Dissolutive Wetting: What Controls Spreading?

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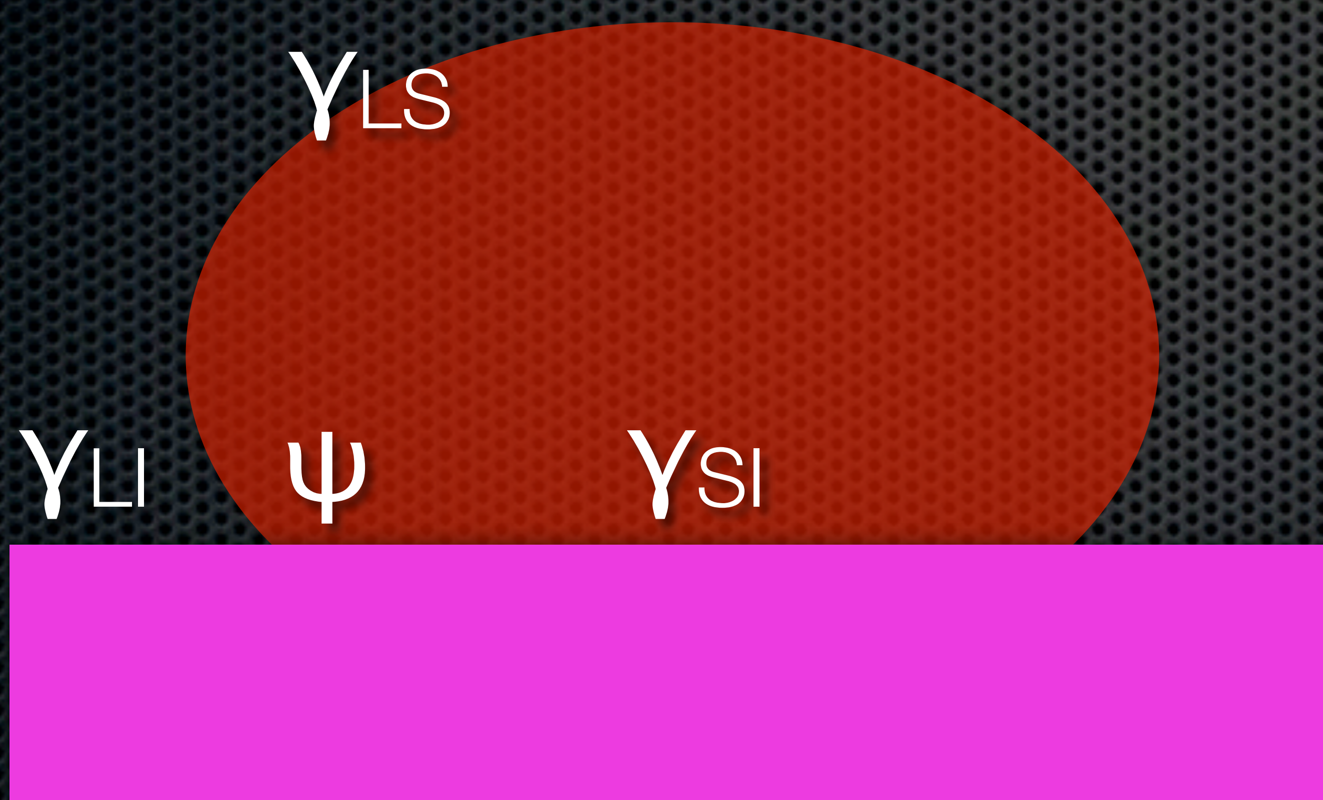
Modeling the early stages of reactive wetting,
Daniel Wheeler, James A. Warren and William J. Boettinger,
PRE (accepted, finally!) 2010

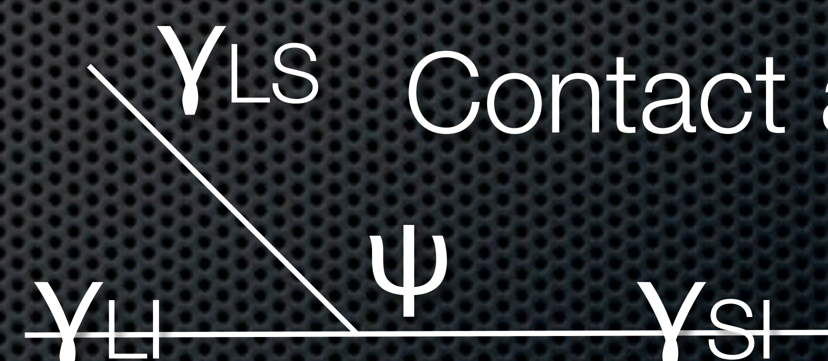
Outline

- Motivation
- Methods, Limitations of prior efforts
- Hydrodynamics, Low Ohnesorge Number flow
- Numerics
- Thick interfaces and intitial conditions
- New metrics of spreading

Good old Wetting

- Surface energies, need: γ_{LI} γ_{SI} γ_{LS}

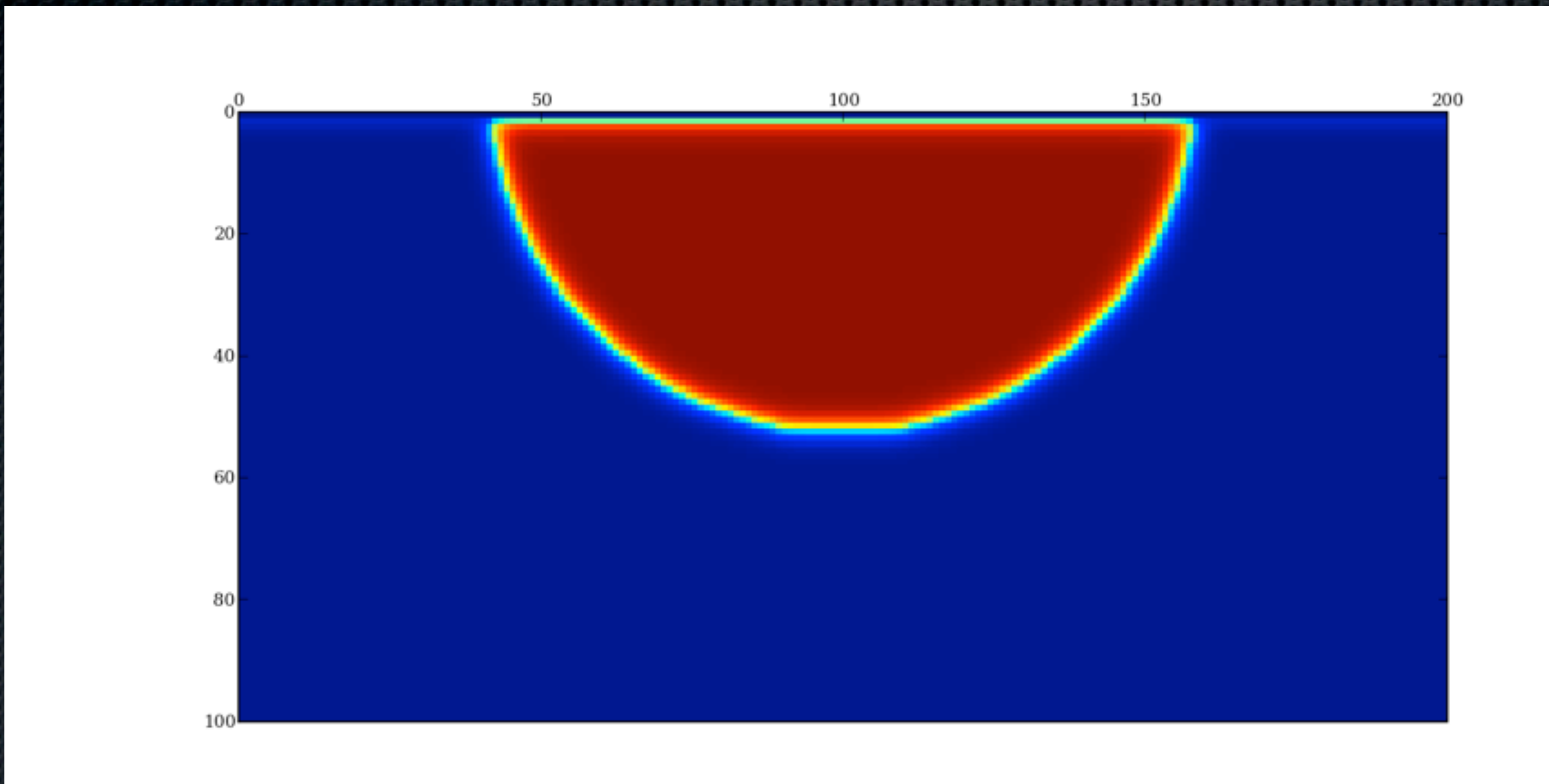




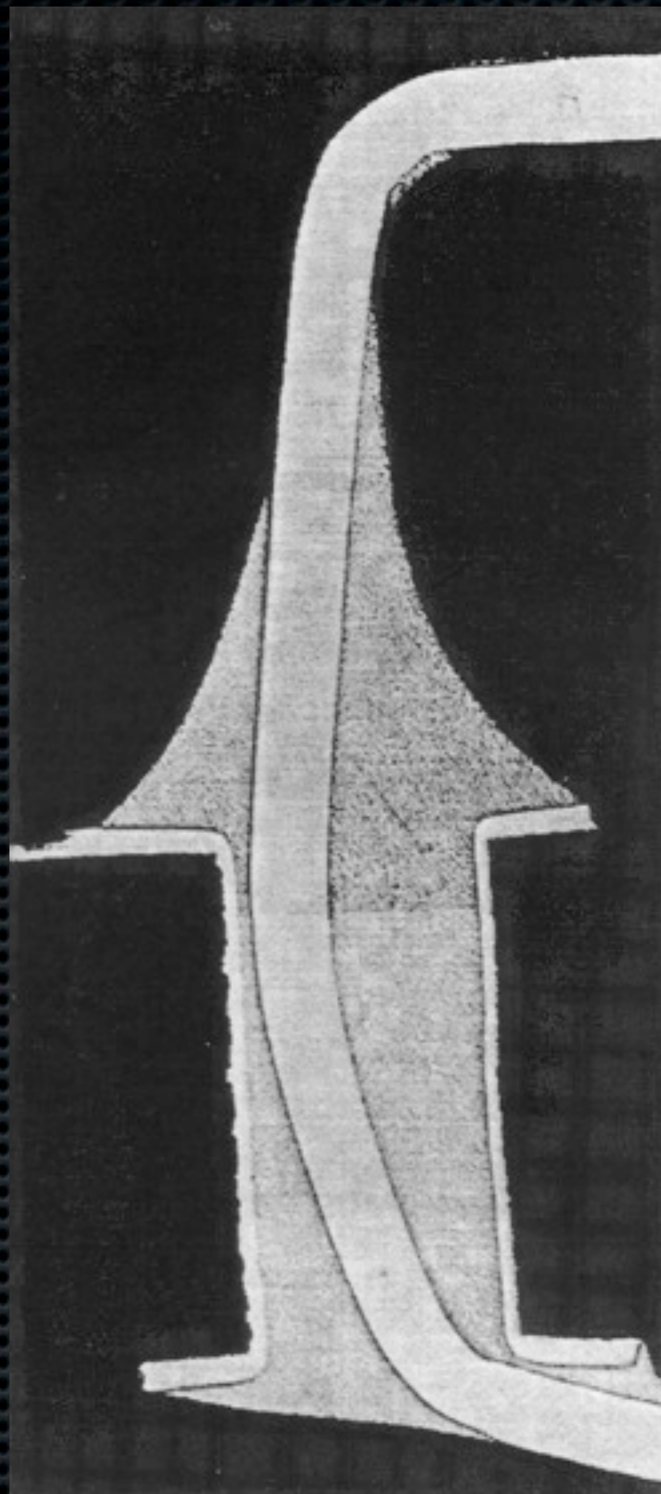
Contact angle ψ

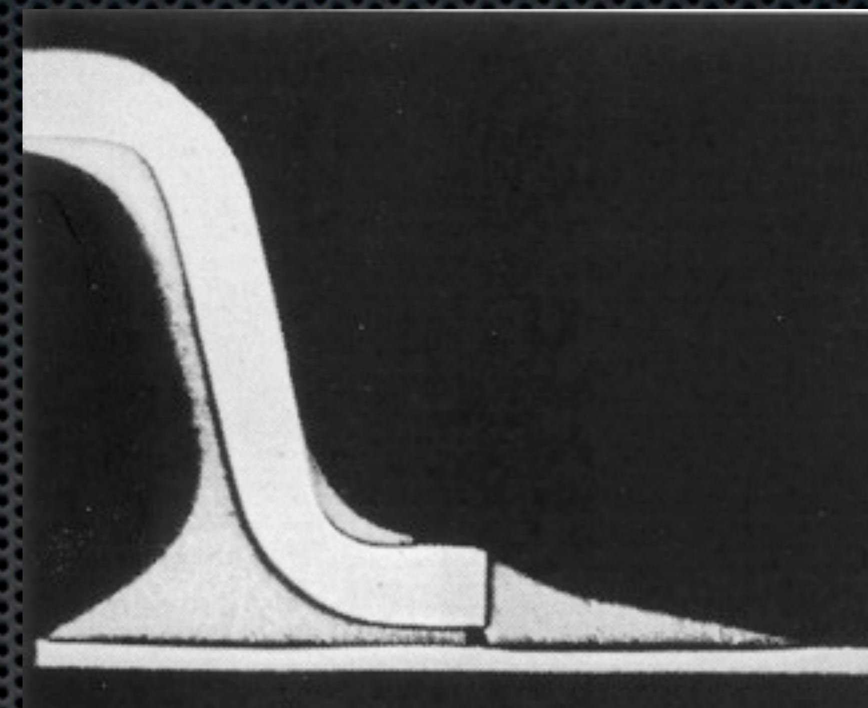
$$\cos(\psi) = \frac{\gamma_{LI} - \gamma_{SI}}{\gamma_{LS}}.$$

Background: Walls in PF

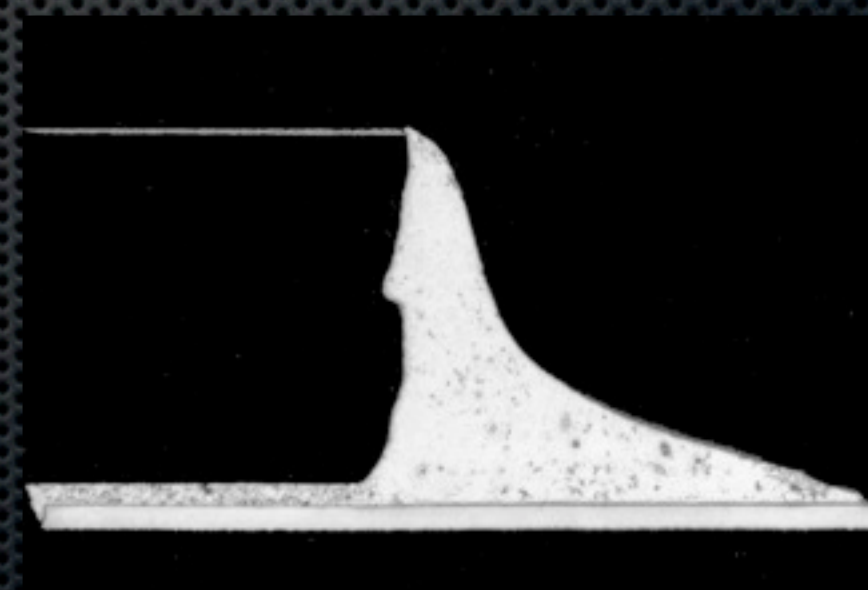


Solder Joints





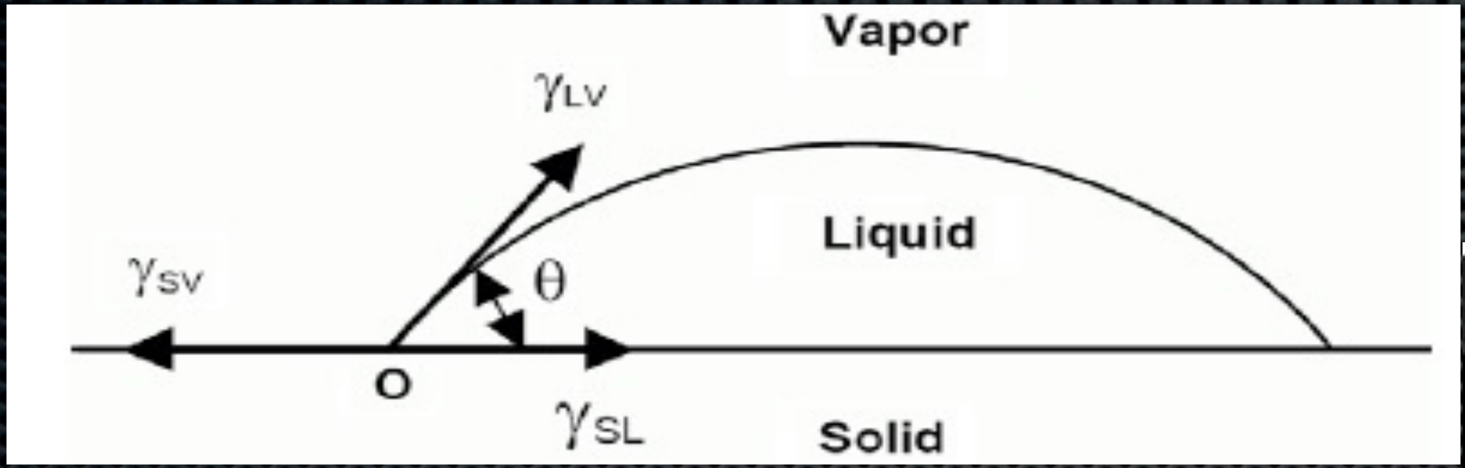
“Surface Mount - Gull Wing”



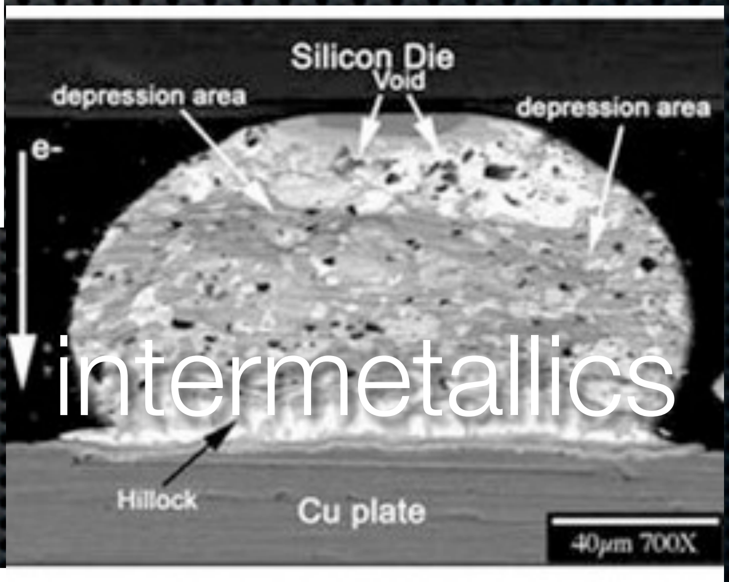
“Through Hole”

“Surface Mount - Leadless”

