MATHEMATICAL MODELING OF REAL WORLD PROCESSES

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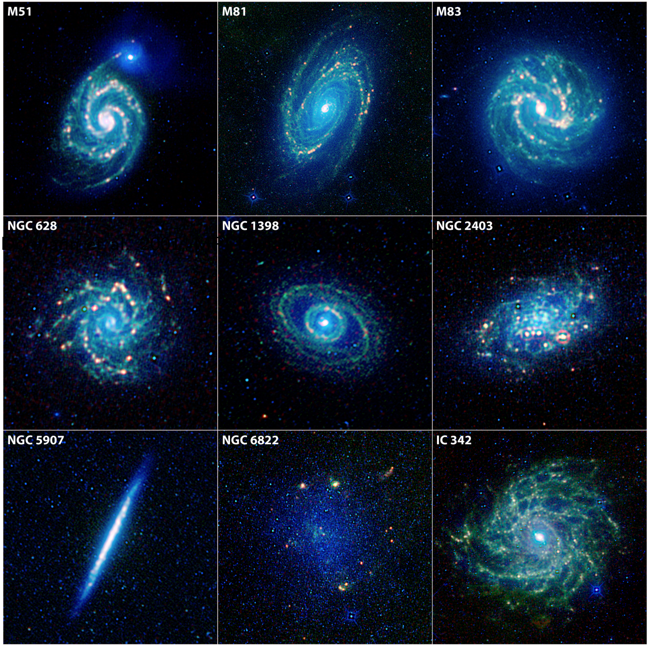
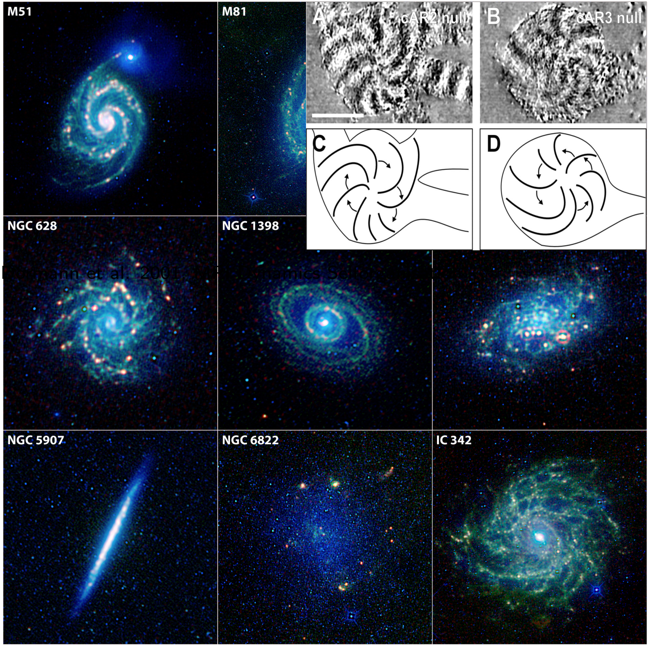
Outline

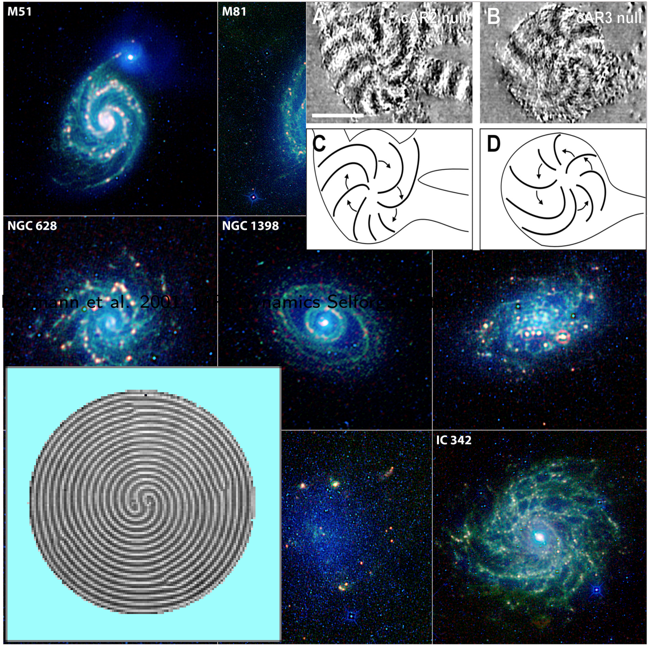
1. Scaling
2. Interface formation
3. Matched asymptotic expansions
4. Multi-scale dynamics

W.I.S.E. NASA,





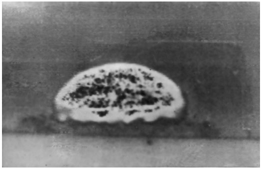
W.I.S.E. NASA, [illegible]mann et al. 2001, [illegible]namics Sc[illegible]



W.I.S.E. NASA, ...mann et al. 2001, ... Dynamics Selforg...

STARS - AMEBEA - LIQUID UNDER THERMAL GRADIENT

- Single to multi-armed spirals
- **Forces** that govern the motion of the indivdual stars or amebea are **very different !!**
- Presently no one can compute millions/billions of 3D paths of interacting stars or amebea, yet
  - on a **large scale** the millions of individuals behave as if their mass were **continuously distributed**
  - forming similar large scale structures
- **Mathematical model** that is able to describe these large scale patterns will have to be able to **reduce the description to the essential most dominant forces** creating these structures and their dynamics
- **Power of Applied Mathematics** is to be able model these (physically unrelated) structures AND analyse them with common mathematical tools
- Derivation of a averaged continuum model, analysis, numerical solution
- Important in modeling: **Know the errors**
- **Dimensional Analysis and Scaling**



- 1945 first atomic explosion in New Mexico: classified[1]
- 1947 movie of explosion appeared
- 1950 G. I Taylor (University of Cambridge) published article on energy (**still classified!!!**) of explosion.

- What effects might be expected during nuclear fission?

