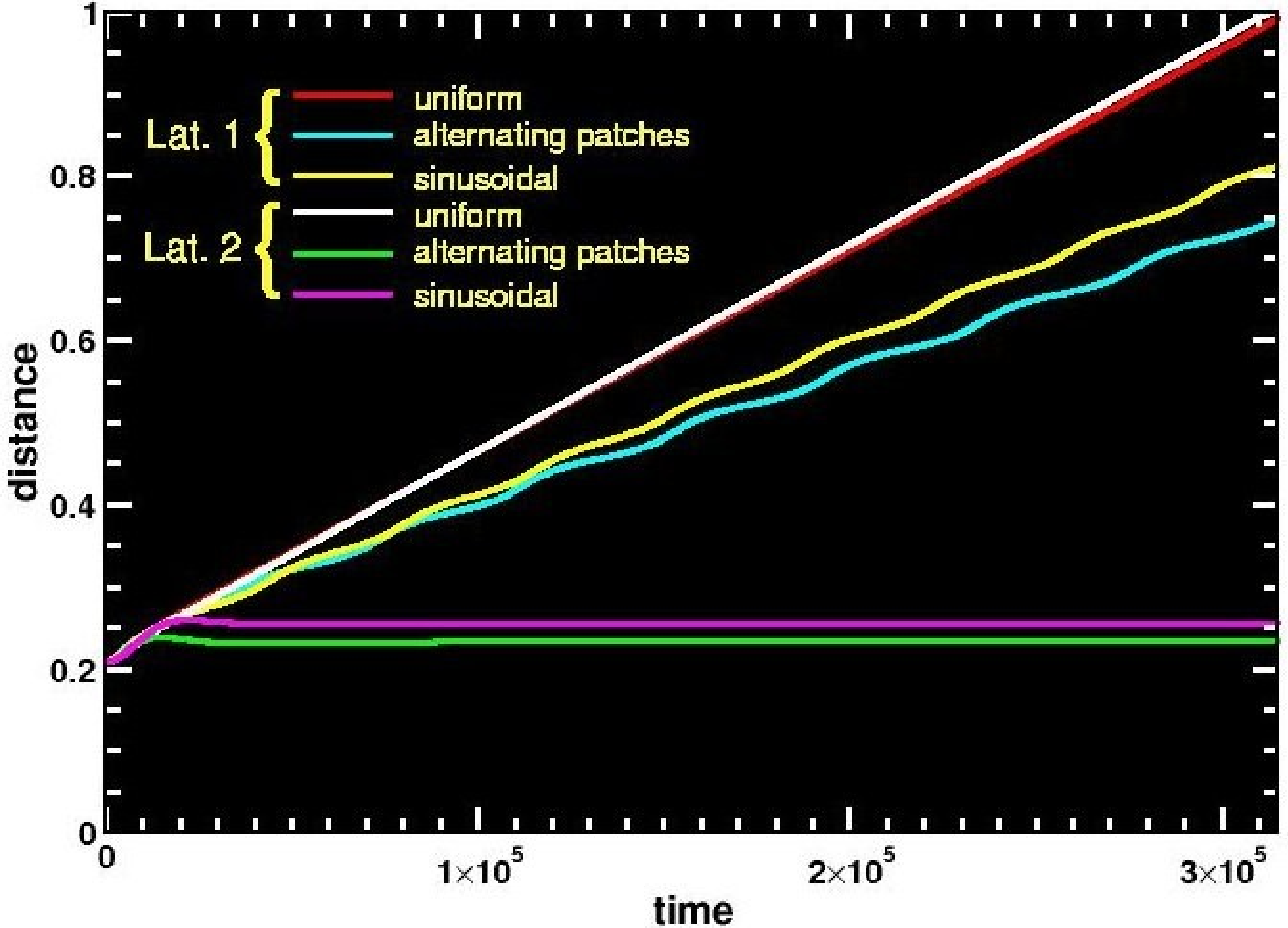

Current Limitations / Challenges

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- Density ratio limited
  - *several models now available addressing this issue, though wetting is still an issue for many*
- Issues with the surface tension and surface energies.
  - *Calculations of surface tension/energy via the thermodynamic (Cahn) approach is for static conditions, can we define a "mechanical" approach for the dynamic situation.*
- Wetting models for moving rough boundaries needed
  - *interface thickness a key factor*

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Conclusions

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- Able to capture qualitatively many wetting phenomena (static contact angle, forced wetting to failure, contact line hysteresis and natural wetting to the point of sticking on a non-uniform surface)
- Simple model and algorithm – only one wetting parameter
- Care needed in understanding effect of interface thickness (as this will dictate the length scale?)
- Work needed to make quantitatively accurate (is the thermodynamic description of surface energy sufficient?)

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