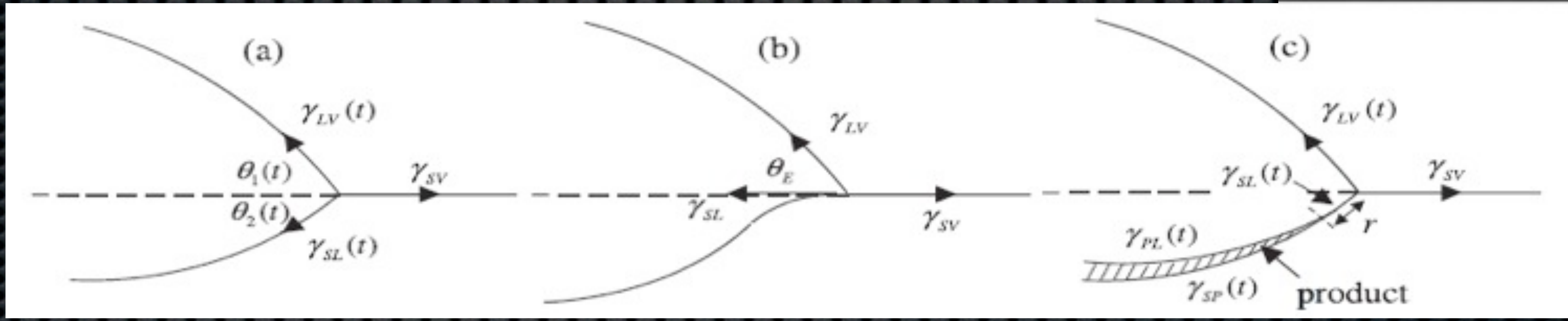
Reactive Wetting



Inert Wetting

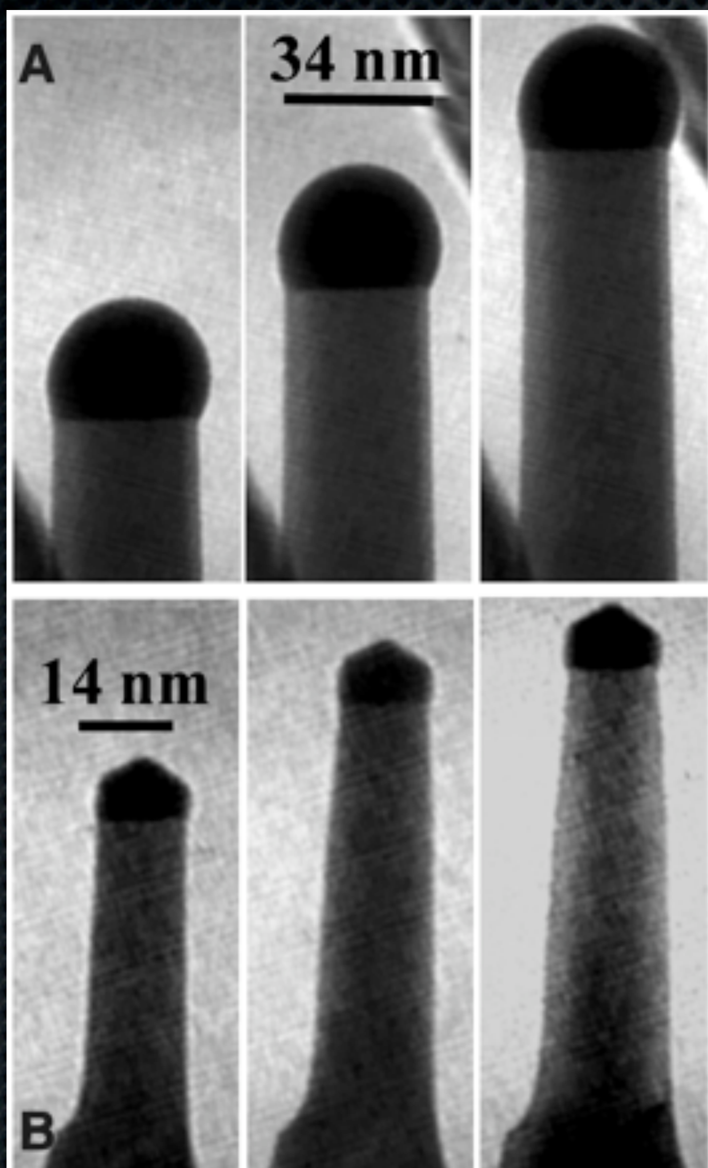


Line images from Yin and Murray, Journal of Physics: Condensed Matter, 2009

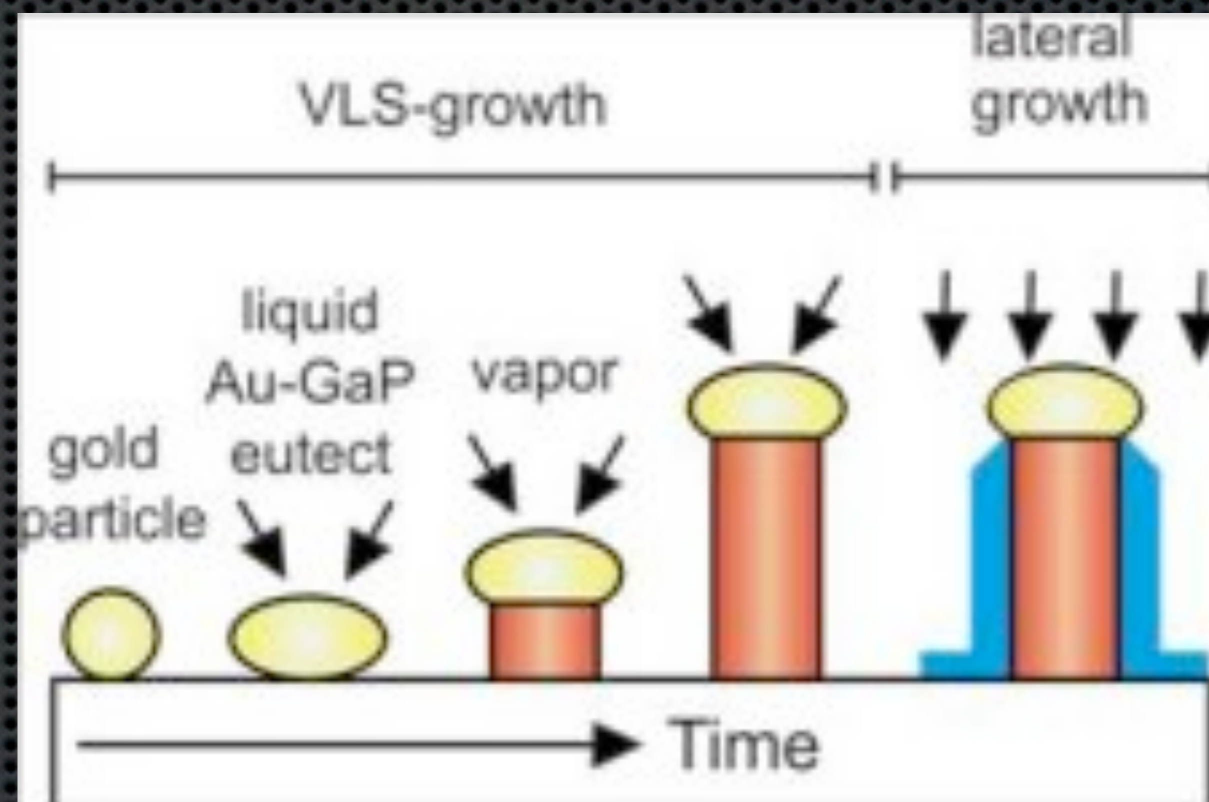


Dissolutive and compound-forming wetting

VLS Growth (NWU Collab)



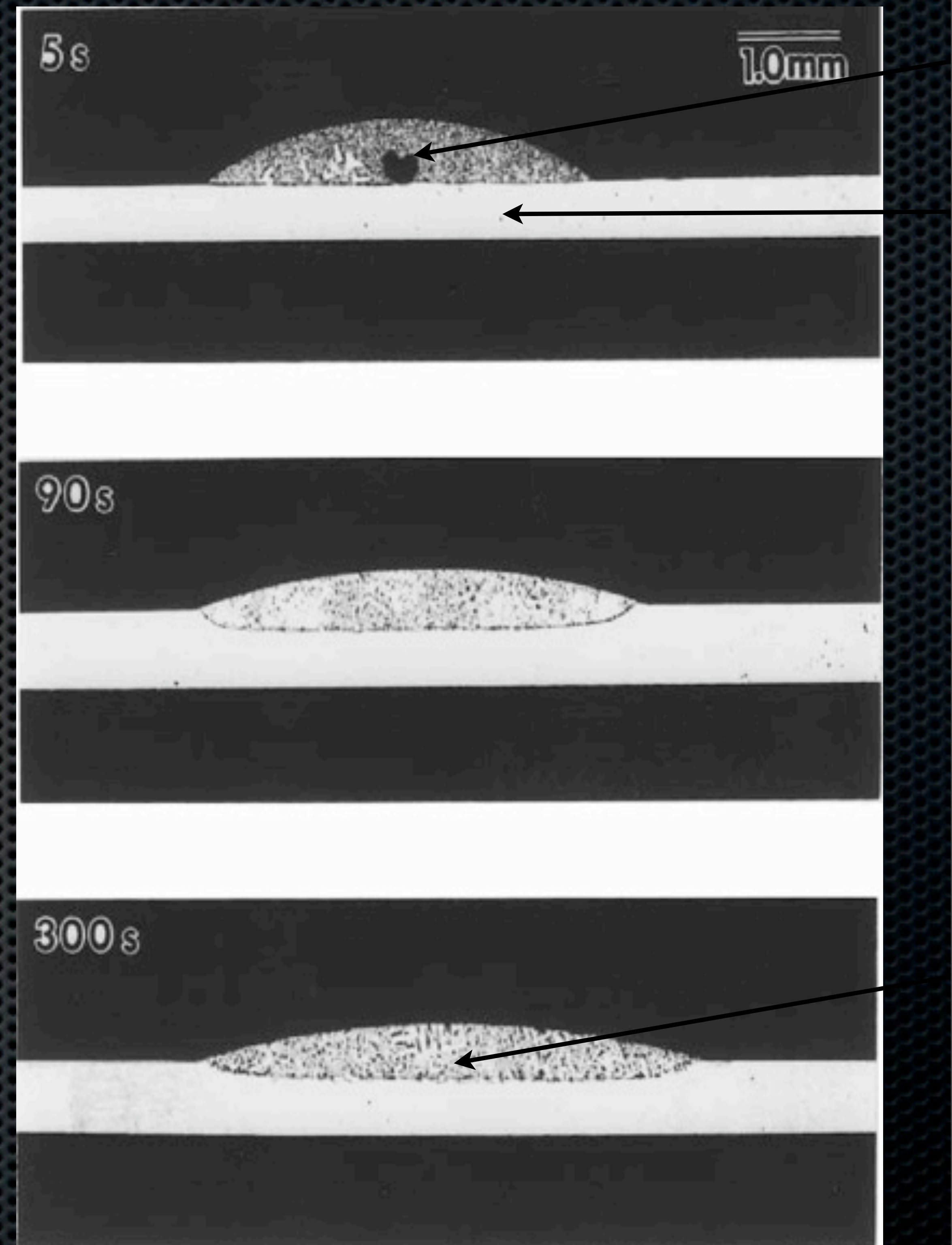
Science 5/4/07
Kodambaka et al.



Nanowirephotonics.com

Observations

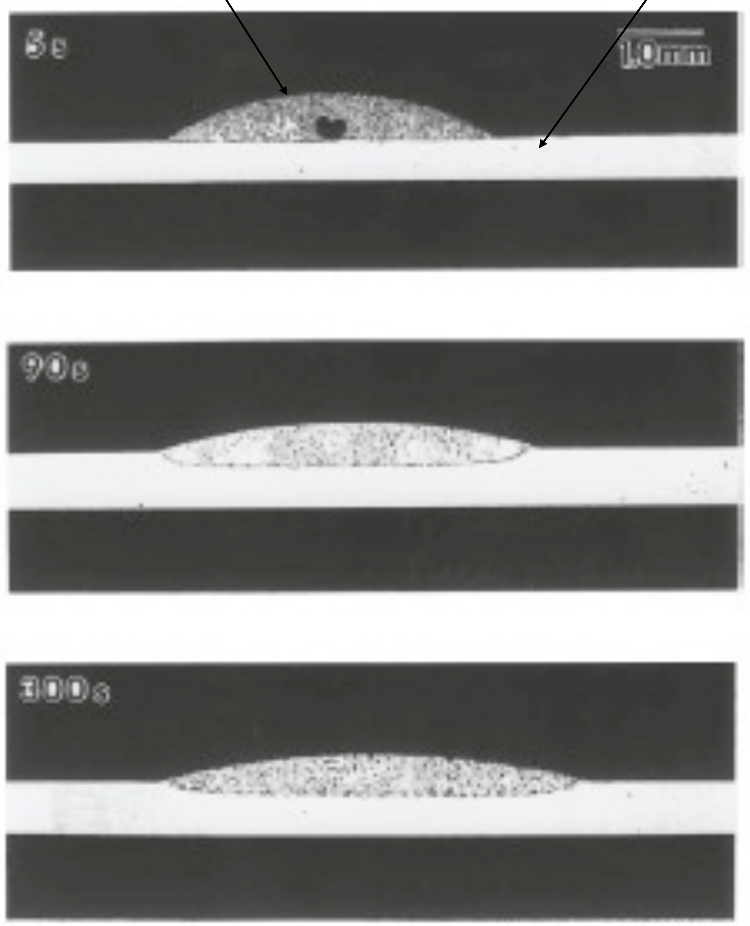
- Most of the spreading happened in <1 ms
- Prior efforts looked at diffusion controlled growth with hydrodynamics *slaved* to the TJ motion
- What is the proper description of the system state after 5 sec?



Experimental Variations

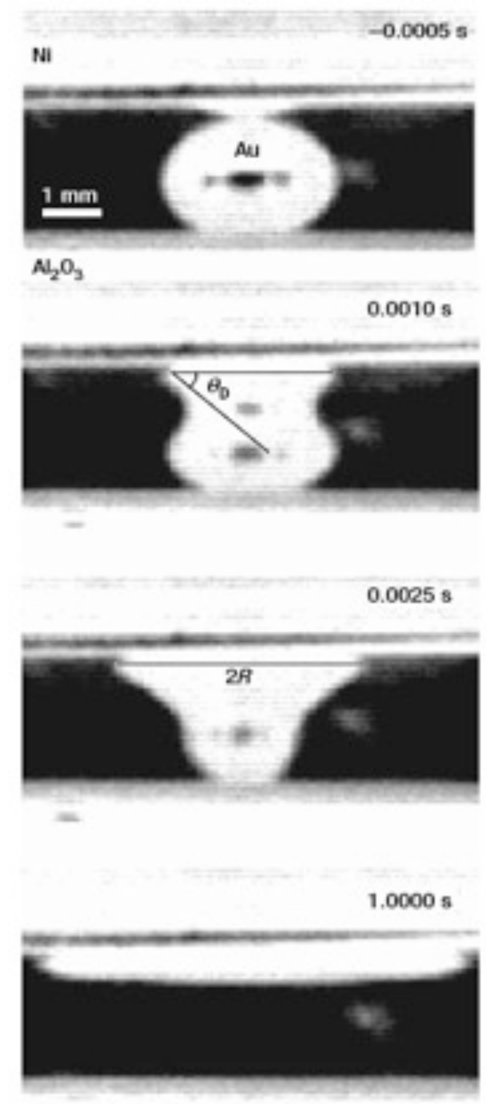
Bi-Sn Solder, Sn rich

Bi substrate



Warren et al.

Slow – lower temperature



Saiz and Tomsia

Fast – higher temperature

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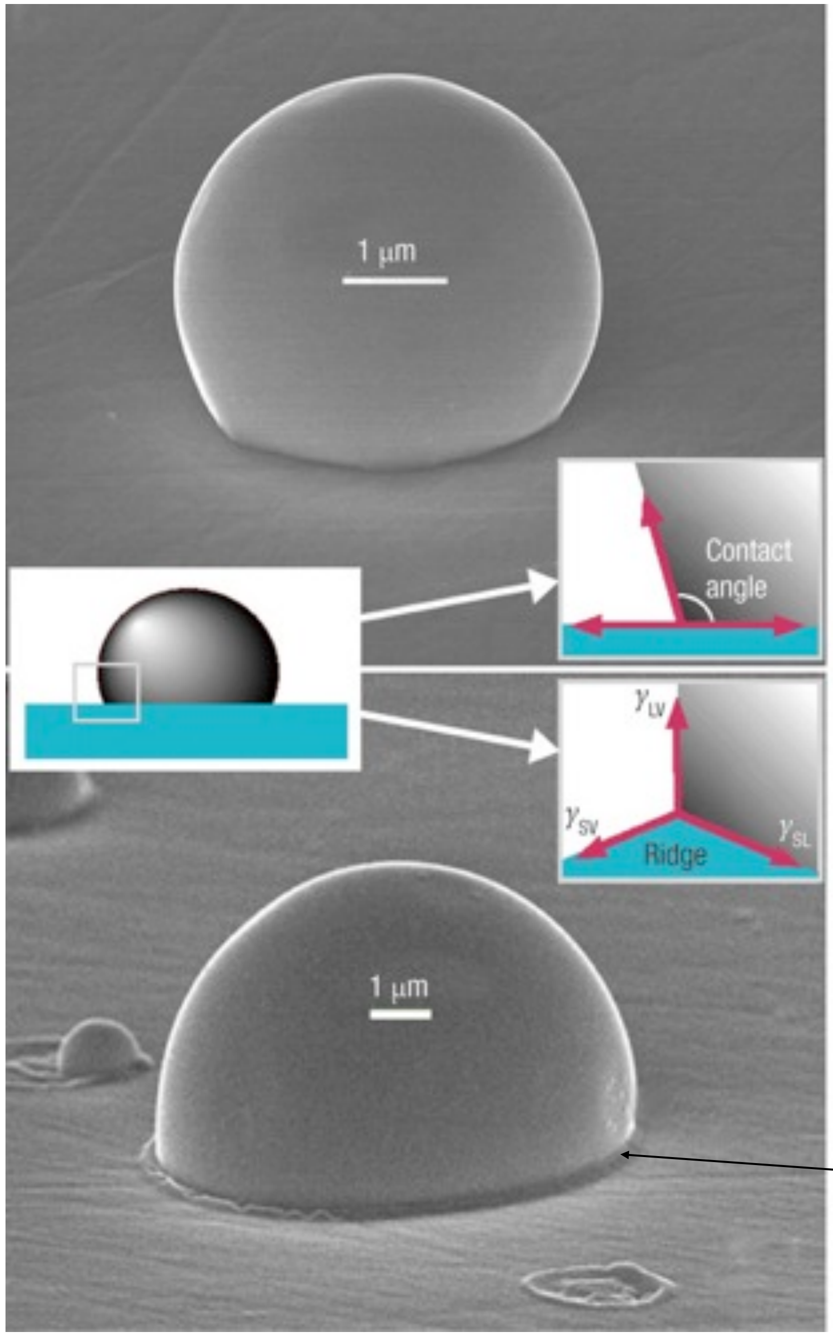
Ridging Effects



Surface must be flat for fast spreading

Our model may help to understand this phenomenon in the future, but requires a really large simulation