  To answer this question:

  Calculate motion and pressure of ambient gas after explosion

  What is known ? **What can be assumed ?**
  - After short, intense initial period: Shock appears
  - Governing equations inside shock wave
  - **Assume:** viscous effects are negligible (at this early stage), spherical symmtry

[1] Barenblatt, "Scaling" (2012)

Governing Equations (Spherical Symmetry)

Conservation of mass $\partial_t \rho + \frac{1}{r^2}\partial_r \left(\rho r^2 u\right) = 0$

Conservation of momentum $\partial_t u + u\partial_r u + \frac{1}{\rho}\partial_r p = 0$

Conservation of energy $\partial_t \left(\frac{p}{\rho^\gamma}\right) + u\partial_r \left(\frac{p}{\rho^\gamma}\right) = 0$

Boundary Conditions

$$\rho_s(u_s - D) = -\rho_0 D$$

$$\rho_s(u_s - D)^2 + p_s = p_o + \rho_0 D^2$$

$$\rho_s(u_s - D)\left(\frac{\gamma}{\gamma-1}\frac{p_s}{\rho_s} + \frac{(u_s-D)^2}{2}\right) = -\rho_0 D\left(\frac{\gamma}{\gamma-1}\frac{p_0}{\rho_0} + \frac{D^2}{2}\right)$$

Initial Conditions

$$\rho(r,0) = \rho_0(r), \quad p(r,0) = p_0(r), \quad u(r,0) = 0 \quad r \geq r_0$$

$$\rho(r,0) = \rho_i(r), \quad p(r,0) = p_i(r), \quad u(r,0) = u_i(r) \quad r < r_0$$

$$E = 4\pi \int_0^{r_0} \rho_i \left(\frac{u_i^2}{2} + \frac{1}{\gamma-1}\frac{p_i}{\rho_i}\right) r^2\, dr$$

Scaling

(i) Location of shock r_s depends on: $E, \rho_0, t, t_0, p_0, \gamma$

(ii) Assume: energy is suddenly released in infinitely concentrated form

$\Rightarrow$ point source i.e. $r_0 \ll r_s$

Assume: pressure of moving gas $p_s \gg p_0$ $\Rightarrow$ neglect terms with p_0 at shock

Units $[E] = \frac{gcm^2}{s^2}$, $[\rho_0] = \frac{g}{cm^3}$, $[t] = s$, $[r_0] = cm$, $[p_0] = \frac{g}{cms^2}$

(i) & (ii) $\Rightarrow$ neglect r_0, p_0

$\Rightarrow$ $S = \left(\frac{Et^2}{\rho_0}\right)^{1/5}$ $\Leftarrow$ dimension of length

$\Rightarrow$ $I := \frac{r_s}{S} = F(S, \rho_0, t, \gamma)$ dimensionless !

$\Rightarrow$ depends only on constant γ

$\Rightarrow$ **Taylor's Scaling Law** $r_s = C(\gamma)\left(\frac{Et^2}{\rho_0}\right)^{1/5}$

$\Rightarrow$ $\frac{5}{2}\log_{10} r_s = \frac{5}{2}\log_{10} C + \frac{1}{2}\log_{10}\left(\frac{E}{\rho_0}\right) + \log_{10} t$ $\Rightarrow$ E

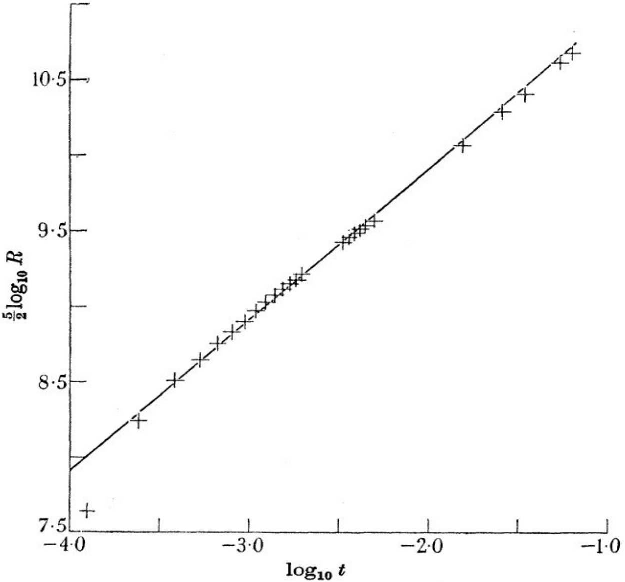


Figure 1. Logarithmic plot showing that $R^{\frac{5}{2}}$ is proportional to t.

Assumptions

(i) A quantity u to be determined in terms of measurable quantities $\{w_1, ..., w_n\}$:

$$u = f(w_1, ..., w_n) \tag{1}$$

(ii) $\{u, w_1, ..., w_n\}$ involve m fundamental dimensions $L_1, ..., L_m$

(iii) The dimension of a quantity z is a product of powers of the fundamental dimensions

$$[z] = L_1^{\alpha_1} L_2^{\alpha_2} \cdots L_m^{\alpha_m} \quad \alpha_i \in \mathbb{R}$$

Conclusions

(i) (1) can be expressed in terms of dim'less quantities.

(ii) $b_i = \begin{bmatrix} b_{1i} \\ \vdots \\ b_{mi} \end{bmatrix}$ dimension of w_i, $\quad B = \begin{bmatrix} b_{11} & \dots & b_{1n} \\ \vdots & & \vdots \\ b_{m1} & \dots & b_{mn} \end{bmatrix}$ dimension of problem.

Number of dim'less quantities is

$$k + 1 = n + 1 - r(B), \text{ where } r(B) = \text{rank of B.}$$

Exactly k of these depend on $\{w_1, ..., w_n\}$

(iii) Let x_i, $i = 1, ...k$ be $k = n - r(B)$ linearly independent solutions x of $Bx = 0$. Let a be the dimension vector of u and y a solution of $By = -a$. Then (1) reduces to

$$\pi = g(\pi_1, ..., \pi_k), \tag{2}$$

where

$$\pi = uw_1^{y_1} \cdots w_n^{y_n} \text{ and } \pi_i = uw_1^{x_{1i}} \cdots w_n^{x_{ni}}$$

are dim'less quantities and (1) becomes

$$u = w_1^{-y_1} \cdots w_n^{-y_n} g(\pi_1, ..., \pi_k) \tag{3}$$

Homework !

- Let $u = R$ radius of shock wave, with $R = f(w_1, ..., w_4)$ and $w_1 = E$, $w_2 = t$, $w_3 = \rho_0$, $w_4 = p_0$
- Using fundamental dimensions, obtain dimension matrix

$$B = \begin{bmatrix} 2 & 0 & -3 & -1 \\ 1 & 0 & 1 & 1 \\ -2 & 1 & 0 & -2 \end{bmatrix}$$

- **Apply Buckingham-Pi:** $r(B) = 3 \quad \Rightarrow \quad k = n - r(B) = 4 - 3 = 1.$

  Solution to $Bx = 0$ is

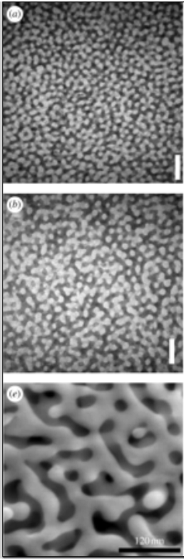
  $x_1 = -\frac{2}{5}x_4, \quad x_2 = \frac{6}{5}x_4, \quad x_3 = -\frac{3}{5}x_4$ where x_4 arbitrary (e.g. $x_4 = 1$)

  $\Rightarrow$ Dimensionless quantity: $\pi_1 = p_0 \left(\frac{t^6}{E^2 \rho_0^3} \right)^{1/5}$

  Solution of $By = -a$ is $y = \frac{1}{5}\begin{bmatrix} -1 \\ -2 \\ 1 \\ 0 \end{bmatrix}$, dimension of R is $a = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$

  $\Rightarrow$ Dimensional Analysis: $R = \left(\frac{Et^2}{\rho_0} \right)^{1/5} g(\pi_1)$

Interface formation and dynamics



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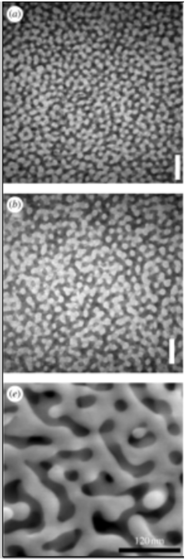

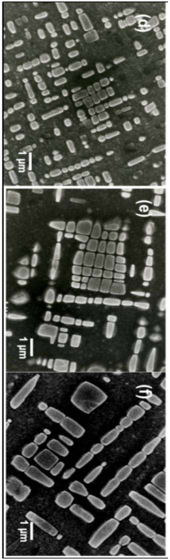

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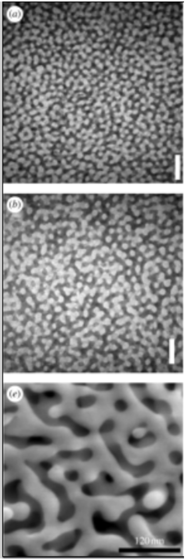

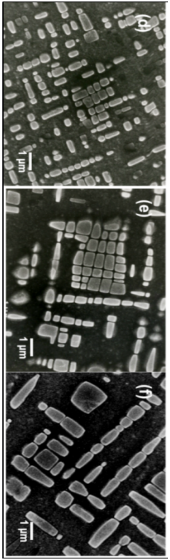

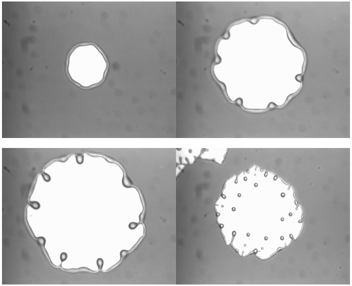

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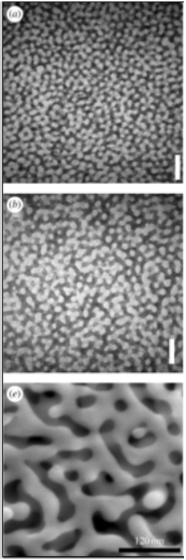

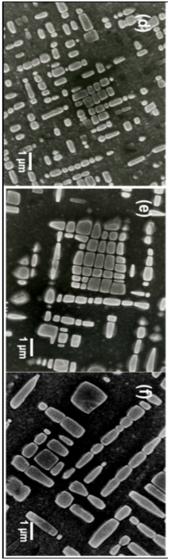

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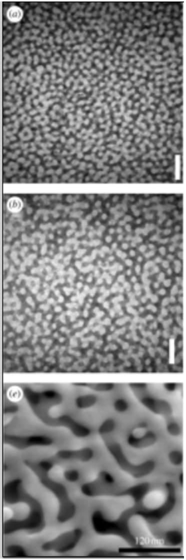

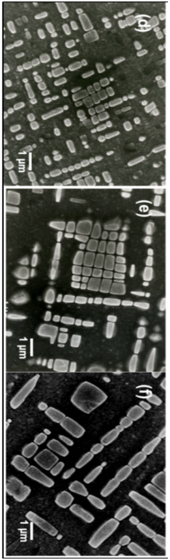

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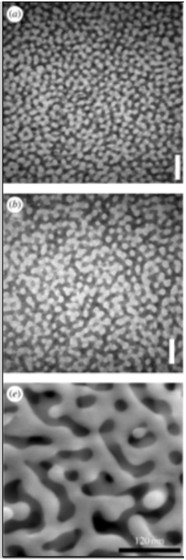

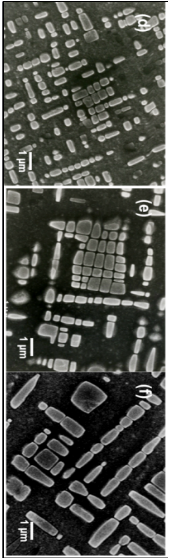

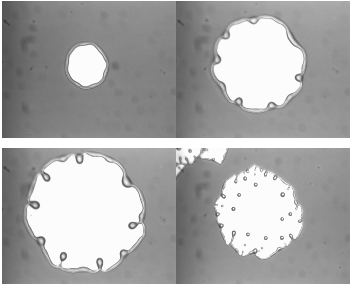

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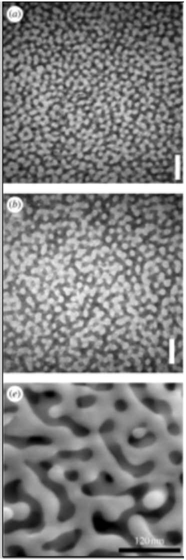
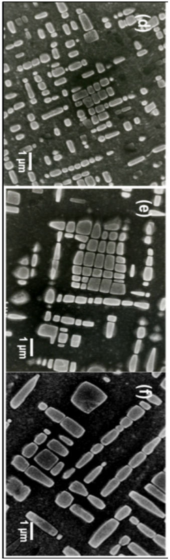
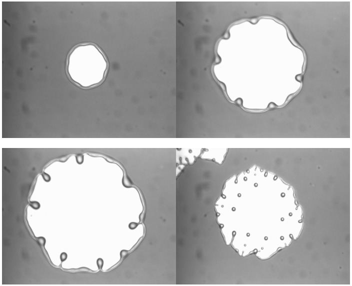
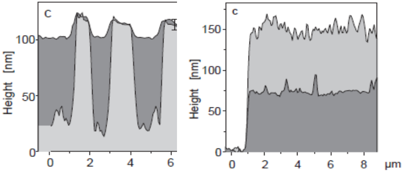
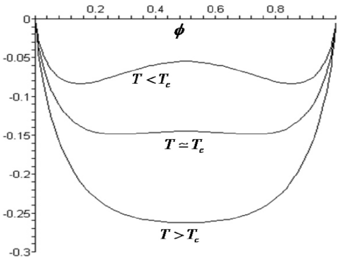
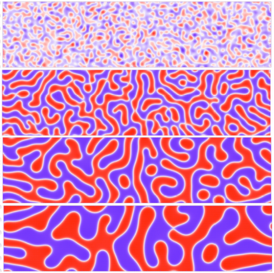