Ridge retards spreading

Chatain and Carter, Nature Materials 2004

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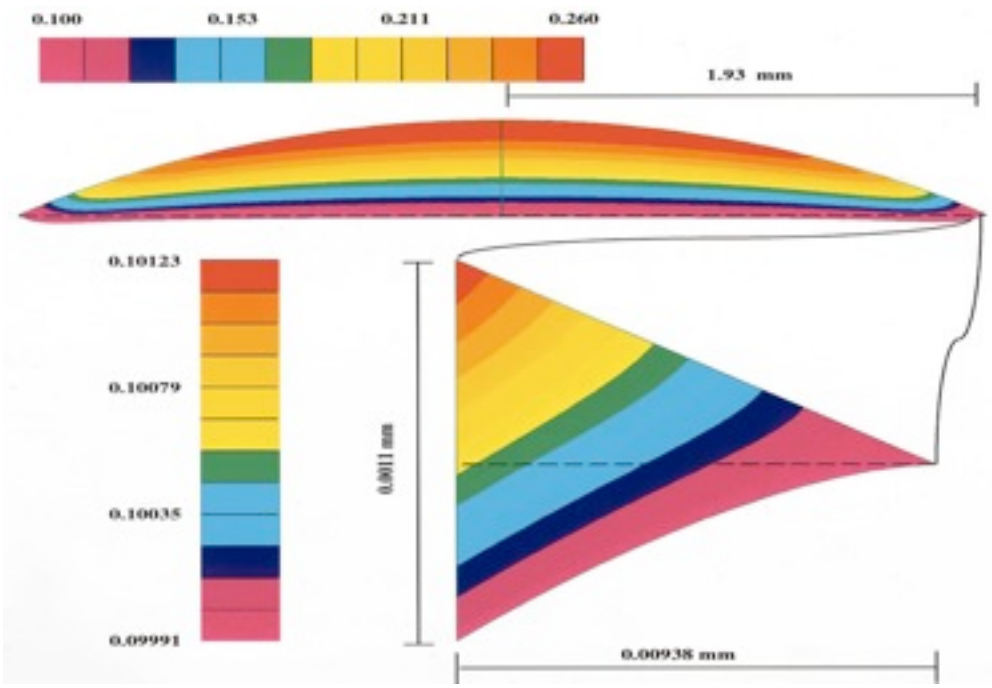
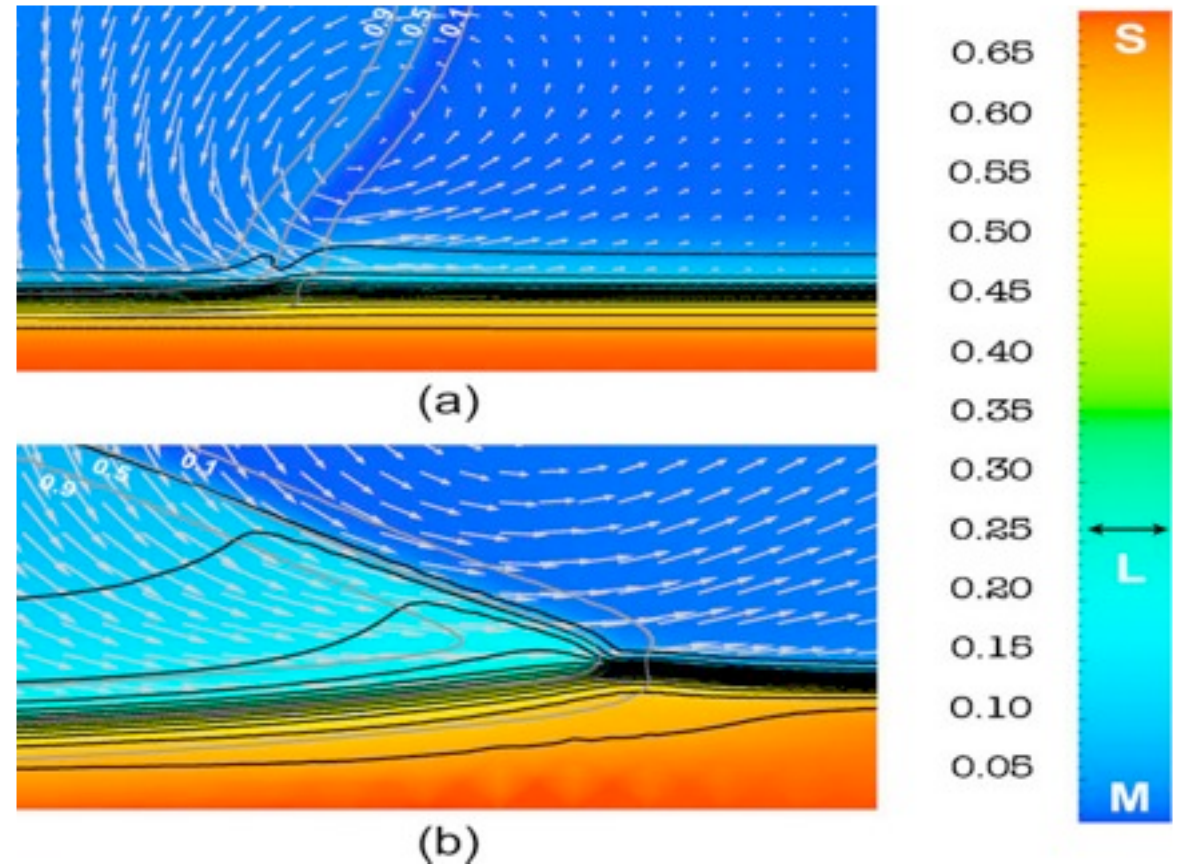
Viscous Dissipation



Lubrication approximation,
Warren et al.



Small viscous drops using
phase field method,
Villanueva et al.

$$t_c = \frac{R\mu}{\gamma} = 1 \times 10^{-6}\mathrm{s}$$

Cannot be correct timescale
for mm sized drops

What about inertial effects?

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2 Approaches

$$\phi_s + \phi_l + \phi_v = 1$$
$$\phi_s, \phi_l, u_i, P$$
$$R = 1 \times 10^{-8}\mathrm{m}$$
$$\delta = 1 \times 10^{-9}\mathrm{m}$$

viscous, three phase fields

- Use the phase field method
- No special algorithms
- Fundamental
- Based on thermo (not ad-hoc)
- nano? -- micro -- macro?

incompressible, pure phase field
Villanueva

Inertial, 1 phase field

$$\phi_s, u_i, \rho$$
$$R = 1 \times 10^{-6}\mathrm{m}$$
$$\delta = 1 \times 10^{-7}\mathrm{m}$$

compressible, van der Waals + phase field

Wheeler

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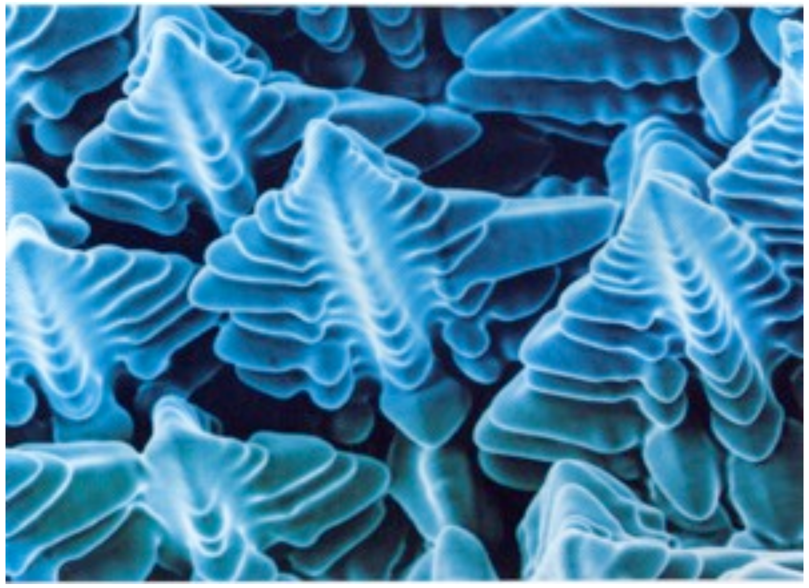
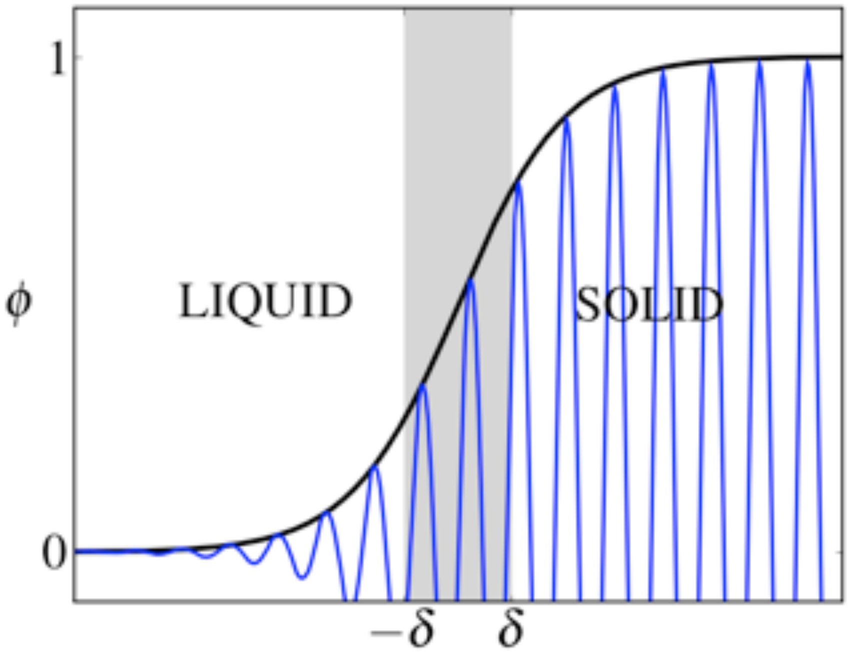
Outline

- Motivation and Introduction
- Phase Field Method intro/Fundamentals
- Thermodynamic derivation
- Numerical approach (FiPy digression)
- Results
- Conclusions

Phase Field Method



Dendrites



Derive from fundamental thermodynamics

Step 1: write down the free energy

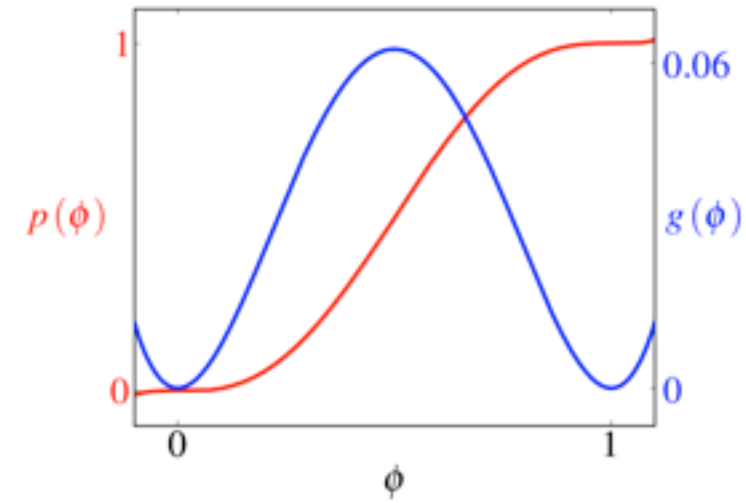
$$f(\phi, T) = L\frac{T_M - T}{T_M}(1 - p(\phi)) + Wg(\phi)$$

Step 2: write down the functional

$$F = \int_V \left[f(\phi, T) + \frac{\epsilon^2}{2} |\nabla\phi|^2 \right] dV$$

Step 3: minimize F

$$\frac{\partial \phi}{\partial t} = -M_\phi \frac{\delta F}{\delta \phi}$$



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Write down the laws of nature

- Mass is conserved

$$\frac{D\rho}{Dt} = -\rho\nabla\cdot\mathbf{v} \qquad \frac{D\rho_i}{Dt} = -\rho_i\nabla\cdot\mathbf{v} - \nabla\cdot\mathbf{J_i}$$

- Momentum is conserved

$$\rho\frac{D\mathbf{v}}{Dt} = \nabla\cdot\sigma$$

- Energy is conserved

$$\frac{Du}{Dt} + u\nabla\cdot\mathbf{v} + \nabla\cdot\mathbf{J_h} = \sigma : \nabla\mathbf{v}$$

- Entropy is maximized (locally in a continuum sense with appropriate fluxes)

NEED TO ENSURE ENTROPY PRODUCTION IS POSITIVE BY POSTULATING CONSTITUTIVE LAWS FOR THE STRESS AND FLUXES

Assume a non-classical entropy

$$S = \int dV\, s^{NC}$$

$$s^{NC} = s(u, \phi, \rho_i) - \frac{1}{2}\left[\epsilon_\phi \Gamma^2(\nabla\phi) + \epsilon_i |\nabla\rho_i|^2\right], \qquad \xi = \frac{\partial \Gamma}{\partial \nabla\phi}$$

SOLID - FLUID PHASE FIELD WHERE THE FLUID CAN UNDERGO A LIQUID-VAPOR TRANSITION (VAN DER WAALS)

$$s_{\text{prod}} = \mathbf{J}_e \cdot \nabla \frac{1}{T} - \mathbf{J}_i \cdot \nabla \left(\frac{\bar{\mu}_i}{T}\right)^{\text{NC}} + \frac{\tau}{T} : \nabla \mathbf{v} + \frac{D\phi}{Dt}\frac{\delta S}{\delta \phi}$$

Turn the Crank: Dynamics

$$s_{\mathrm{prod}} \quad = \quad \mathbf{J}_e \cdot \nabla \frac{1}{T} - \mathbf{J}_i \cdot \nabla \left(\frac{\bar{\mu}_i}{T}\right)^{\mathrm{NC}} + \frac{\tau}{T} : \nabla \mathbf{v} + \frac{D\phi}{Dt}\frac{\delta S}{\delta \phi}$$

$$\frac{D\phi_k}{Dt} = M_{\phi_k} \frac{\delta S}{\delta \phi_k} \qquad \frac{\delta S}{\delta \phi} = \frac{\partial s}{\partial \phi} + \epsilon_\phi \nabla \cdot (\Gamma \xi)$$

$$\left(\frac{\bar{\mu}_i}{T}\right)^{\mathrm{NC}} = \frac{\mu_i - \mu_n}{T} - \epsilon_i \nabla^2 \rho_i + \epsilon_n \nabla^2 \rho_n$$

$$\mathbf{J}_{\mathbf{i} \neq \mathbf{n}} = -M_i \nabla \left[\frac{\mu_i - \mu_n}{T} - \epsilon_i \nabla^2 \rho_i + \epsilon_n \nabla^2 \rho_n\right]$$

$$\mathbf{J}_e = K \nabla \frac{1}{T}$$

Still need $s(\phi, \rho)$

$$\xi = \frac{\partial \Gamma}{\partial \nabla \phi}$$

Last Term $\tau : \nabla \mathbf{v}$

$$\tau = \sigma + \left[P - T\epsilon_i\left(\rho_i\nabla^2\rho_i + \frac{1}{2}|\nabla\rho_i|^2\right) - T\frac{\epsilon_\phi}{2}|\nabla\phi|^2\right]I$$
$$+ T\epsilon_i\nabla\rho_i \otimes \nabla\rho_i + T\epsilon_\phi\nabla\phi\otimes\nabla\phi,$$

$$\tau = \mu\left(\nabla\mathbf{v} + (\nabla\mathbf{v})^T\right) + \left(K - \frac{2}{3}\mu\right)I\nabla\cdot\mathbf{v}$$

Non-Classical
Newtonian
Fluid

Outline

- Motivation and introduction
- Phase field method intro
- Thermodynamics (local)
- Numerical approach (FiPy digression)
- Results
- Conclusions

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Reactive Wetting – More Complicated

Interpolation between solid and fluid phases

$$f\left(\phi,\rho_1,\rho_2\right) = \left(1-p\left(\phi\right)\right) f^F\left(\rho_1,\rho_2\right) + p\left(\phi\right) f^S\left(\rho_1,\rho_2\right) + W g\left(\phi\right)$$

Use van der Waals model for fluid phase

$$f^F\left(\rho_1,\rho_2\right) = \frac{e_1\rho_1^2}{m^2} + \frac{e_{12}\rho_1\rho_2}{m^2} + \frac{e_2\rho_2^2}{m^2} + \frac{RT}{m}\left[\rho_1 \ln\rho_1 + \rho_2 \ln\rho_2 - \rho \ln\left(m-\bar{v}\rho\right)\right]$$

Long range attraction

$$PV = nRT$$

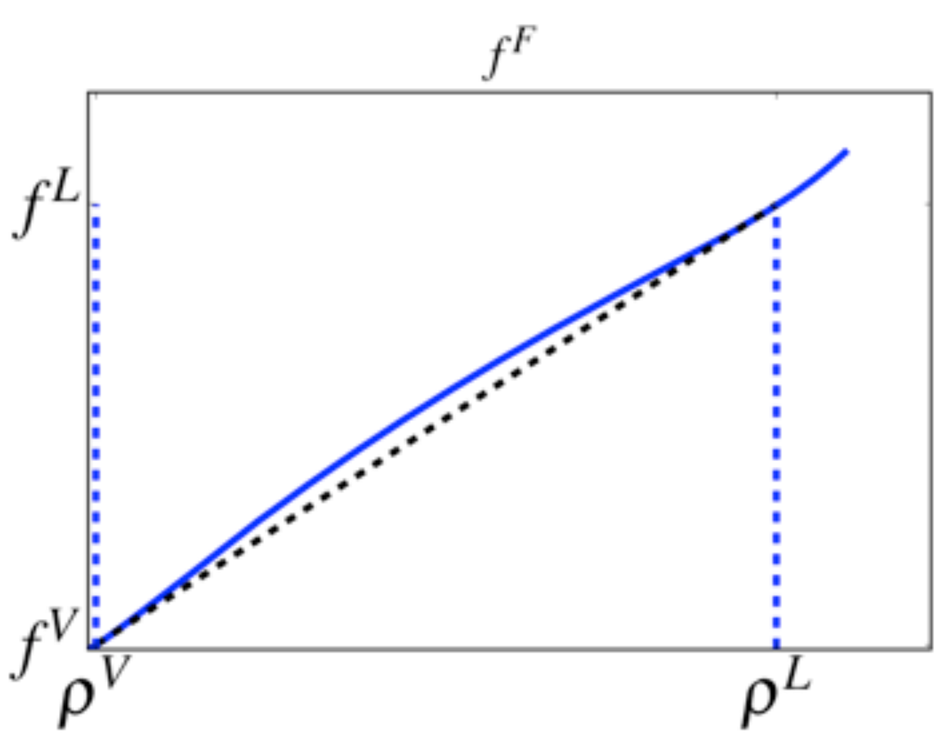
Ideal gas law

$$\left(P - e_1\frac{n^2}{V^2}\right)\left(V - \bar{v}n\right) = nRT$$

Van der Waals equation of state

Short range repulsion

Common tangent construction for pure system



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Reactive Wetting – More Complicated

Interpolation between solid and fluid phases

$$f\left(\phi,\rho_1,\rho_2\right)=\left(1-p\left(\phi\right)\right)f^F\left(\rho_1,\rho_2\right)+p\left(\phi\right)f^S\left(\rho_1,\rho_2\right)+Wg\left(\phi\right)$$

Solid free energy

Short range repulsion

$$f^S\left(\rho_1,\rho_2\right)=\frac{A_1\rho_1}{m}+\frac{A_2\rho_2}{m}+\frac{RT}{m}\left(\rho_1\ln\rho_1+\rho_2\ln\rho_2-\rho\ln\rho\right)+\frac{Bm}{\rho v_s^2}\left(1-\frac{\rho v_s}{m}\right)^2$$