Cahn-Hilliard equation $\quad \dfrac{\partial \phi}{\partial t} = \nabla \cdot \left(M \, \nabla \dfrac{\delta f}{\delta \phi} \right)$

Total free energy: Ginzburg-Landau free energy

$$f[\phi, T] = \int_V F(\phi(\mathbf{x}), T(\mathbf{x})) + \frac{1}{2}\epsilon |\nabla \phi|^2 \, d\mathbf{x}$$

Bulk free energy:

$$F = \phi(1-\phi) + k_B T(\phi \ln \phi + (1-\phi)\ln(1-\phi))$$

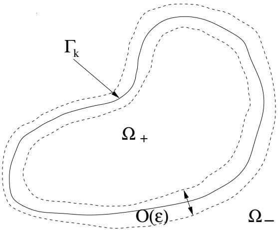
Simplest free energy, combining bulk contribution from a binary mixture and interfacial energy.

Mass conservation: $\quad \dfrac{\partial \phi}{\partial t} = -\nabla \cdot \boldsymbol{J}$

$$\boldsymbol{J} = -M \nabla \cdot \mu \quad \text{with} \quad \mu = \frac{\delta f}{\delta \phi}$$

Phase separation: Cahn-Hilliard equation

$$\begin{aligned} \frac{\partial u}{\partial t} &= \Delta\,\mu \quad \text{in} \quad \Omega = \Omega_+ \cup \Omega_- \\ \mu &= F'(u) - \epsilon^2 \Delta u \\ n \cdot \boldsymbol{\nabla}\mu &= 0\,, \quad \boldsymbol{n} \cdot \boldsymbol{\nabla} u = 0 \quad \text{on} \quad \partial\Omega \end{aligned}$$



- Solutions reach near phase equilibrium after $O(1)$ time.
- Near phase equilibrium:

  solution has developed an interface between precipitates Ω_+, Ω_- of width of $O(\varepsilon)$
- approaching a sharp interfaces Γ_k as $\epsilon \to 0$
- Dynamics of the precipitates evolves on the slow time-scale $\tau = \varepsilon t$

$$\Rightarrow \quad \epsilon \frac{\partial u}{\partial \tau} = \Delta\,\mu$$

Analysis $\Rightarrow$ **Matched Asymptotic Expansions**

Definitions

(i) Let $u(\mathbf{x};\epsilon)$ and $v(\mathbf{x};\epsilon)$ be functions defined in $D \subset \mathbb{R}^n$ and $I : 0 \le \epsilon \le \epsilon_0(\mathbf{x})$. Then

$$u(\mathbf{x};\epsilon) = O(v(\mathbf{x};\epsilon)), \quad \text{in D, as} \quad \epsilon \to 0$$

if for each $\mathbf{x} \in D$ there exists $k(\mathbf{x})$ and and I such that $|u| \le k|v|$ for each $\epsilon \in I$.

(ii)

$$u(\mathbf{x};\epsilon) = o(v(\mathbf{x};\epsilon)), \quad \text{in D, as} \quad \epsilon \to 0$$

if for each $\mathbf{x} \in D$ and given $\delta > 0$, there exists $I : 0 \le \epsilon \le \epsilon(\mathbf{x},\delta)$ s.t. $|u| \le \delta|v|$ for all $\epsilon \in I$ and denote this by $u \ll v$.

(iii) An **asymptotic sequence** $\{\phi_n(\epsilon)\}$, $n = 1, 2, ...$ is a sequence such that $\phi_{n+1}(\epsilon) = o(\phi_n(\epsilon))$ as $\epsilon \to 0$.

(iv) The series $\sum_{n=1}^{N} \phi_n(\epsilon) u_n(\mathbf{x})$ is called an **asymptotic expansion** of u w.r.t. $\{\phi_n(\epsilon)\}$ for $\epsilon \to 0$, if for each $M = 1, ..., N$

$$u(\mathbf{x};\epsilon) - \sum_{n=1}^{N} \phi_n(\epsilon) u_n(\mathbf{x}) = o(\phi_M), \quad \text{as} \quad \epsilon \to 0$$

Asymptotics expansions

Example[2]**:** Consider $\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-t^2)\, dt$

- $\exp(-t^2)$ is analytic in the entire complex plane $\mathbb{C}$ so that its Taylor series

$$\mathrm{erf}(x) = \frac{2}{\pi} \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n+1}}{(2n+1)!} = \frac{2}{\sqrt{\pi}} \left(x - \frac{x^3}{3} + \frac{x^5}{10} - \frac{x^7}{42} + \frac{x^9}{216} - \frac{x^{11}}{1320} + \cdots \right)$$

  converges with infinite radius of convergence.

- Accuracy: For an accuracy of 10^{-5}

  upto $x = 2$ need 16 terms, upto $x = 3$ need 31 terms, upto $x = 5$ need 75 terms

  For round-off error 10^{-7}: At $x = 5$ largest term is $6.6 \cdot 10^8 \Rightarrow$ WRONG answer!

- ALTERNATIVE: Integrate by parts

$$\mathrm{erf}(x) = 1 - \frac{2}{\sqrt{\pi}} \int_x^{\infty} \exp(-t^2)\, dt = 1 - \frac{\exp(-x^2)}{x\sqrt{\pi}} \left(1 - \frac{1}{2x^2} + \frac{1 \cdot 3}{(2x^2)^2} - \frac{1 \cdot 3 \cdot 5}{(2x^2)^3} + \cdots \right)$$

  $\Rightarrow$ series diverges for all x and radius of convergence is zero! BUT:
  $x = 2.5$ need 3 terms for accuracy of 10^{-5}, $x = 3$ need 2 terms for accuracy of 10^{-5}

- This series is an asymptotic expansion!

[2] Jon Chapman, Univ. of Oxford

A simple but instructive example:

$$\epsilon\, y'' + 2\, y' + 2\, y = 0 \quad \text{in} \quad 0 < x < 1, \quad \epsilon \ll 1$$
$$y(0) = 0 \quad y(1) = 1$$

- As $\epsilon \to 0$ order of ODE decreases $\Rightarrow$ one BC can't be satisfied
  $\Rightarrow$ singular perturbation problem
- Region where $\epsilon = 0$-problem does not have solution: **Boundary layer**
- Where is the boundary layer (BL)?
- Let BL be at $x = x_0$: $x = x_0 + \epsilon^\alpha \bar{x}$ or

  Inner (BL) variable

$$\bar{x} = \frac{x - x_0}{\epsilon^\alpha}, \quad \alpha > 0$$

- Assume $x_0 = 0$, define $Y(\bar{x}; \epsilon) = y(x; \epsilon)$
  Inner (BL) problem

$$\epsilon^{1-2\alpha} \frac{d^2 Y}{d\bar{x}^2} + 2\epsilon^{-\alpha} \frac{dY}{d\bar{x}} + 2Y = 0, \quad 0 < \bar{x} < \infty, \quad Y(0) = 0$$

Outer expansion Assume solution of outer problem has asymptotic expansion

$$y(x;\epsilon) = y_0(x) + \epsilon\, y_1(x) + O(\epsilon^2)$$

Note: iterative method
Leading order problem (O(1)):

$$y_0' + y_0 = 0 \quad y_0(1) = 1$$

$$\Rightarrow \quad y_0(x) = \exp(1-x)$$

Inner expansion
Assume

$$Y(\bar{x};\epsilon) = Y_0(\bar{x}) + \epsilon^{\gamma} Y_1(\bar{x}) + O(\epsilon^{\delta}), \quad \delta > \gamma, \quad \gamma > 0$$

Leading order problem:

$$\epsilon^{1-2\alpha}\frac{d^2}{d\bar{x}^2}\,(Y_0 + h.o.t.) + 2\,\epsilon^{-\alpha}\,\frac{d}{d\bar{x}}\,(Y_0 + h.o.t.) + 2\,(Y_0 + h.o.t.) = 0$$

Dominant balance $\Rightarrow$ leading order problem

(i) 1st and 3rd term balance and 2nd term is of smaller order as $\epsilon \to 0$

$\Rightarrow \quad 1 - 2\alpha = 0 \quad \Rightarrow \quad \alpha = \frac{1}{2}$

$\Rightarrow$ 1st and 3rd are $O(1)$ and 2nd of $O(\epsilon^{-1/2})$ as $\epsilon \to 0$ $\lightning$

(ii) 1st and 2nd term balance and 3rd is smaller

$\Rightarrow \quad \alpha = 1 \quad \Rightarrow$ 1st& 2nd are $O(\epsilon^{-1})$ and 3rd $O(1)$ $\surd$

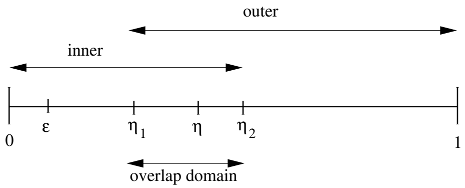
$$\frac{d^2Y_0}{d\bar{x}^2} + 2\frac{dY_0}{d\bar{x}} = 0 \quad \text{for} \quad 0 < \bar{x} < \infty$$
$$Y_0(0) = 0$$

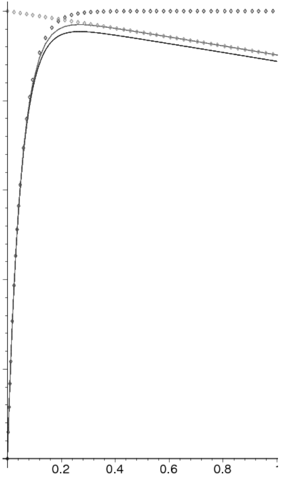
$$\Rightarrow \quad Y_0(\bar{x}) = A(1 - \exp(-2\bar{x}))$$

Matching

- There exist a domain where inner and outer solutions approximate same function
  - ⇒ **Overlap-Domain**
  - ⇒ there exist an **intermediate variable** x_η such that

$$x_\eta = \frac{x}{\eta(\epsilon)} \quad \text{such that} \quad \epsilon \ll \eta(\epsilon) \ll 1$$





Matched asymptotic expansions

Theorem

Kaplun's Extension Theorem

Let $\epsilon \ll \eta(\epsilon) \ll 1$ *such that* $x_\eta = x/\eta(\epsilon)$

(i) *There exist an* $\eta_1(\epsilon)$ *such that for* x_η *fixed*

$$\lim_{\epsilon \to 0} y_{outer}(x_\eta) - y_0(\eta(\epsilon) \quad x_\eta) = 0 \text{ for any } \eta(\epsilon) \text{ that satisfies } \quad \eta_1(\epsilon) \ll \eta(\epsilon) \ll 1.$$

(ii) *There exist an* $\eta_2(\epsilon)$ *such that for* x_η *fixed*

$$\lim_{\epsilon \to 0} y_{inner}(x_\eta) - Y_0(\epsilon\eta(\epsilon)\, x_\eta) = 0 \quad \text{for any } \eta(\epsilon) \text{ that satisfies } \quad \epsilon \ll \eta(\epsilon) \ll \eta_2(\epsilon).$$

Remark

Kaplun's Hypothesis

The domain of validity of y_{outer} *and* y_{inner} *overlap, i.e.* $\eta_1 \ll \eta_2$*. In this overlap domain the leading orders of* y_{outer} *and* y_{inner} *agree.*

Proofs: P. Lagerstrom, "Matched asymptotic expansions: Ideas and Techniques", Spriner-Verlag, 1988.