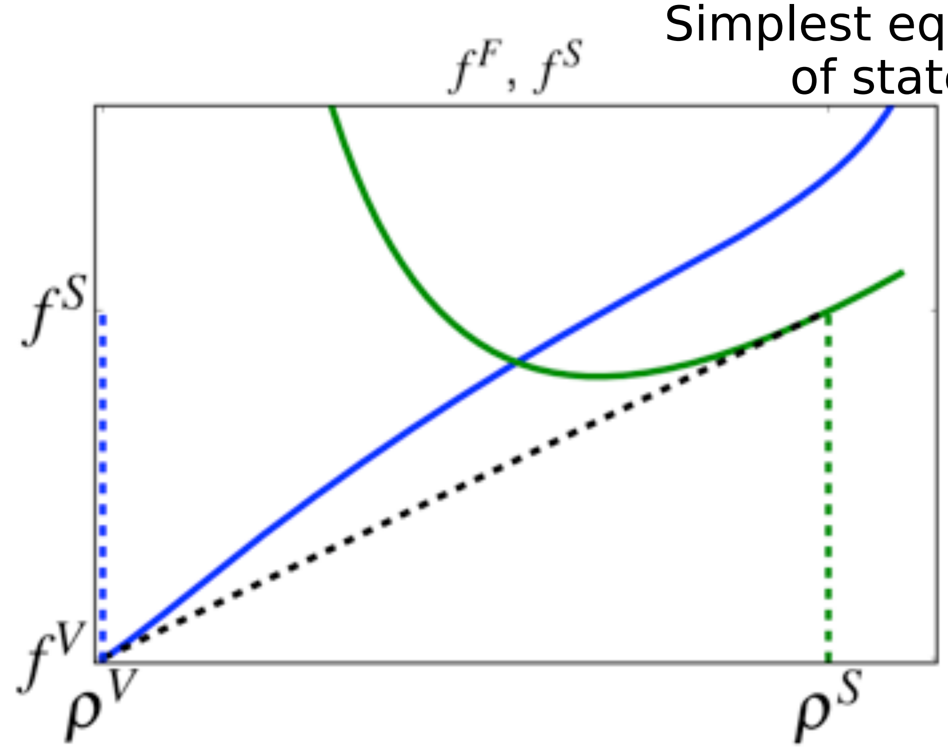
Solid offset constant

Entropy of mixing

$$\boxed{PV_s=2Bn\frac{V_s-V}{V_s}}$$

Simplest equation of state

Common tangent construction for pure system



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Derivation

Interpolation between solid and fluid phases

$$f\left(\phi,\rho_1,\rho_2\right)=\left(1-p\left(\phi\right)\right)f^F\left(\rho_1,\rho_2\right)+p\left(\phi\right)f^S\left(\rho_1,\rho_2\right)+Wg\left(\phi\right)$$

Solid free energy

$$f^S\left(\rho_1,\rho_2\right)=\frac{A_1\rho_1}{m}+\frac{A_2\rho_2}{m}+\frac{RT}{m}\left(\rho_1\ln\rho_1+\rho_2\ln\rho_2-\rho\ln\rho\right)+\frac{Bm}{\rho V_s^2}\left(1-\frac{\rho V_s}{m}\right)^2$$

Solid offset constant

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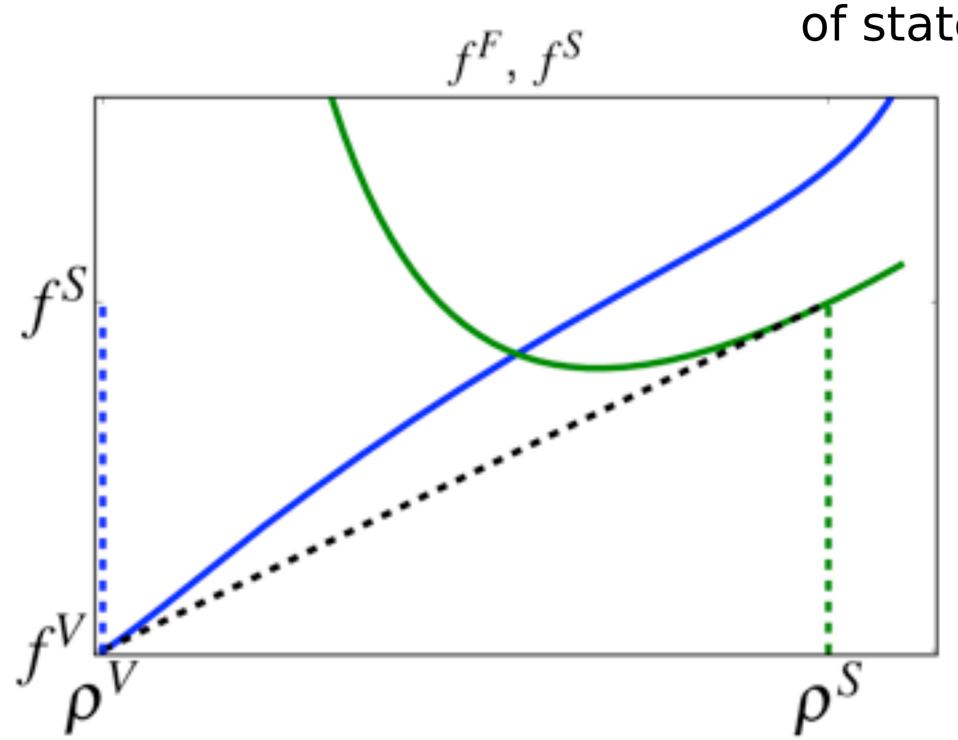

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Reactive Wetting - Functional

$$F = \int_V \left[f\left(\phi, \rho_1, \rho_2\right) + \frac{\epsilon_\phi T}{2} \left|\nabla \phi\right|^2 + \frac{\epsilon_i T}{2} \left|\nabla \rho_i\right|^2 \right] dV$$

Van der Waals liquid-vapor transistion

Turn the crank

mass

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot \left(\vec{u} \rho_i\right) = -\nabla \cdot \vec{J}_i$$

$$\vec{J}_1 = -\vec{J}_2 = -M \nabla \left(\frac{\mu_1 - \mu_2}{T} \right)$$

$$\mu_i = \frac{\delta F}{\delta \rho_i}$$

phase field

$$\frac{D\phi}{Dt} = -\frac{M_\phi}{T} \frac{\delta F}{\delta \phi}$$

momentum

$$\frac{\partial \left(\rho u_i\right)}{\partial t} + \partial_j \left(\rho u_i u_j\right) = \partial_j \left(\eta \left[\partial_i u_j + \partial_i u_j\right]\right) - \rho_j \partial_i \mu_j - \partial_i \phi \frac{\delta F}{\delta \phi}$$

Time Scales

Time scale	Symbol	Expression	Value (s)
instantaneous convection	t_a^*	R_0/U^*	.
convection	t_a	R_0/U	1.97×10^{-8}
viscous	t_v	$\rho_l^{\mathrm{equ}} R_0^2/\eta_l$	3.68×10^{-6}
inertial	t_i	$\sqrt{\rho_l^{\mathrm{equ}} R_0^3/\gamma_{lv}}$	1.97×10^{-8}
phase field	t_ϕ	$\delta^2/\epsilon_\phi M_\phi$	1.0×10^{-9}
perceptible diffusion	t_{diff}	$\delta^2/4K^2 D_f$	7.69×10^{-4}
bulk diffusion	t_{d}	R_0^2/D_f	1.04×10^{-3}
solid deformation	t_s	$\delta\eta_s/\gamma_{lv}$	1.05×10^{-2}
capillary	t_c	$\eta_f R_0/\gamma_{lv}$	1.05×10^{-10}
interface equilibration			?.??

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So Now we have Equations

- Just solve them!
- What does that mean?
- The Usual Scheme:
  - Variables on LHS
  - Finite Difference
  - Iterate
- All of these choices have consequences (poor convergence, instability, etc.)

$$\frac{D\rho_i}{Dt} = -\rho_i \nabla \cdot \mathbf{v} - \nabla \cdot \mathbf{J_i}$$

$$\rho \frac{D\mathbf{v}}{Dt} = \nabla \cdot \sigma$$

$$\frac{D\phi_k}{Dt} = M_{\phi_k} \frac{\delta S}{\delta \phi_k}$$

Solve Them!

THIS IS FAR EASIER SAID THAN DONE!!

- The equations formulated/chosen might be a “bad” choice
- Finite differencing---Stability Finite Difference turns equations PDEs into Ax=b

$$\frac{\partial \phi}{\partial t} \rightarrow \frac{\phi^{n+1} - \phi^{n}}{\Delta t} = RHS(\phi^{?}, c^{?}, ...)$$

- Choice of backwards/forwards is about stability
- Usual Scheme will yield a number of matrix equations
- What order do I solve them in?

$$\frac{D\rho_i}{Dt} = -\rho_i \nabla \cdot \mathbf{v} - \nabla \cdot \mathbf{J_i}$$

$$\frac{D\phi_k}{Dt} = M_{\phi_k} \frac{\delta S}{\delta \phi_k} \qquad \rho \frac{D\mathbf{v}}{Dt} = \nabla \cdot \sigma$$

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Numerical Approach

Segregated picard iterations

$$\begin{pmatrix} \frac{\partial \rho}{\partial t} + \dots & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\partial \rho}{\partial t} + \dots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\partial}{\partial t} + \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\partial}{\partial t} + \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\partial}{\partial t} + \dots \end{pmatrix} \begin{pmatrix} u \\ v \\ \rho_1 \\ \rho_2 \\ \mu_1 \\ \mu_2 \\ \phi \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \mu_1^* \\ \mu_2^* \\ 0 \end{pmatrix}$$

FiPy

The segregated solver did not work for low viscosities and binary materials (worked for pure materials)

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Numerical Approach

Fully coupled picard iterations

$$
\begin{pmatrix}
\frac{\partial\rho}{\partial t}+\dots & 0 & 0 & 0 & \rho_1\partial_x & \rho_2\partial_x & 0 \\
0 & \frac{\partial\rho}{\partial t}+\dots & 0 & 0 & \rho_1\partial_y & \rho_2\partial_y & 0 \\
0 & 0 & \frac{\partial}{\partial t}+\dots & 0 & -\partial_j\frac{M}{T}\partial_j & \partial_j\frac{M}{T}\partial_j & 0 \\
0 & 0 & 0 & \frac{\partial}{\partial t}+\dots & \partial_j\frac{M}{T}\partial_j & -\partial_j\frac{M}{T}\partial_j & 0 \\
0 & 0 & -\frac{\partial\mu_1^*}{\partial\rho_1}+\epsilon_1 T\partial_j^2 & -\frac{\partial\mu_1^*}{\partial\rho_2} & 1 & 0 & 0 \\
0 & 0 & -\frac{\partial\mu_2^*}{\partial\rho_1} & -\frac{\partial\mu_2^*}{\partial\rho_2}+\epsilon_2 T\partial_j^2 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \frac{\partial}{\partial t}+\dots
\end{pmatrix}
\begin{pmatrix} u \\ v \\ \rho_1 \\ \rho_2 \\ \mu_1 \\ \mu_2 \\ \phi \end{pmatrix}
=
\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \mu_1^* \\ \mu_2^* \\ 0 \end{pmatrix}
$$

FiPy

- FiPy is the frontend
- Using Trilinos solvers and preconditioners as the backend
- FiPy is modified for both coupled and parallel solutions
- Limited by CFL condition (not speed of sound)
- Worked with Aaron Lott (UMD) on optimizing Trilinos precondtioners

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Numerical Approach

Fully coupled picard iterations

$$\begin{pmatrix} \frac{\partial \rho}{\partial t} + \dots & 0 & 0 & 0 & \rho_1 \partial_x & \rho_2 \partial_x & 0 \\ 0 & \frac{\partial \rho}{\partial t} + \dots & 0 & 0 & \rho_1 \partial_y & \rho_2 \partial_y & 0 \\ 0 & 0 & \frac{\partial}{\partial t} + \dots & 0 & -\partial_j \frac{M}{T} \partial_j & \partial_j \frac{M}{T} \partial_j & 0 \\ 0 & 0 & 0 & \frac{\partial}{\partial t} + \dots & \partial_j \frac{M}{T} \partial_j & -\partial_j \frac{M}{T} \partial_j & 0 \\ 0 & 0 & -\frac{\partial \mu_1^*}{\partial \rho_1} + \epsilon_1 T \partial_j^2 & -\frac{\partial \mu_1^*}{\partial \rho_2} & 1 & 0 & 0 \\ 0 & 0 & -\frac{\partial \mu_2^*}{\partial \rho_1} & -\frac{\partial \mu_2^*}{\partial \rho_2} + \epsilon_2 T \partial_j^2 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\partial}{\partial t} + \dots \end{pmatrix} \begin{pmatrix} u \\ v \\ \rho_1 \\ \rho_2 \\ \mu_1 \\ \mu_2 \\ \phi \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \mu_1^* \\ \mu_2^* \\ 0 \end{pmatrix}$$

$$\frac{M_f}{M_s} = 1 \times 10^4 \qquad \frac{\nu_s}{\nu_f} = 1 \times 10^7$$

FiPy

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Parasitic Currents

momentum conserving

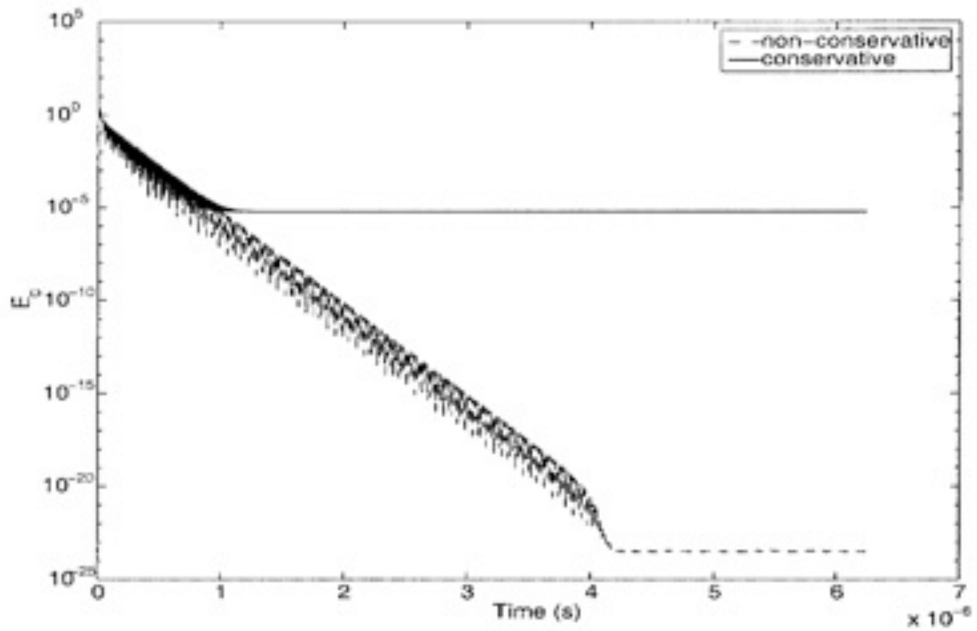
$$\frac{\partial\left(\rho u_i\right)}{\partial t}+\partial_j\left(\rho u_i u_j\right)=\partial_j\left(\eta\left[\partial_i u_j+\partial_i u_j\right]\right)-\boxed{\partial_i P+\epsilon T\rho_k\partial_i\partial_j^2\rho_k}$$

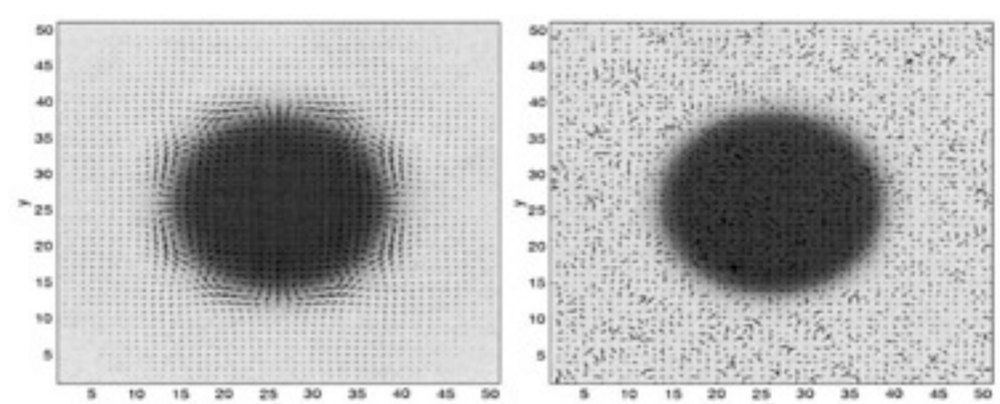
$$P=\rho_i\mu_i^c-f$$

$$\mu_k=\mu_k^c-\epsilon T\partial_j^2\rho_k$$

$$\frac{\partial\left(\rho u_i\right)}{\partial t}+\partial_j\left(\rho u_i u_j\right)=\partial_j\left(\eta\left[\partial_i u_j+\partial_i u_j\right]\right)-\boxed{\rho_k\partial_i\mu_k}$$

energy conserving





Jamet et al., JCP, 2002

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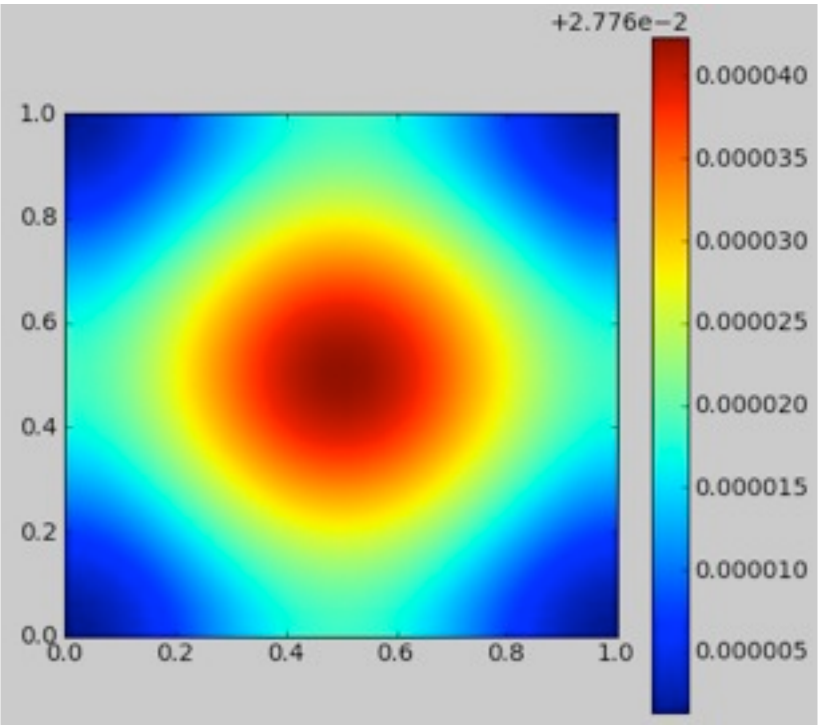
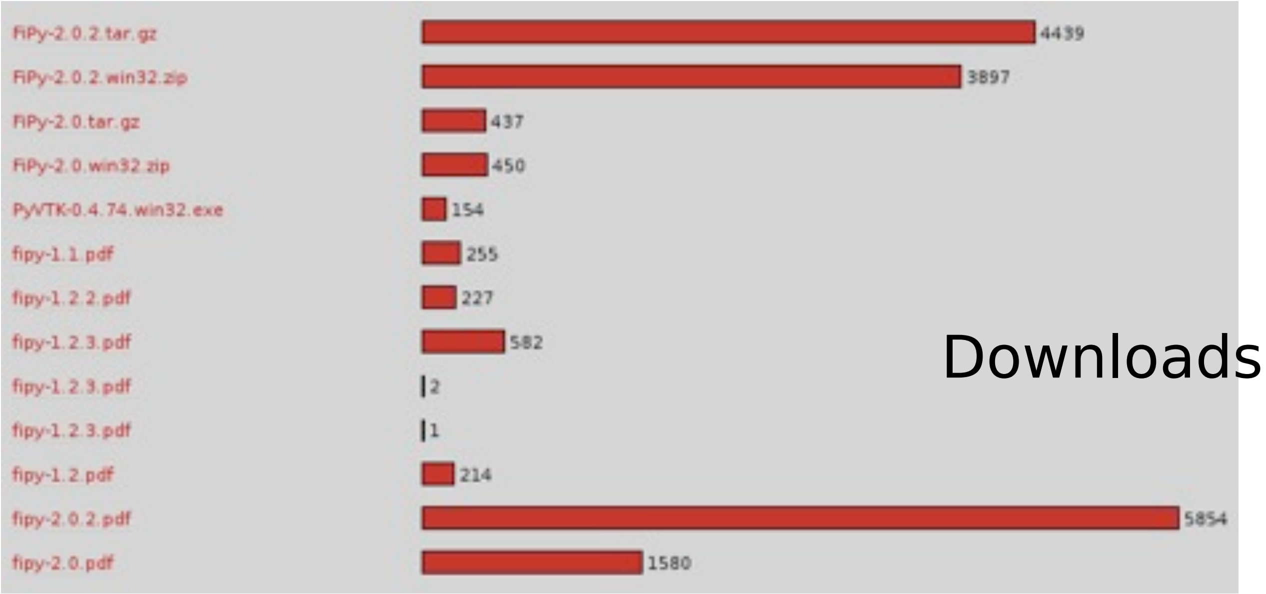
FiPy

```
In [1]: from fipy import *

In [2]: m = Grid2D(nx = 100, ny = 100, dx=0.01, dy=0.01)

In [3]: x, y = m.getCellCenters()

In [4]: v = CellVariable(mesh=m, value=x * y * (1 - x) * (1 - y))

In [5]: vi = Viewer(v)

In [6]: e = TransientTerm() == DiffusionTerm()

In [7]: e.solve(v)

In [8]: vi.plot()

In [9]: e.solve(v)

In [10]: vi.plot()
```