Matching

Let $\eta(\epsilon) = \epsilon^{\beta}$ with $0 < \beta < 1$ so that $\epsilon \ll \epsilon^{\beta} \ll 1$ and define the intermediate variable

$$x_\eta = \frac{x}{\epsilon^\beta}.$$

Then

$$y_{inner} = A\left[1 - \exp\left(-2\frac{x_\eta}{\epsilon^{1-\beta}}\right)\right] + h.o.t. \;\rightarrow\; A + e.s.t. + h.o.t. \quad \text{as } \epsilon \rightarrow 0, x_\eta \text{ fixed}$$

and

$$y_{outer} = \exp\left(1 - x_\eta \epsilon^{\beta}\right) + h.o.t. \;\rightarrow\; \exp(1) + h.o.t. \quad \text{as } \epsilon \rightarrow 0, x_\eta \text{ fixed}$$

$$\Rightarrow \quad A = \exp(1).$$

Uniformly valid (composite) expansion

To leading order the asymptotic solution valid in the whole domain:

$$y_c(x;\epsilon) = y_0(x) + Y_0\left(\frac{x}{\epsilon}\right) - \text{matched part} + h.o.t.$$

Matched part: $y_0(0)$.

$$\Rightarrow \quad y_c(x;\epsilon) = \exp(1-x) - \exp\left(1 - \frac{2\,x}{\epsilon}\right) + h.o.t.$$

Next order problem

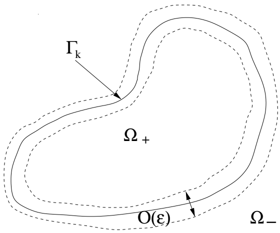
$$\frac{dy_1}{dx} + y_1 = -\frac{1}{2}\frac{d^2 y_0}{dx^2}, \quad y_1(1) = 0, \qquad \frac{d^2 Y_1}{d\bar{x}^2} + 2\frac{dy_1}{d\bar{x}} = -2Y_0, \quad Y_1(0) = 0$$

- also needed to estimate validity of leading order result
- multiple BL, corner layers, transition layers, ...

Sharp-interface

Outer problem

$$
\begin{aligned}
u(\tau, \mathbf{x}; \varepsilon) &= u_o(\tau, \mathbf{x}) + \varepsilon u_1(\tau, \mathbf{x}) + \varepsilon^2 u_2(\tau, \mathbf{x}) + O(\varepsilon^3) \\
\mu(\tau, \mathbf{x}; \varepsilon) &= \mu_o(\tau, \mathbf{x}) + \varepsilon \mu_1(\tau, \mathbf{x}) + \varepsilon^2 \mu_2(\tau, \mathbf{x}) + O(\varepsilon^3)
\end{aligned}
$$



Leading order

$$0 = \Delta \mu_o = \Delta F'(u_o)$$

$O(\varepsilon)$

$$\frac{\partial u_o}{\partial \tau} = \Delta \mu_1 = \Delta \left(F''(u_o) u_1 \right)$$

$O(\varepsilon^2)$

$$\frac{\partial u_1}{\partial \tau} = \Delta \mu_2 = \Delta \left(F''(u_o) u_2 + \frac{1}{2} F'''(u_o) u_1^2 - \Delta u_o \right)$$

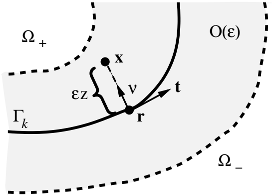
- + boundary conditions on $\partial\Omega$
- Boundary conditions on $\Gamma_k \Rightarrow$ matching to 'inner' problem near Γ_k

Inner problem

Define boundary layer with z ='inner' variable

Parametrization of curve Γ_k:

$\boldsymbol{r}(\tau, s) = (r_1(\tau, s), r_2(\tau, s))$, s is arclength



$$\mathbf{x}(\tau, s, z) = \boldsymbol{r}(\tau, s) + \epsilon\, z\, \boldsymbol{\nu}(\tau, s)$$

$$\mathbf{x} = (x_1, x_2) = (x, y),\ \boldsymbol{r}(\tau, s) = (r_1(\tau, s), r_2(\tau, s))$$

$$\boldsymbol{\nu}(\tau, s) = \left(-\frac{\partial r_2}{\partial s}(\tau, s), \frac{\partial r_1}{\partial s}(\tau, s)\right), \quad \boldsymbol{t}(\tau, s) = \left(\frac{\partial r_1}{\partial s}(\tau, s), \frac{\partial r_2}{\partial s}(\tau, s)\right)$$

Sharp-interface model

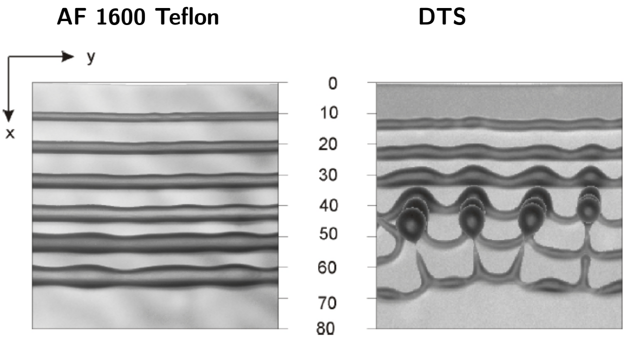
$$\Delta\mu_1^- = 0 \text{ in } \Omega^-, \quad \boldsymbol{n}\cdot\boldsymbol{\nabla}\mu_1^- = 0 \text{ on } \partial\Omega^-, \quad \mu_1^\pm = \tilde{\mu}_1(\tau, \boldsymbol{r}), \quad \Delta\mu_1^+ = 0 \text{ in } \Omega^+$$

Interfacial velocity

$$V^{\boldsymbol{\nu}} = -\frac{[[\boldsymbol{\nu}\cdot\boldsymbol{\nabla}_x\mu_1^\pm(\tau, \boldsymbol{r})]]}{[[u_o^\pm]]}$$

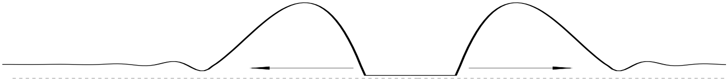
Sharp-interface model governs the long-time dynamics of the phase field model

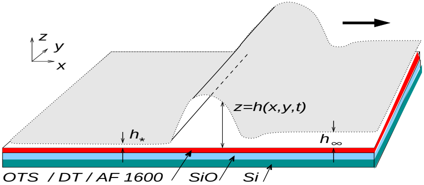
Multi-scale dynamics of patterns

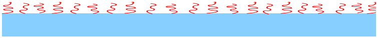


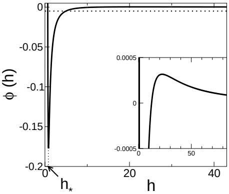
Karin Jacobs and group:
Condensed Matter Physics, Saarland University

Liquid dewetting: Driving force









$$\phi(h) = \frac{c_s}{8h^8} - \frac{A}{2h^2}$$

Liquid dewetting: Mathematical model

Bulk $(0 < z < h)$:

$$\rho\left(\partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = -\nabla p + \mu\Delta\mathbf{u}, \quad \nabla\cdot\mathbf{u} = 0,$$
$$\mathbf{u} = (u, w), \qquad \mathbf{x} = (x, z)$$