FiPy

- Open source
- Python
- Finite volume



Downloads

113 mailing list members

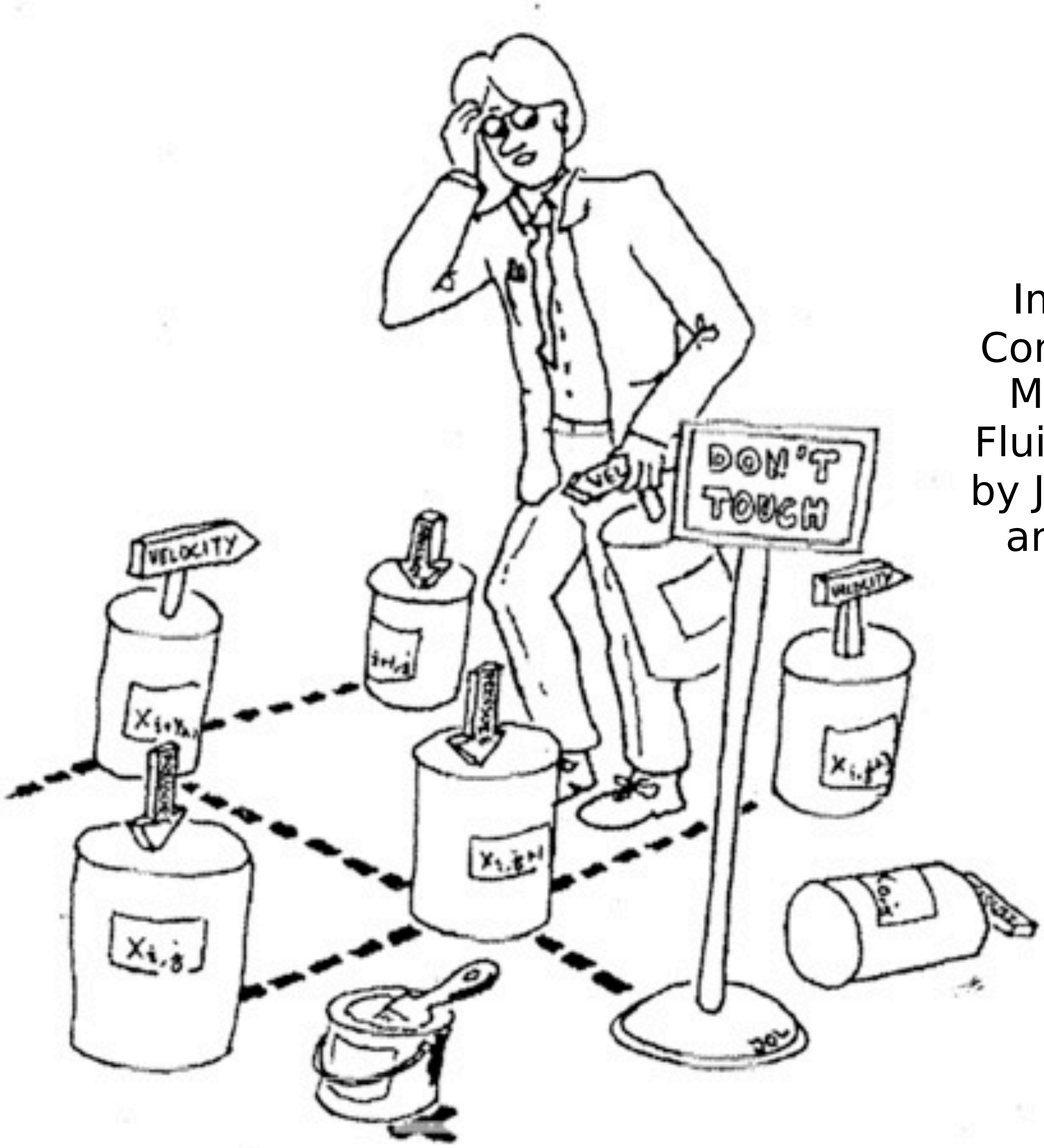
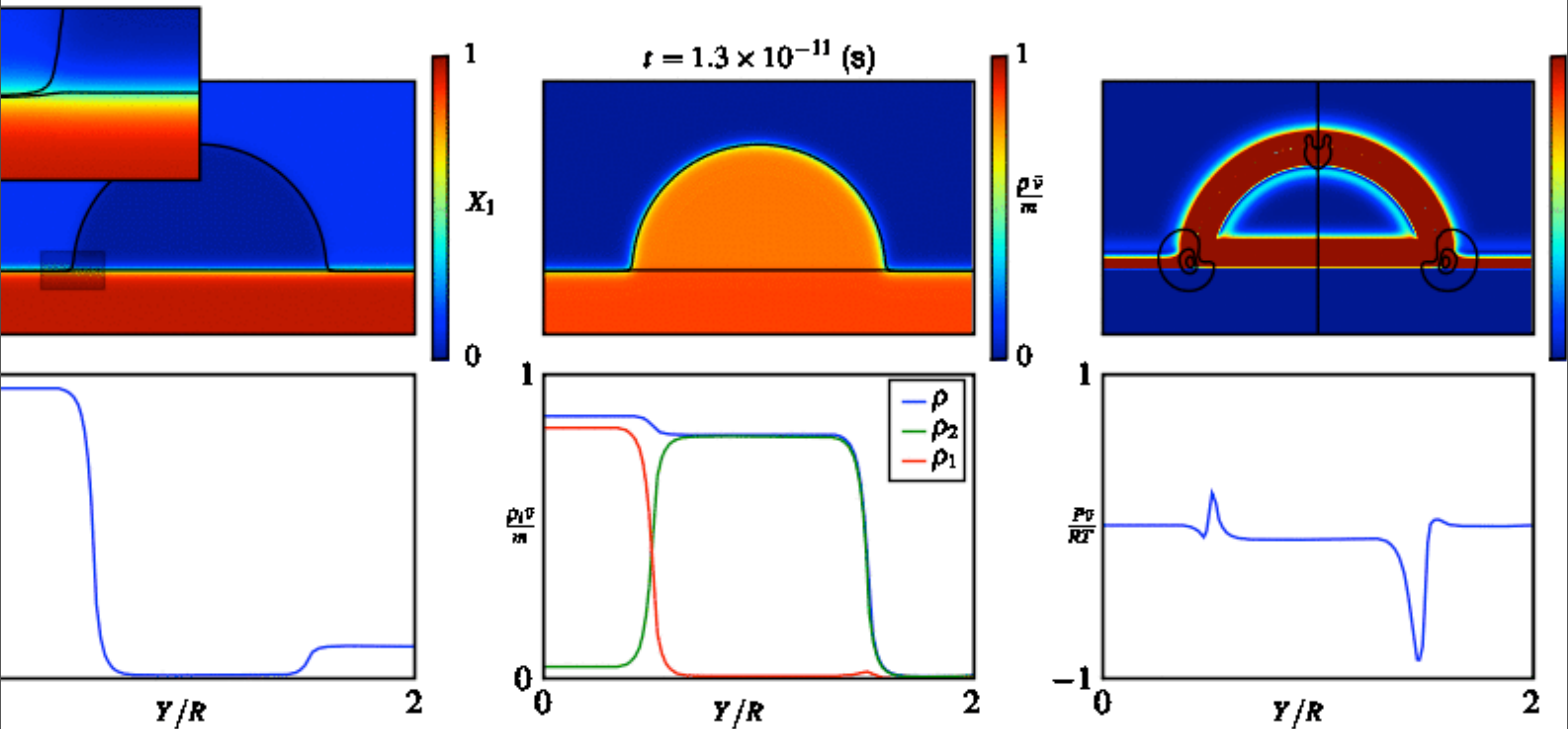


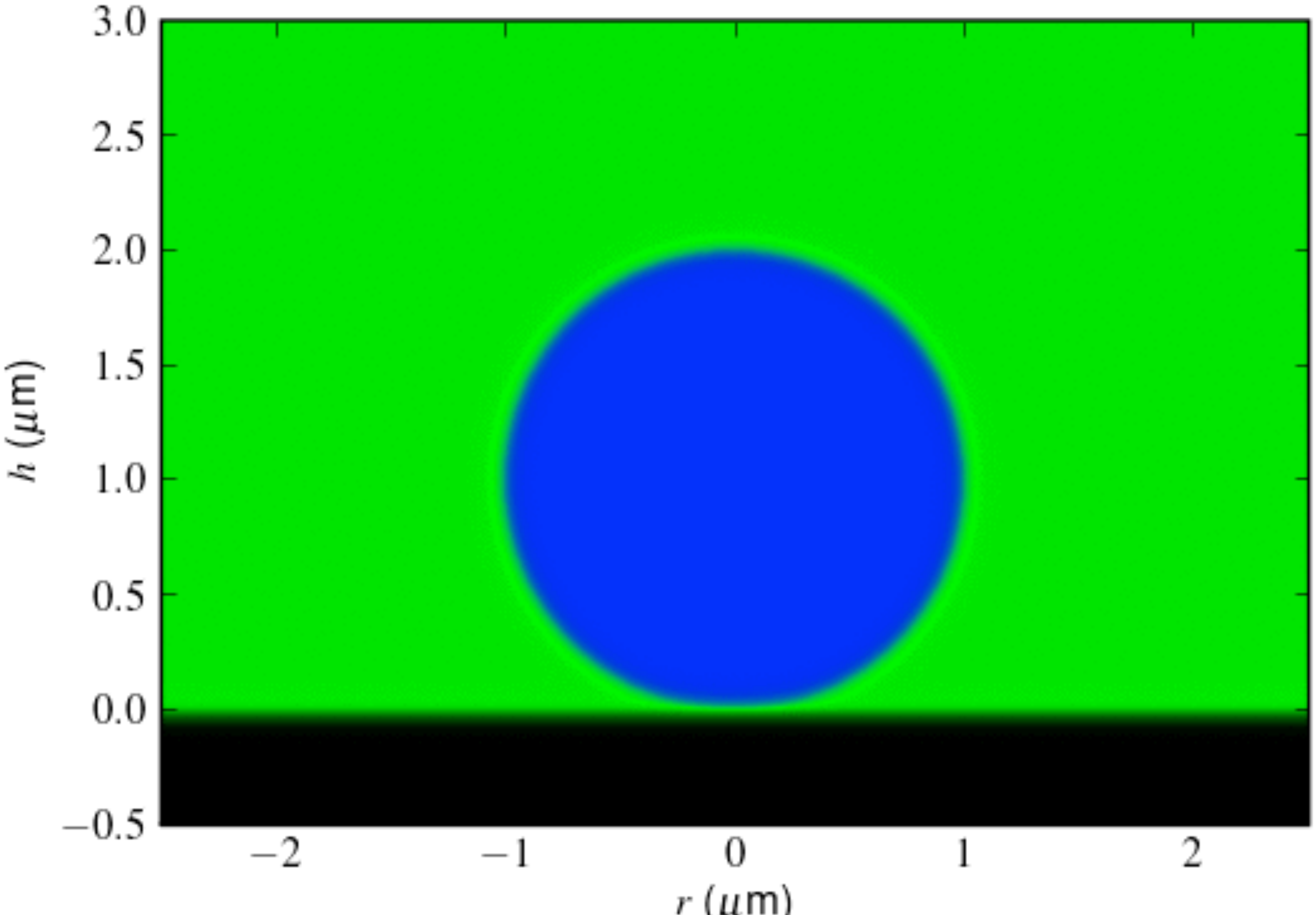
Image from Computational Methods for Fluid Dynamics by J. H. Ferziger and M. Peric

- Motivation and Introduction
- Phase Field Method
- Thermodynamic derivation
- Numerical approach (FiPy digression)
- Results
- Conclusions

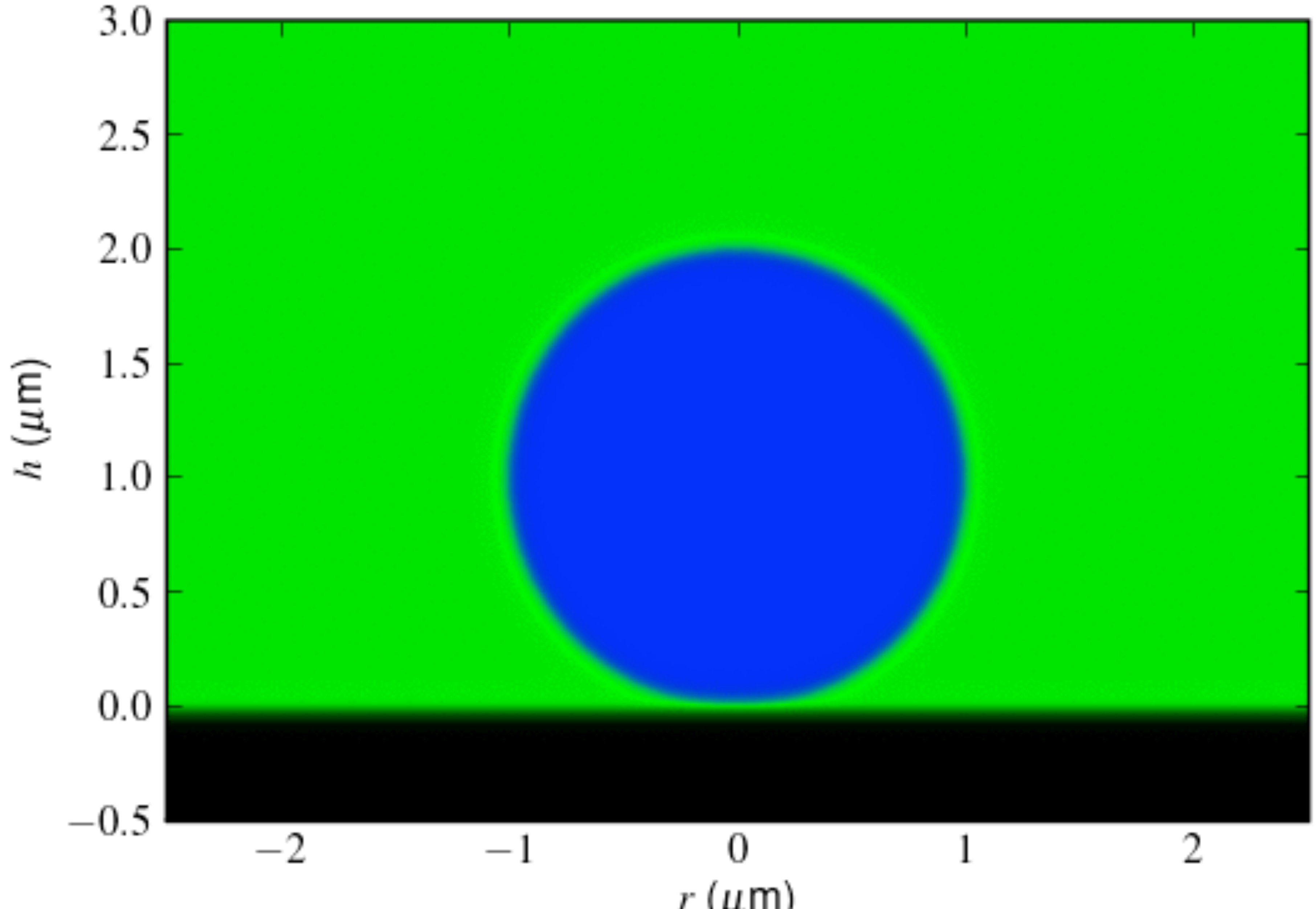
Too Viscous Liquid (Less physical)



Nearly Inviscid Liquid (physical)

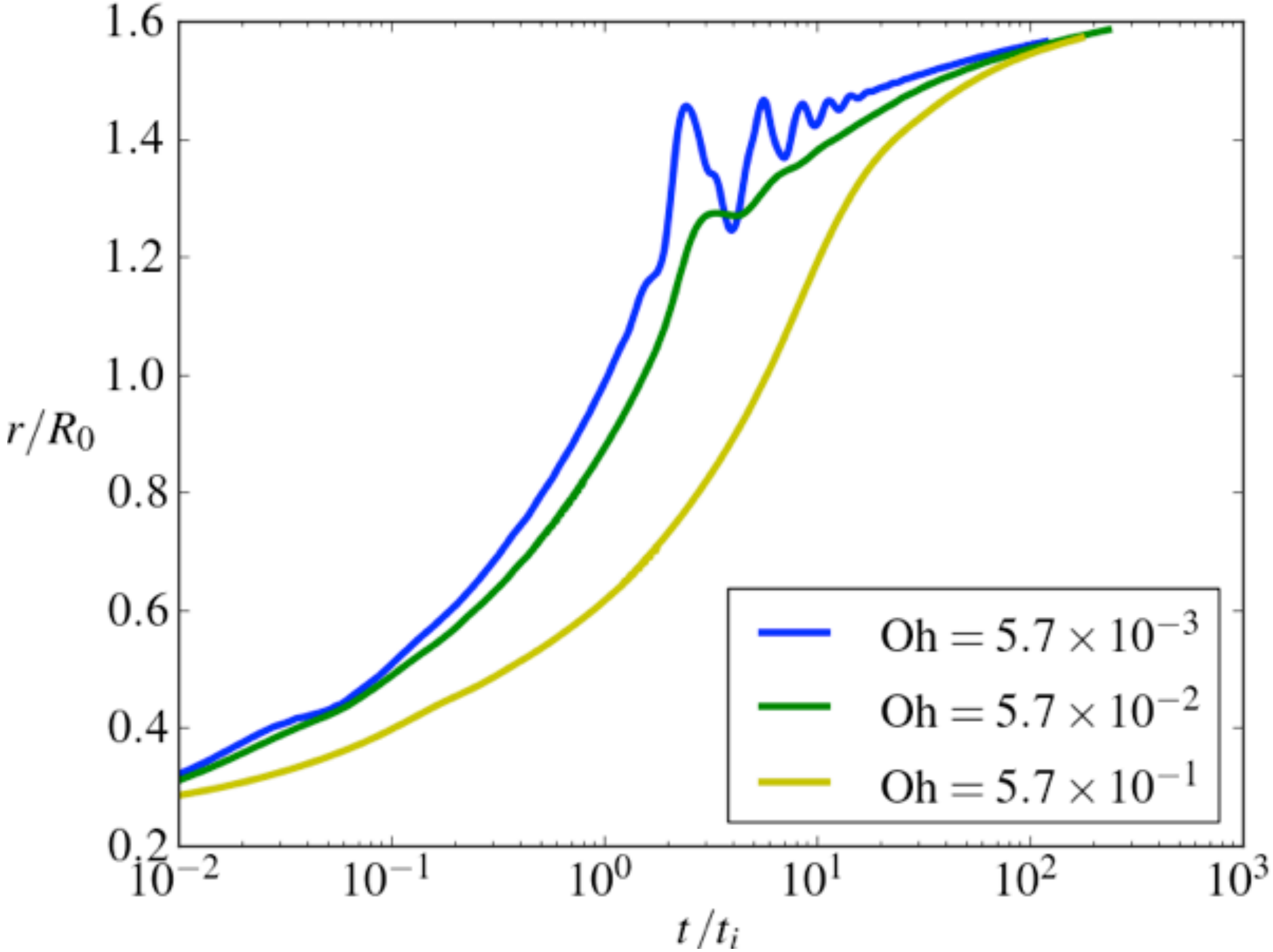


Nearly Inviscid Liquid (physical)



Note Oscillations!

Oscillations



$$t_i = \sqrt{\frac{\rho R_0^3}{\gamma}} \quad t_c = \frac{\eta R_0}{\gamma}$$

$$\mathrm{Oh} = t_c/t_i$$

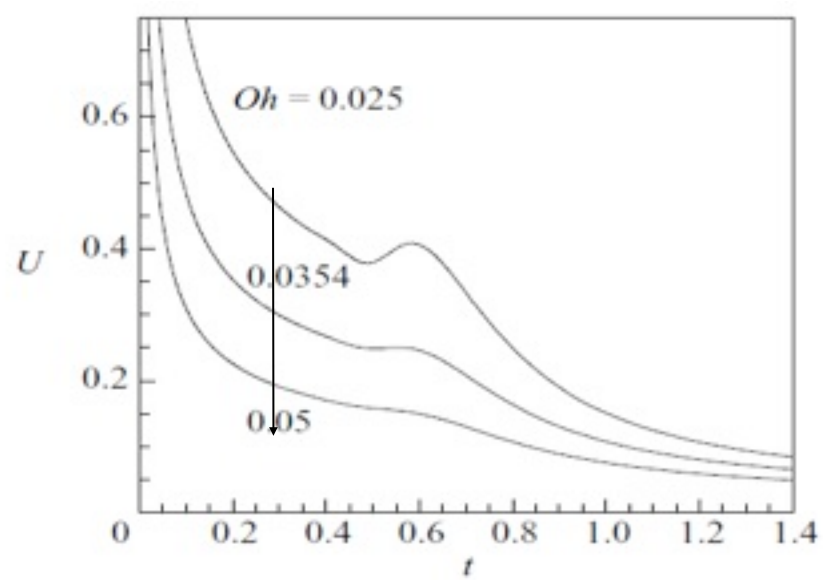
Ohnesorge number

Schiaffino & Sonin, POF 1997
Water on glass

$$0.01 < \mathrm{Oh} < 1$$

transition

Ding & Spelt, JFM, 2007



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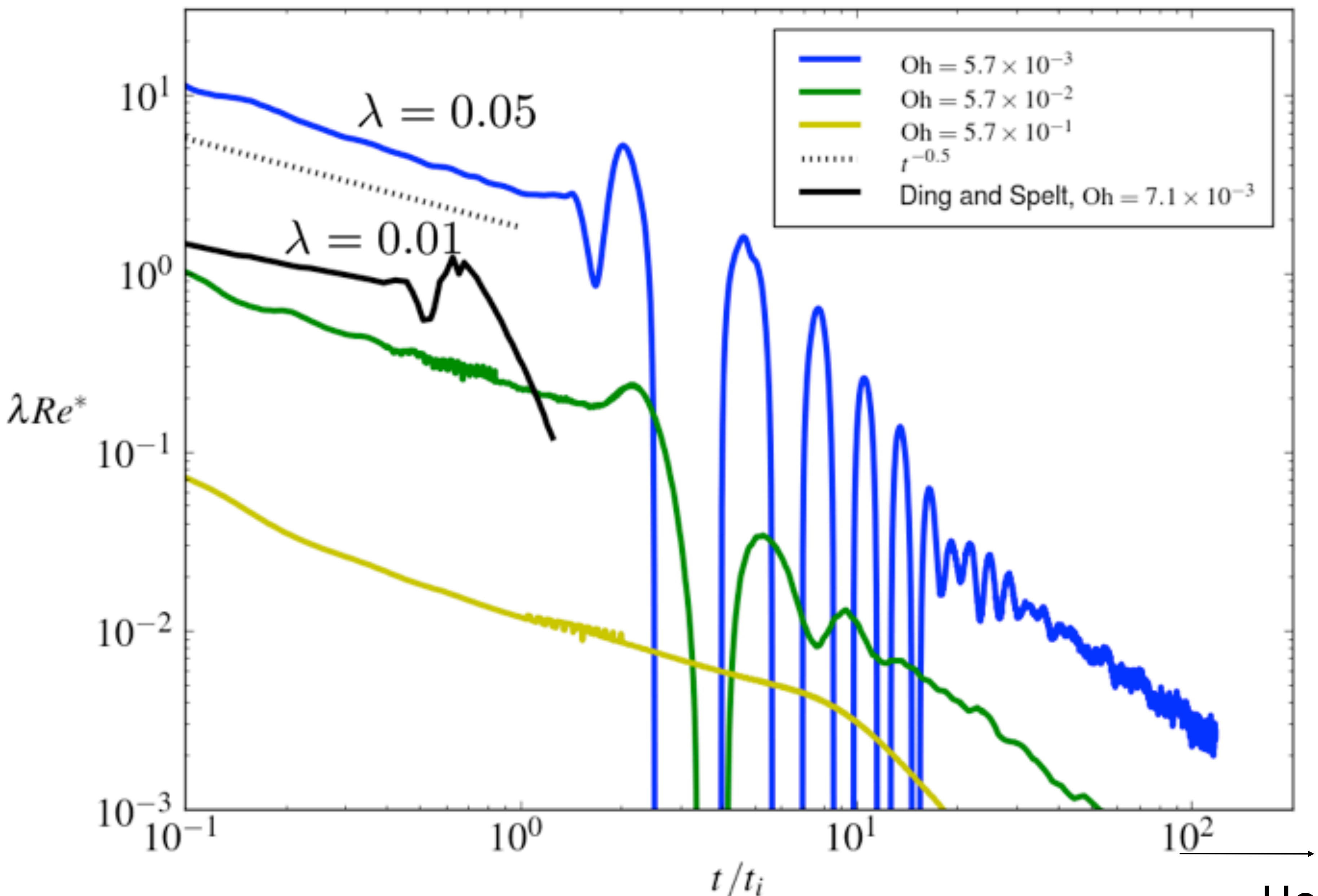
Spreading Rate



Biance et al., PRE 2004

water on glass

$$\frac{r^2(t)}{R_0^2} \sim \frac{t}{t_i}$$

Hocking & Davis, JFM 2002

monotonic decreasing

dimensionless slip-length

diffuse interface width

$$\mathrm{Re}^* = \frac{U \rho R_0}{\eta} > \mathrm{Re}_{\mathrm{ocsillatory}} \left(\lambda = \frac{\delta}{R_0} \right)$$

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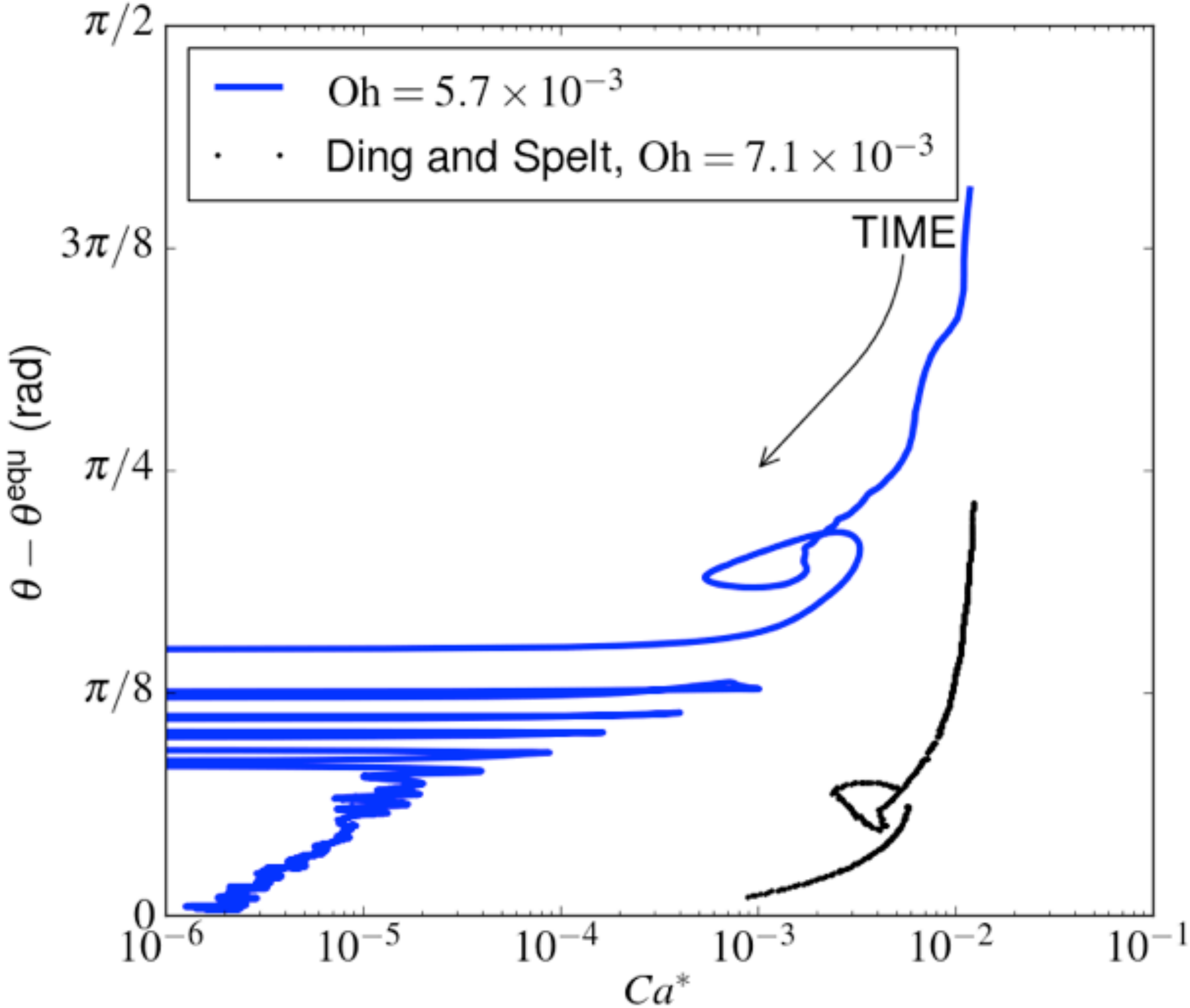
Contact Angle



Hoffman-Voinov-Tanner law

$$\mathrm{Ca}^* = \frac{U\eta}{\gamma} \sim \theta^3 - \theta^3_{\mathrm{equ}}$$

not valid for inertial systems

Hocking & Davis, JFM 2002

For sufficiently high Reynolds there is no simple relation connecting the dynamic contact angle and contact-line speed.

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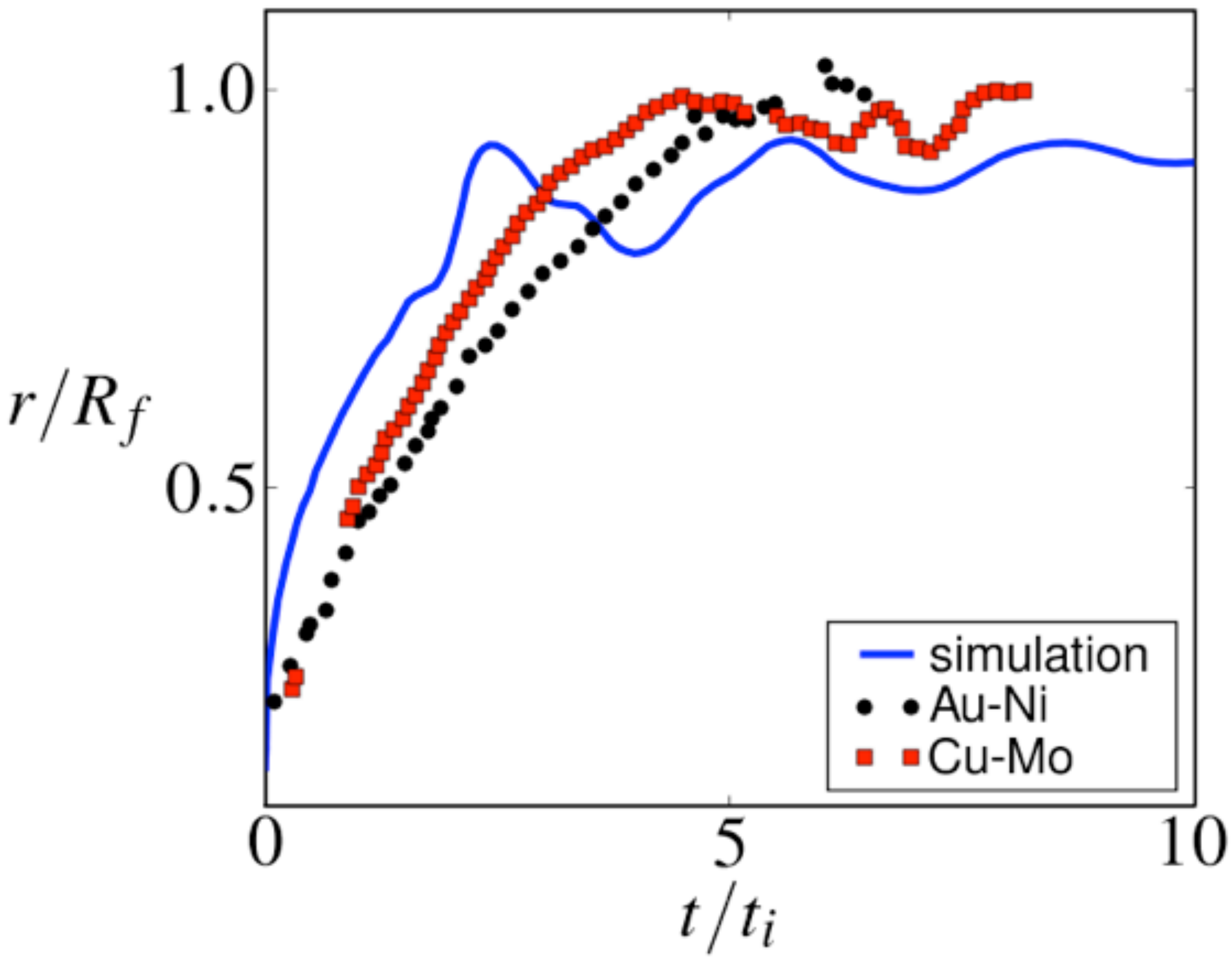
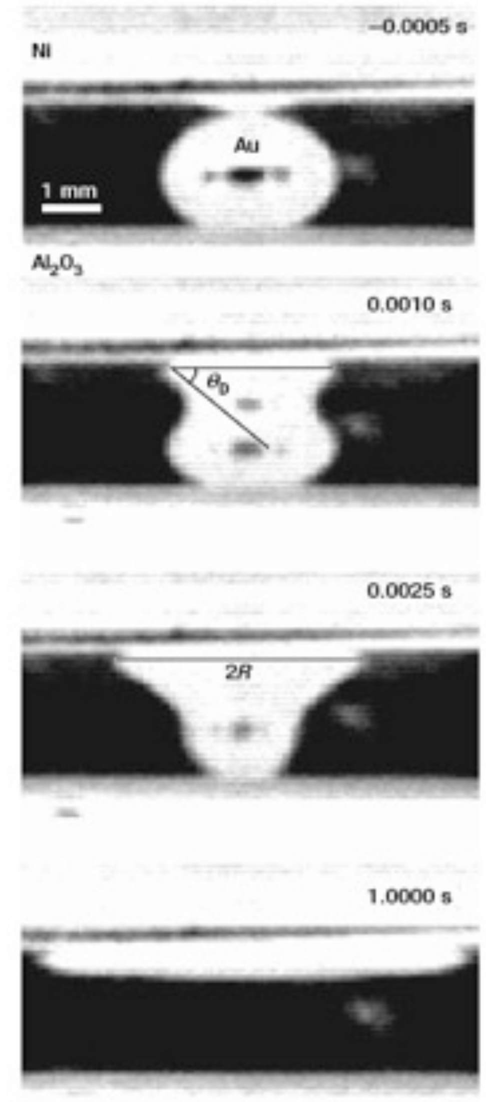
Au-Ni, Cu-Mo experiments