Capillary interface $(z = h(x,t))$:

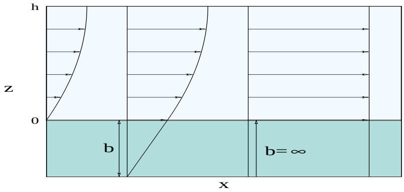
$$\mathbf{n}\cdot\underline{\Pi}\cdot\mathbf{t} = 0, \quad \mathbf{n}\cdot\underline{\Pi}\cdot\mathbf{n} = \sigma\kappa - \phi'(h), \quad (0, \partial_t h)\cdot\mathbf{n} = \mathbf{u}\cdot\mathbf{n}.$$

$$\kappa = \frac{\partial_{xx}h}{(1+(\partial_x h)^2)^{3/2}},\ \mathbf{t} = \frac{(1,\partial_x h)^T}{(1+(\partial_x h)^2)^{1/2}},\ \mathbf{n} = \frac{(-\partial_x h, 1)^T}{(1+(\partial_x h)^2)^{1/2}},$$

$$\underline{\Pi} = -p\,\mathrm{id} + \mu\begin{pmatrix} 2\partial_x u & \partial_z u + \partial_x w \\ \partial_z u + \partial_x w & \partial_z w \end{pmatrix}.$$

Liquid/solid interface $(z = 0)$: $\quad w = 0$

Navier-Slip condition: $\quad u = b\,\partial_z u$



Liquid dewetting: Thin film models

- No-slip ($b = 0$):

$$\partial_t h = -\partial_x \left[h^3 \partial_x \left(\partial_{xx} h - \phi'(h)\right)\right]$$

- Weak-slip ($b \sim 1$):

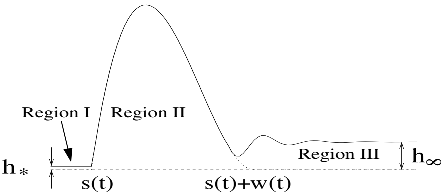
$$\partial_t h = -\partial_x \left[\left(h^3 + bh^2\right) \partial_x \left(\partial_{xx} h - \phi'(h)\right)\right]$$

- Intermediate-slip ($1 \ll b \ll \epsilon_\ell^{-2}$):

$$\partial_t h = -\partial_x \left[h^2 \partial_x \left(\partial_{xx} h - \phi'(h)\right)\right]$$

- Strong-slip ($b = \beta/\epsilon_\ell^2$):

$$\begin{aligned} \mathrm{Re}\left(\partial_t u + u\partial_x u\right) &= \frac{4\,\partial_x(h\partial_x u)}{h} + \partial_x\left(\partial_{xx} h - \phi'(h)\right) - \frac{u}{\beta h} \\ \partial_t h + \partial_x (hu) &= 0 \end{aligned}$$



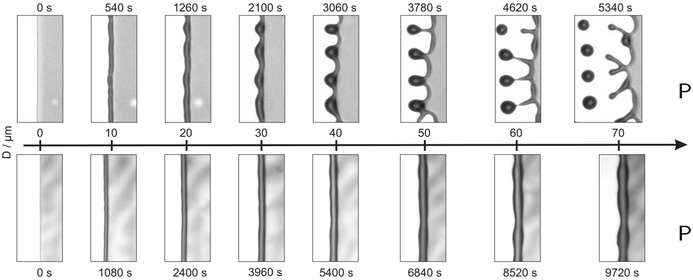
Matched asymptotics for $t \to \infty$.

- No slip $(n = 3)$: $s(t) \sim c\, t/(c \ln t + 1)$, (Flitton, King 2004)
- Intermediate slip $(n = 2)$: $s(t) \sim Ct^{2/3}$ (FK04; Münch., W, Witelski 05)
- Strong slip: $s(t) \sim C\, t^{\alpha}$, $\alpha \sim 1$ (Evans, King, Münch, 2006)

$\Longrightarrow$ **Dewetting Rates:** $\begin{cases} \sim C & \text{(no slip \& strong slip)} \\ \sim Ct^{-1/3} & \text{(intermediate slip)} \end{cases}$

Implications for contact-line instability?

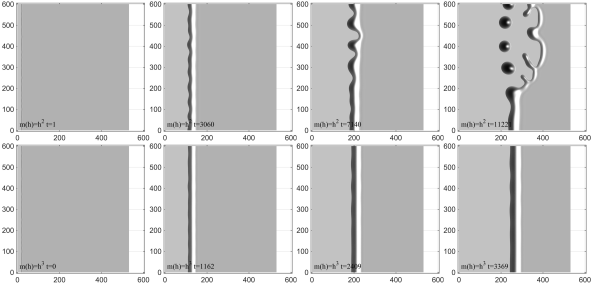
Liquid dewetting of polymer films: Experiments



PS on **DTS**/SiO_2/Si

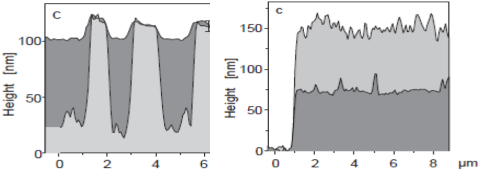
PS on **AF1600**/SiO_2/Si

Source: Karin Jacobs' group, Univ. Saarland

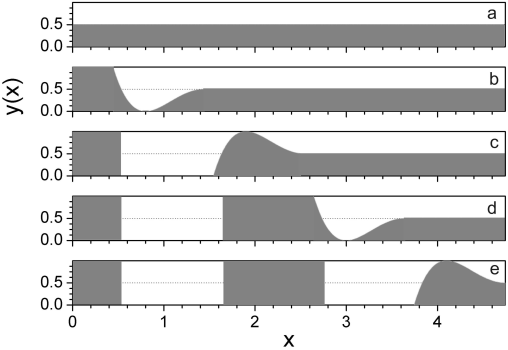


Surface directed spinodal decomposition

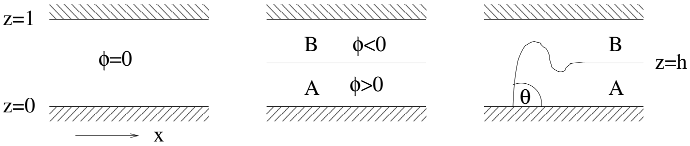
Surface directed spinodal decomposition



Confined bulk diffusion



Phase-field model



ϕ order parameter, μ chemical potential, F bulk free energy

$$\phi_t = \Delta\mu, \qquad \mu = F'(\phi) - \epsilon^2 \Delta\phi,$$
$$F(\phi) = -\chi\phi^2 + \phi^4/6, \qquad \chi = (1-T)/T$$