Saiz and Tomsia,
Nature Materials 2004

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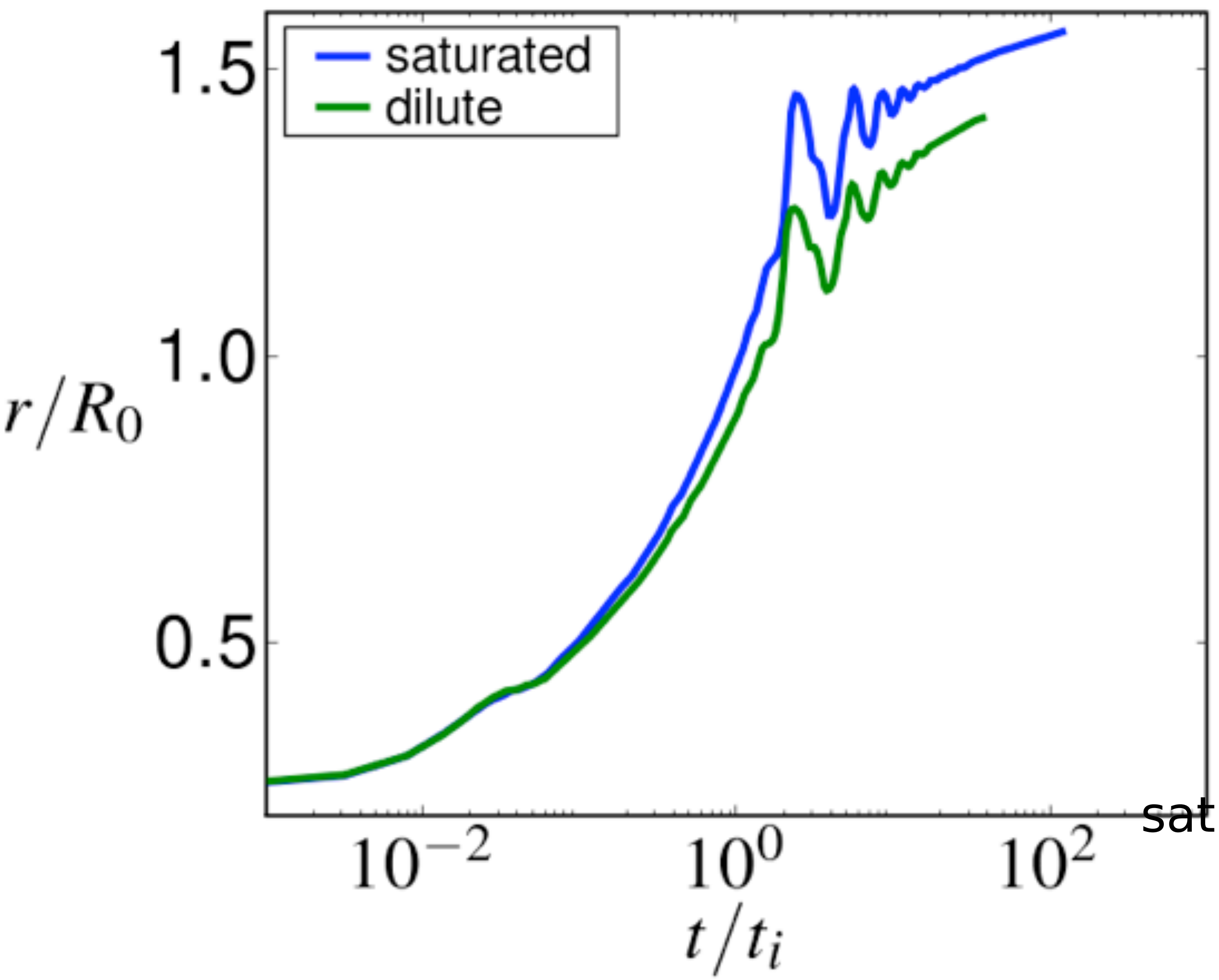
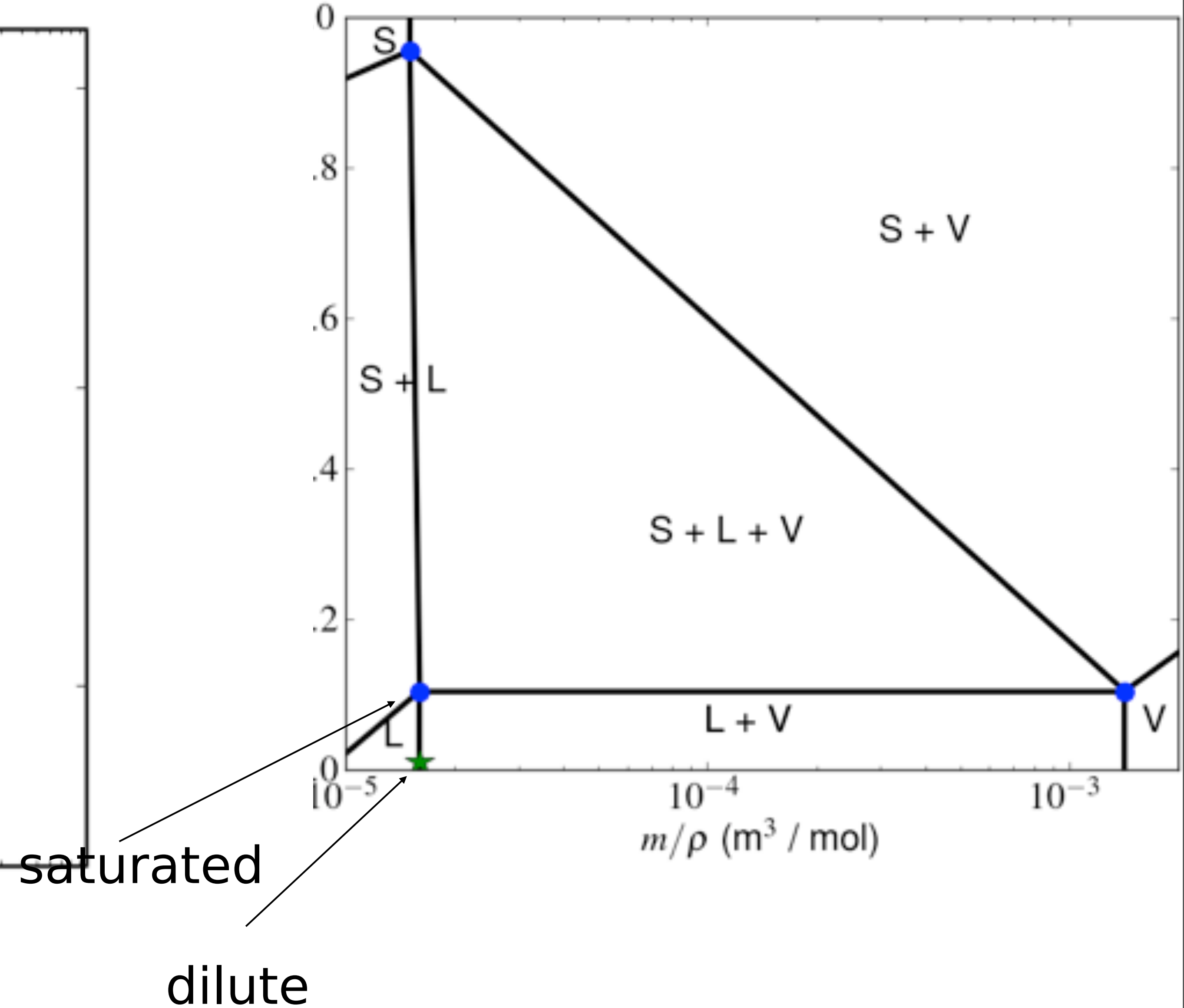
Concentration Effects





Time scale	Symbol	Expression	Value (s)
inertial	t_i	$\sqrt{\rho_l^{\mathrm{equ}} R_0^3/\gamma_{lv}}$	1.97×10^{-8}
perceptible dissolution	t_{diff}	$\delta^2/4K^2 D_f$	7.69×10^{-4}

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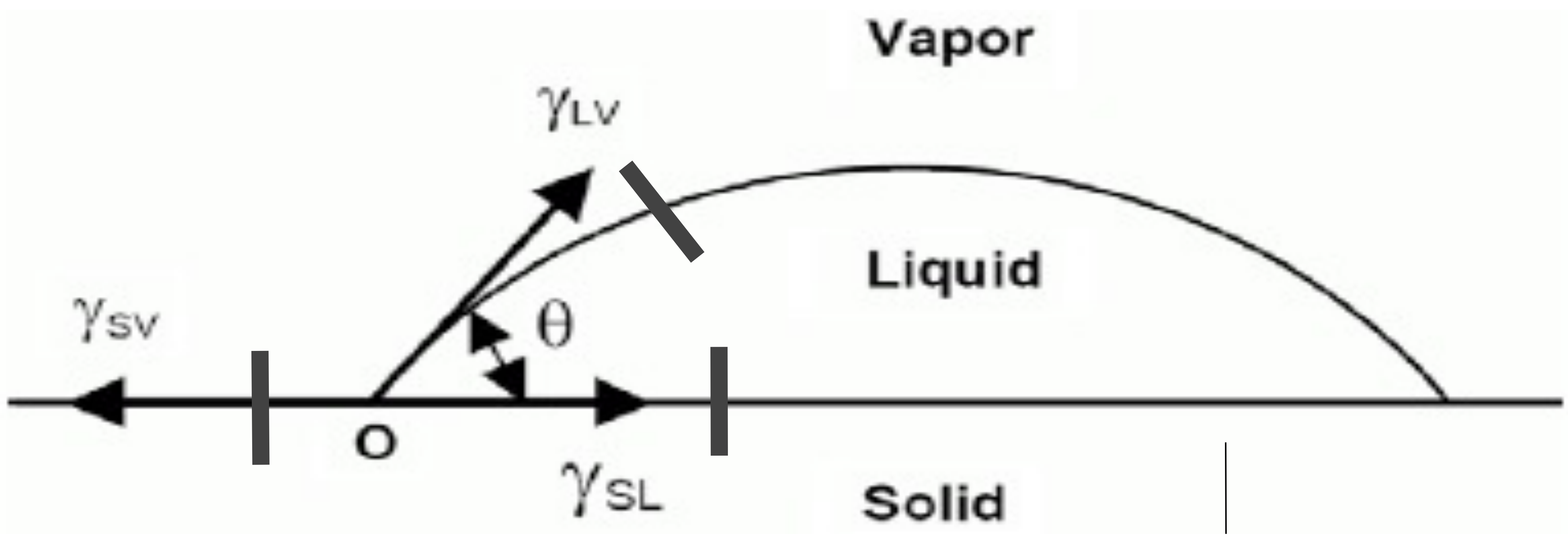
Spreading Coefficient

$$S^{\mathrm{equ}}\left(t\right) = \gamma_{sv}^{\mathrm{equ}} - \left(\gamma_{sl}^{\mathrm{equ}} + \gamma_{lv}^{\mathrm{equ}}\cos\theta\left(t\right)\right)$$

$$\tilde{\gamma}\left(t\right) = \int_{l(t)} \left[\epsilon_k T |\nabla \rho_k(t)|^2 + \epsilon_\phi T |\nabla \phi(t)|^2\right] dl$$

$$\gamma^{\mathrm{equ}} = \tilde{\gamma}\left(t \to \infty\right) \qquad \tilde{S}\left(t\right) = \tilde{\gamma}_{sv}\left(t\right) - \left(\tilde{\gamma}_{sl}\left(t\right) + \tilde{\gamma}_{lv}\left(t\right)\cos\theta\left(t\right)\right)$$



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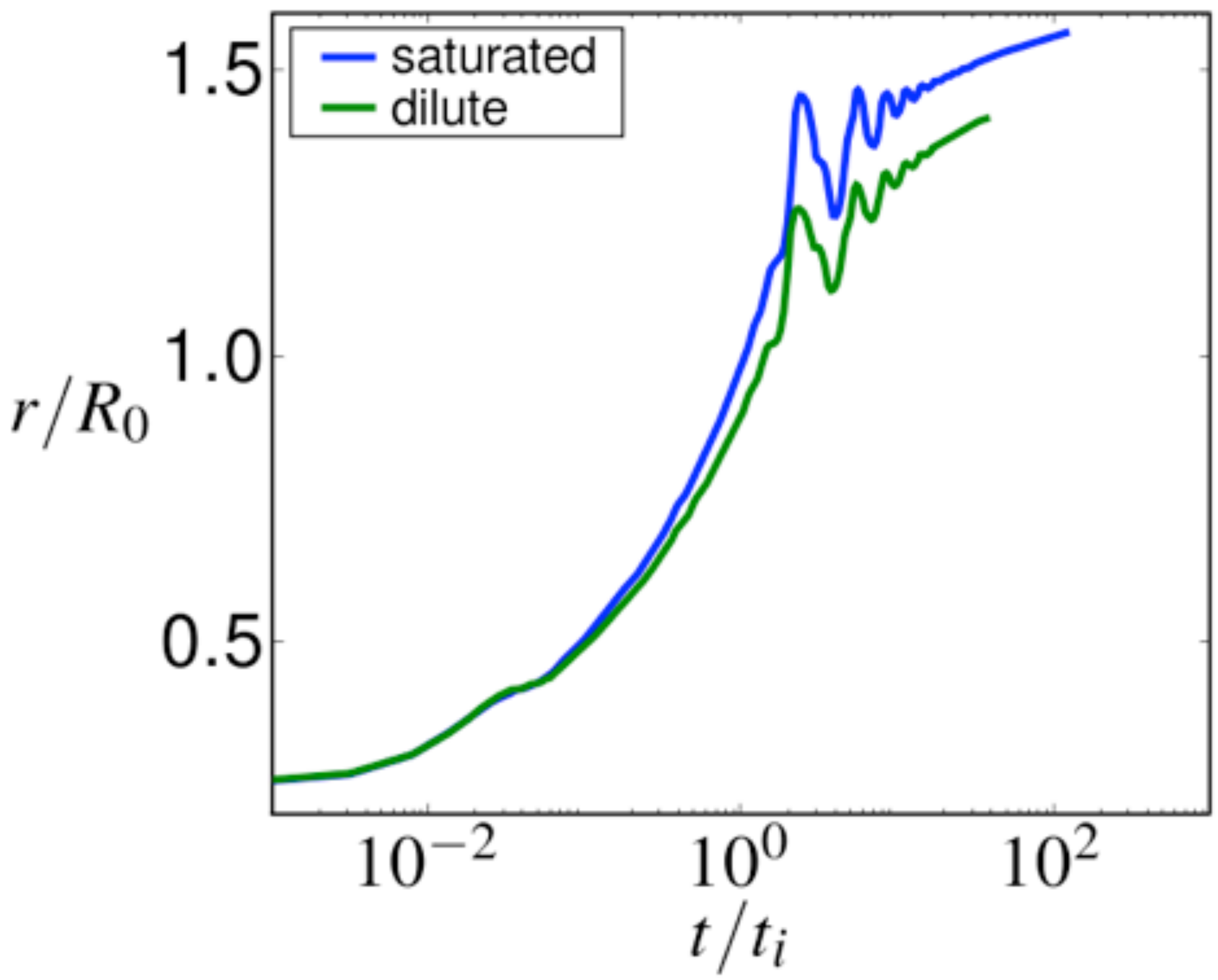
Spreading Coefficient



$$\tilde{S}(t) = \tilde{\gamma}_{sv}(t) - \left(\tilde{\gamma}_{sl}(t) + \tilde{\gamma}_{lv}(t)\cos\theta(t)\right)$$

$$S^{\mathrm{equ}}(t) = \gamma_{sv}^{\mathrm{equ}} - \left(\gamma_{sl}^{\mathrm{equ}} + \gamma_{lv}^{\mathrm{equ}}\cos\theta(t)\right)$$

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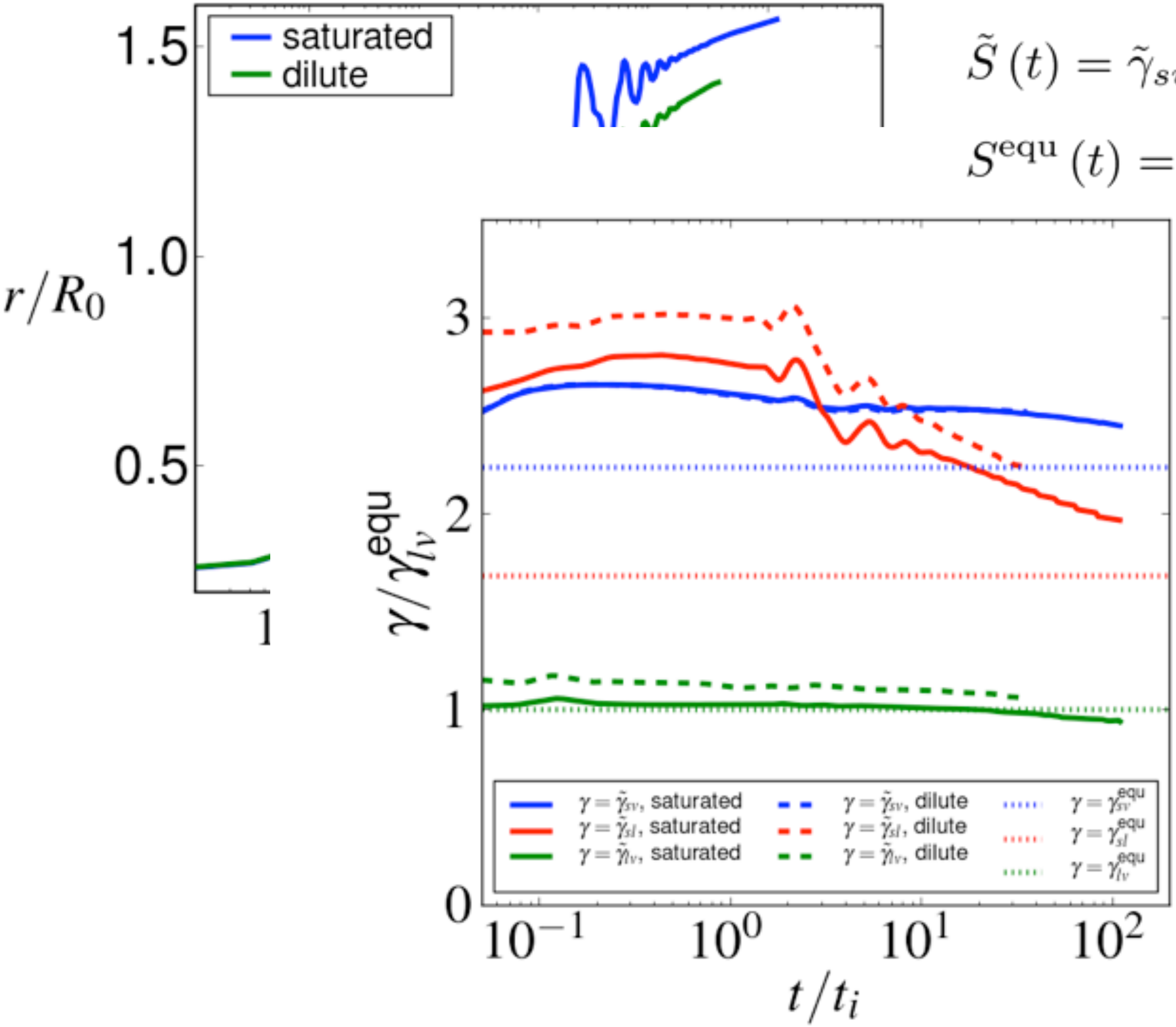
Spreading Coefficient



$$\tilde{S}(t) = \tilde{\gamma}_{sv}(t) - (\tilde{\gamma}_{sl}(t) + \tilde{\gamma}_{lv}(t)\cos\theta(t))$$

$$S^{\mathrm{equ}}(t) = \gamma_{sv}^{\mathrm{equ}} - (\gamma_{sl}^{\mathrm{equ}} + \gamma_{lv}^{\mathrm{equ}}\cos\theta(t))$$

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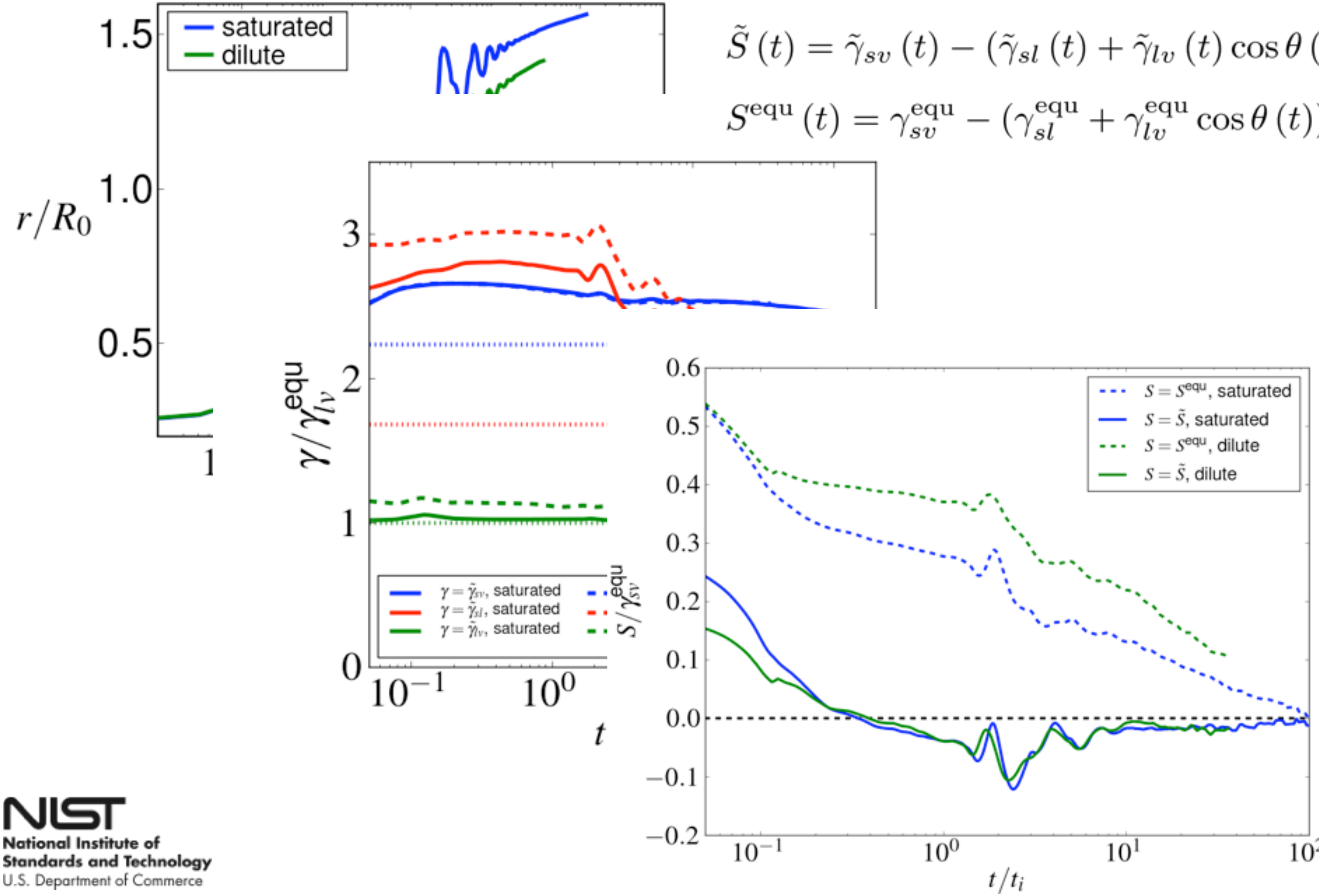
Spreading Coefficient

$$\tilde{S}(t) = \tilde{\gamma}_{sv}(t) - \left(\tilde{\gamma}_{sl}(t) + \tilde{\gamma}_{lv}(t)\cos\theta(t)\right)$$

$$S^{\mathrm{equ}}(t) = \gamma_{sv}^{\mathrm{equ}} - \left(\gamma_{sl}^{\mathrm{equ}} + \gamma_{lv}^{\mathrm{equ}}\cos\theta(t)\right)$$



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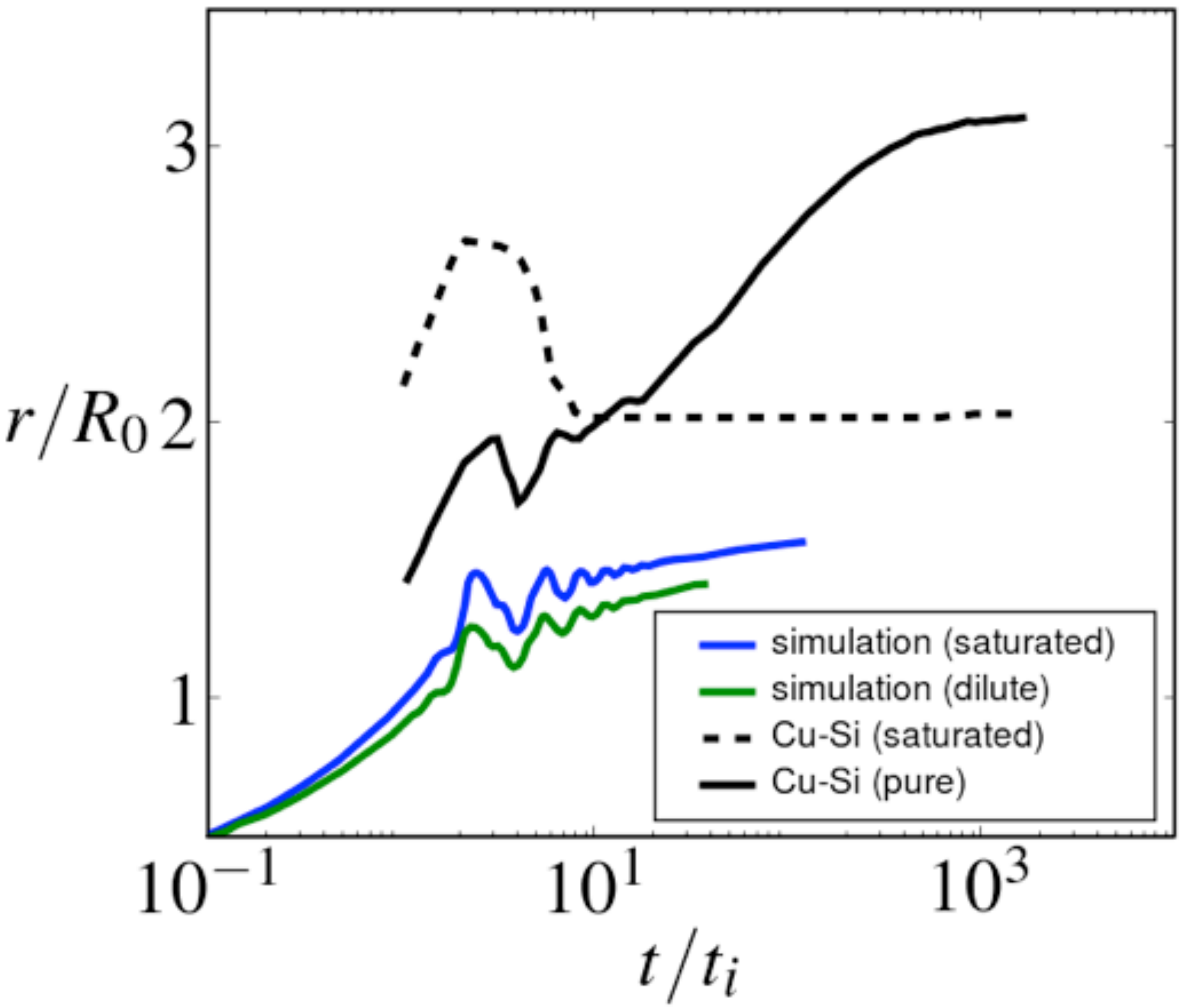
Cu-Si experiments



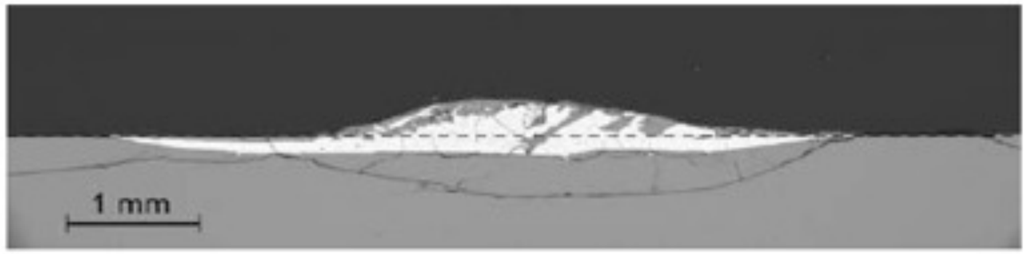
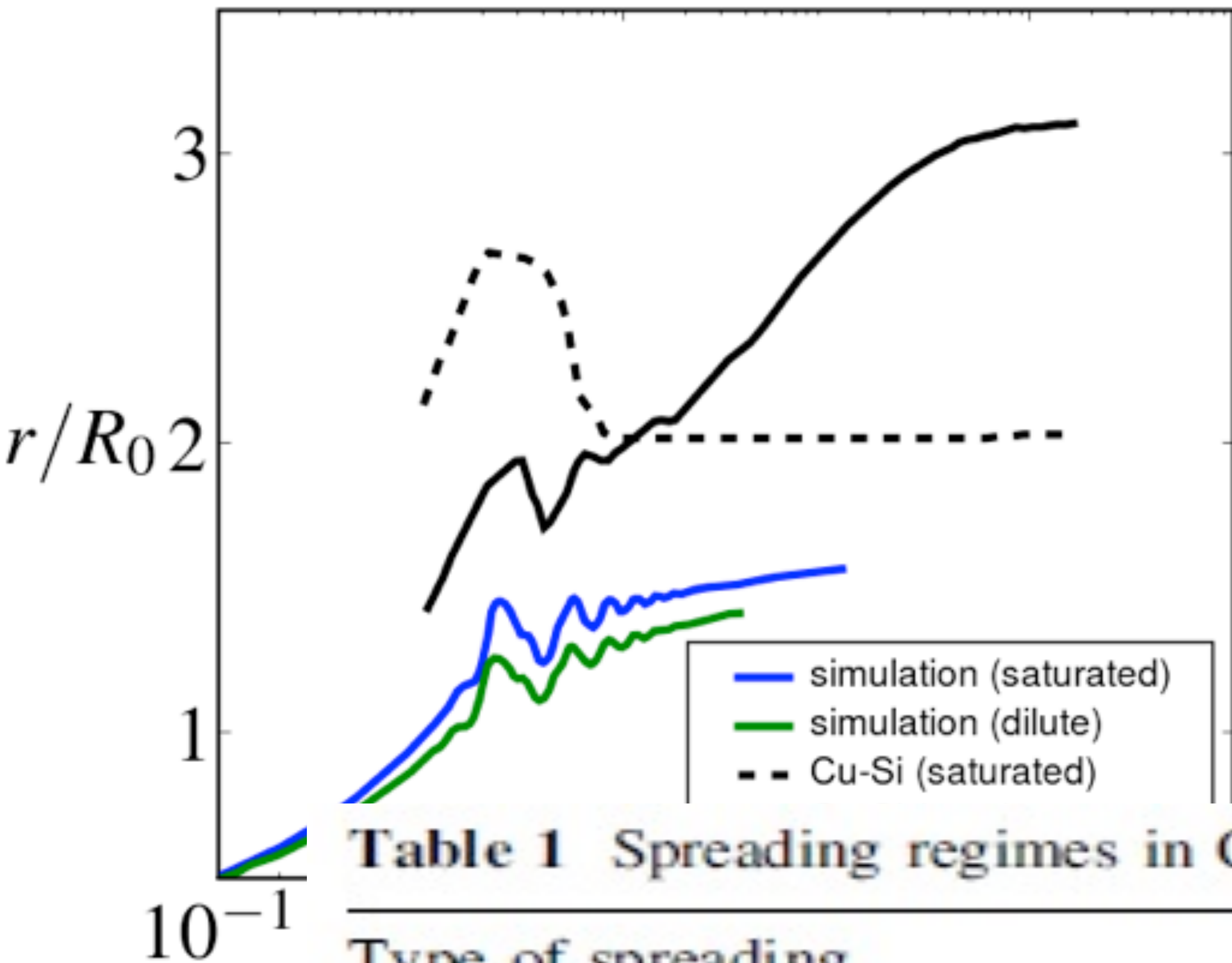


Fig. 2 Cross section of a Cu/Si sample cooled to room temperature from 1100 °C at $t > t_f$ (SEM). The dashed line indicates the initial position of the substrate surface

Protsenko et al., JMS, 2008

Oscillations!!!

Cu-Si experiments



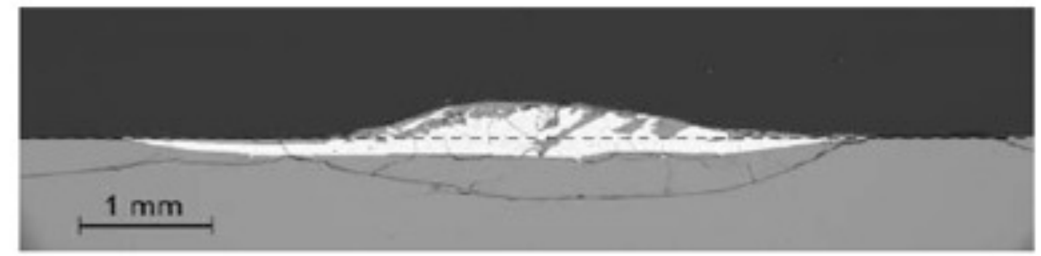


Fig. 2 Cross section of a Cu/Si sample cooled to room temperature from 1100 °C at $t > t_f$ (SEM). The dashed line indicates the initial position of the substrate surface

Protsenko et al., JMS, 2008

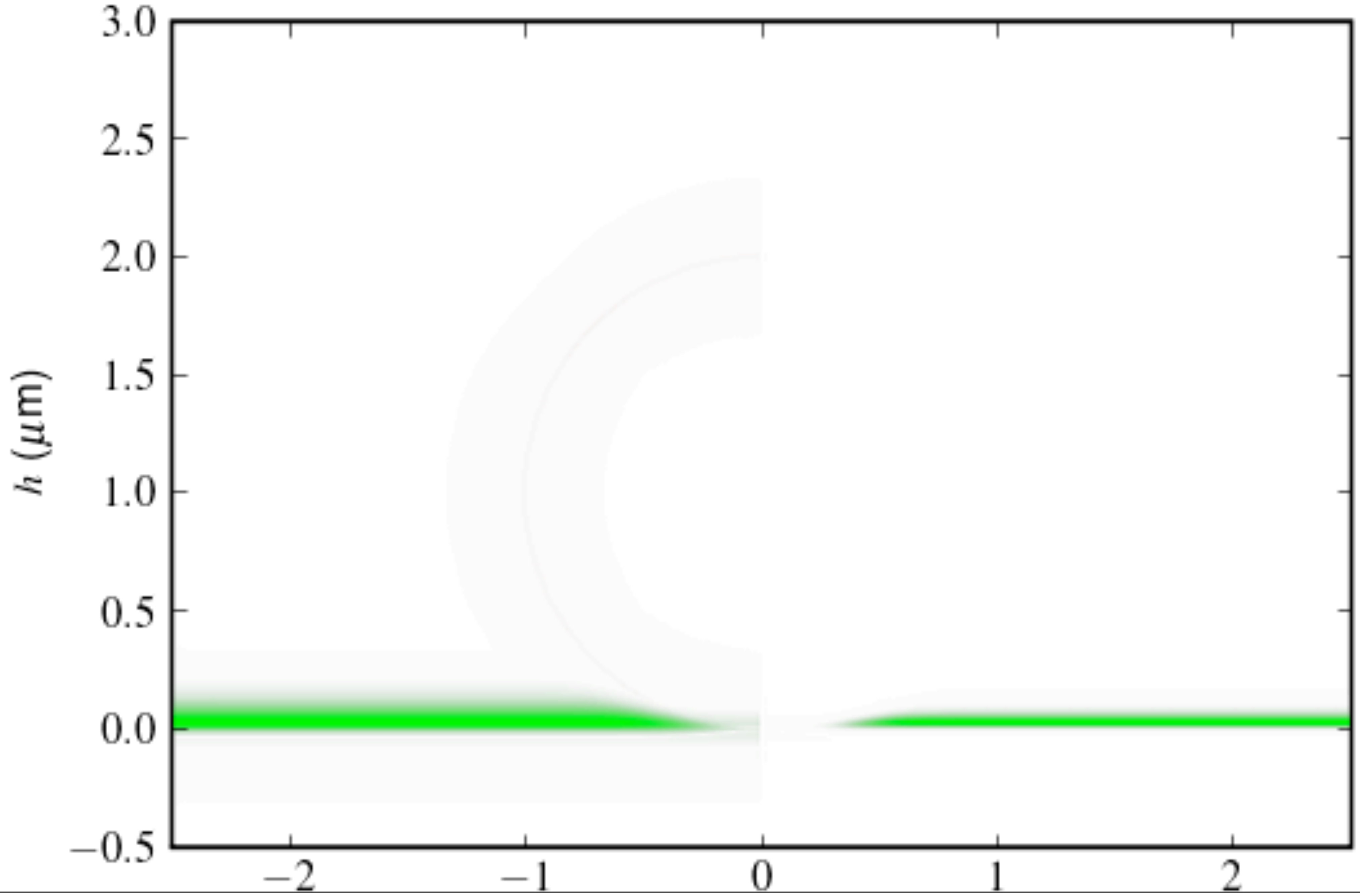
Table 1 Spreading regimes in Cu/Si system at 1100 °C

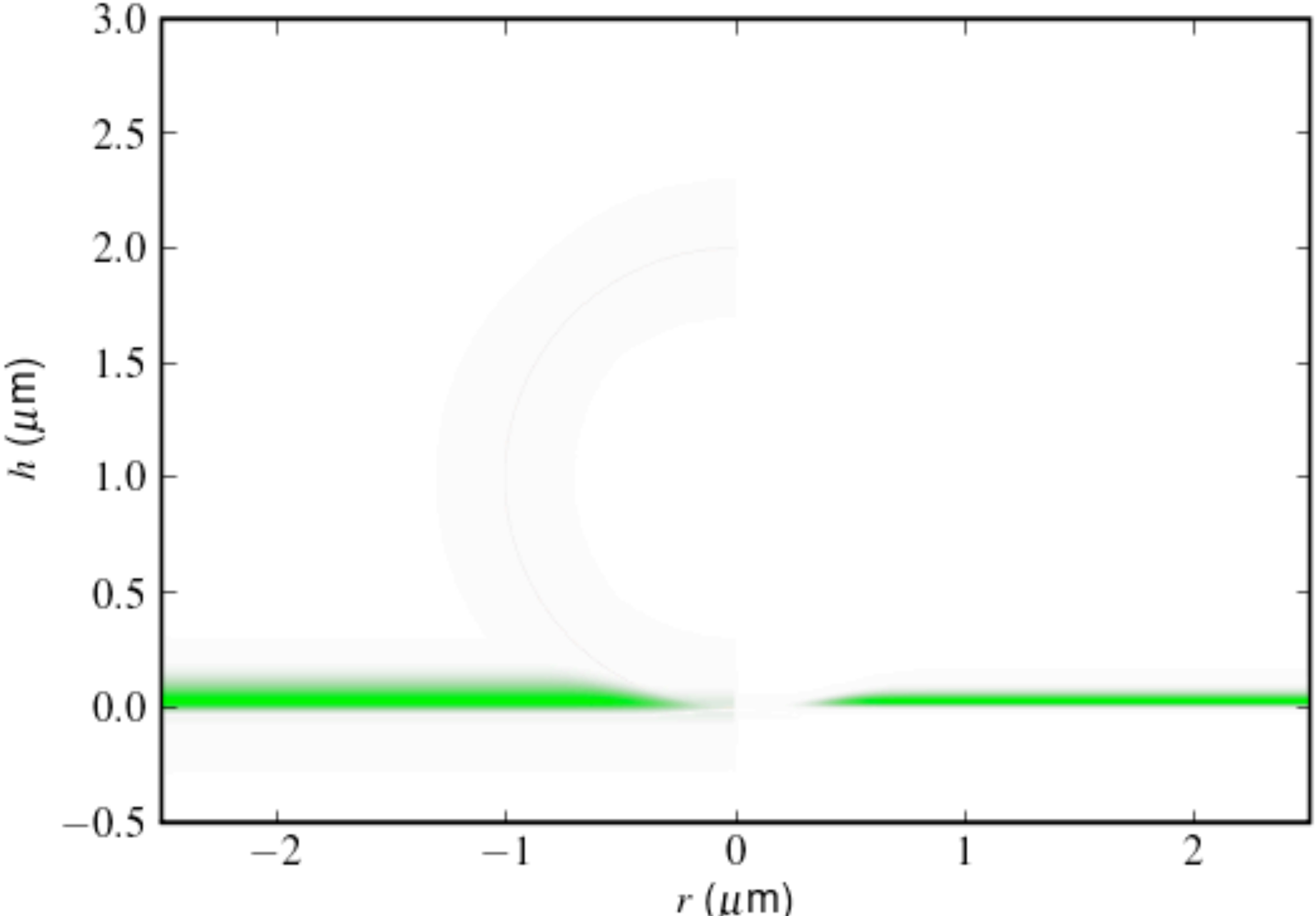
Type of spreading	Spreading time (ms)	Contact angle (deg)
Non-reactive	4–8	45 ± 5
Reactive: towards interfacial equilibrium	30–50	22[a] ± 2
Reactive: towards total equilibrium	1000–2000	6[a] ± 2

[a] Visible contact angle

Dissipation Mechanism

$$\dot{s}_{\text{PROD}} = \underbrace{\frac{M}{T^2}\left(\partial_j\left(\mu_1^{\text{NC}} - \mu_2^{\text{NC}}\right)\right)^2}_{\text{diffusion}} + \underbrace{\frac{M_\phi}{T^2}\left(\frac{\partial f}{\partial \phi} - \epsilon_\phi T \partial_j^2 \phi\right)^2}_{\text{solid-fluid phase change}} + \underbrace{\frac{\nu}{2T}\left(\partial_i u_k + \partial_k u_i\right)\partial_i u_k}_{\text{viscous}}$$




3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
h (μm)
−2
−1
0
1
2
r (μm)

Outline

- Motivation and Introduction
- Thermodynamic derivation
- Numerical approach
- Results
- Conclusions

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Conclusions

- The dissipation mechanism is caused by "triple-line friction" when spreading is inertial.
- The dissipation mechanism is related to interface equilibration after inertial spreading.
- Larger drops, thinner interface, more physical
- Reactive wetting examples available soon with FiPy

Modeling the early stages of reactive wetting,
Daniel Wheeler, James A. Warren and William J. Boettinger,
PRE (accepted for publication) 2010

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