Boundary conditions at $z = 0$, d for antisymmetric walls:

$$\mu_z = 0 \quad \text{(no-flux)},$$
$$\epsilon\phi_z = \beta_1 (1 - \phi^2/(3\chi_0)^{1/2})$$

Initial condition

$$\phi(z, 0) = 0.$$

Cahn 1977, Binder 1995, Puri & Binder (2002, 2007,. . .), Gheoghegan & Krausch (2003)

Cubic surface energy: e.g. Xu & Wang 2011

Sharp Interface Model

$$\partial_{xx}\mu^{(1)} + \partial_{zz}\mu^{(1)} = 0, \qquad \text{on } 0 < z < h \quad \text{and} \quad h < z < d,$$

$$\mu^{(1)} = \frac{\sigma h_{xx}}{(1+h_x^2)^{1/2}}, \quad h_t = \frac{1}{2(3\chi)^{1/2}}\left(\left[\partial_x \mu^{(1)} h_x - \partial_z \mu^{(1)}\right]_-^+\right), \quad \text{at } z = h,$$

$$\partial_z \mu^{(1)} = 0 \qquad \text{at } z = 0,\, d.$$

Conditions at 3-phase contact line $x = s(t)$:

$$h = 0,\ h_x = \tan\theta,\ q = 0,$$

$$\text{with} \quad \cos\theta = \frac{2\beta_1(1+\chi)}{3\sigma} \quad \text{(Cahn 77 - Modica 87).}$$

Conditions for A/B interface at $x \to \infty$:

$$h \to 1, \quad q \to 0.$$

Thin film model

Notice mass conservation:

$$h_t + q_x = 0 \qquad \text{with } q = \partial_x \int_0^d \mu dz.$$

For $\theta \ll 1$, rescale and use thin film approximation.

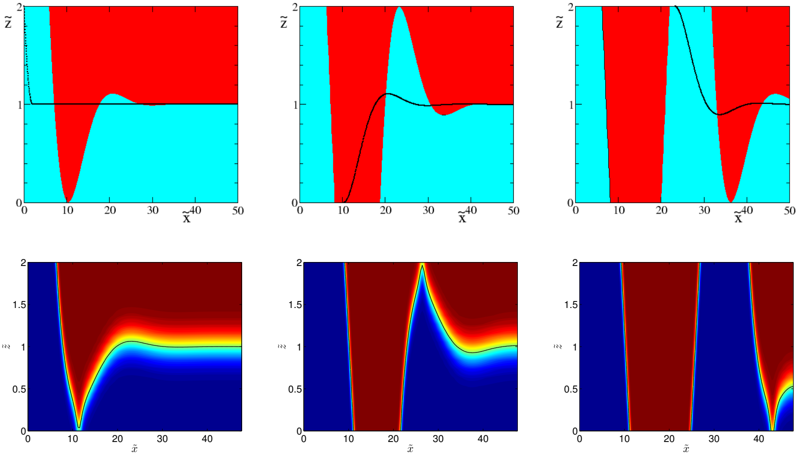
$$\begin{aligned} \partial_{\tilde{z}\tilde{z}}\tilde{\mu} &= 0, \qquad \text{on } 0 < \tilde{z} < h(\tilde{x},\tilde{t}) \text{ and } \tilde{h}(\tilde{x},\tilde{t}) < \tilde{z} < d, \\ \tilde{\mu} &= \tilde{h}_{\tilde{x}\tilde{x}}, \qquad \text{at } \tilde{z} = \tilde{h}(\tilde{x},\tilde{t}), \\ \tilde{h}_{\tilde{t}} &= -\left[\partial_{\tilde{z}}\tilde{\mu}\right]_-^+, \qquad \text{at } \tilde{z} = \tilde{h}(\tilde{x},\tilde{t}), \\ \partial_{\tilde{z}}\tilde{\mu} &= 0 \qquad \text{at } \tilde{z} = 0,\ d; \end{aligned}$$

Integrate and combine with mass conservation:

$$\tilde{h}_{\tilde{t}} + \tilde{h}_{\tilde{x}\tilde{x}\tilde{x}\tilde{x}} = 0.$$

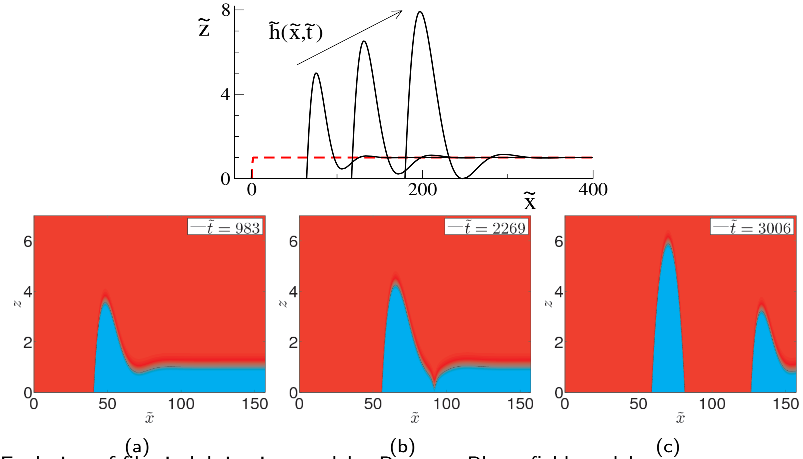
Contact line and far-field conditions:

$$x = s(t): \quad \tilde{h} = 0, \quad \tilde{h}_{\tilde{x}} = 1, \quad \tilde{h}_{\tilde{x}\tilde{x}\tilde{x}} = 0; \quad \tilde{x} \to \infty: \quad \tilde{h} \to 1, \quad \tilde{h}_{\tilde{x}\tilde{x}\tilde{x}} \to 0.$$



Top: Evolution of film in lubrication model – Bottom: Phase field model
Parameters PFM: $\chi_0 = 0.1$, $\beta_1 = 0.11$, $\varepsilon = 0.03$, $\theta = 50^\circ$.

Rim shedding



Top: Evolution of film in lubrication model – Bottom: Phase field model

Parameters PFM: $\chi_0 = 0.1$, $\beta_1 = 0.11$, $\varepsilon = 0.03$, , $\theta = 45°$.

Hennessy et al., EPL 2014, Hennessy et al., SIAP, 2014

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