Multiscale Modelling in Thin Liquid Films
"Spinodal dewetting" Aug 10+11, 2006

$t \longrightarrow$

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J. Becker, G. Grün, R. Seeman, H. Mantz, K. Jacobs, K.R. Mecke, R. Blossey, "Complex dewetting scenarios captured by thin-film models", Nat. Mater 2(1) 2003 : 59-63

note: "dewetting" doesn't mean what you may think it means...

$t=0$

$\uparrow$dry $\uparrow$dry $\uparrow$dry   isn't what's meant.
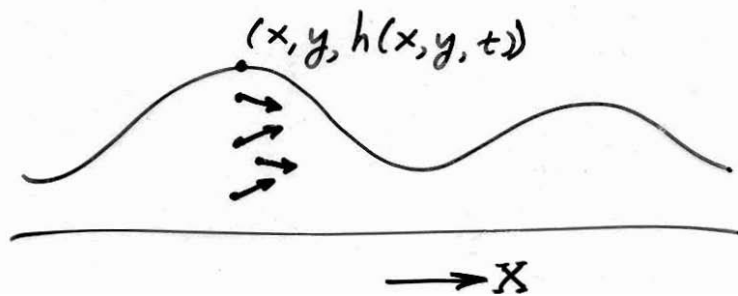
is what's meant   large drops/regions of fluid separated by an ultra-thin film (nanometer)

If one has a thin viscous film of fluid, one can neglect gravity & inertial effects and find a model that captures the driving forces: surface tension & intermolecular forces.

Further, rather than keeping track of the fluid velocity at each point in the fluid,

$(x, y, h(x, y, t))$

$\longrightarrow X$

one can find a model that is fully determined by the location of the (free) air/liquid interface: $h(x, y, t)$

$$\frac{\partial h}{\partial t} = \nabla \cdot (h^3 \nabla p)$$

where $p = \Pi(h) - \Delta h$

↑ arises from surface tension

"disjoining pressure" models intermolecular forces

Goals

Present derivation of model

- Present numerical simulations of the model (1-d)
- Present reduction of PDE model to a system of ODE (1-d)

These two talks are pedagogical---as part of a summer school. The numerics and the PDE to ODE reduction are not my work. They are the work of Glasner and Witelski: "Coarsening dynamics of dewetting films," Phys Rev E 67 (2003) 016302.
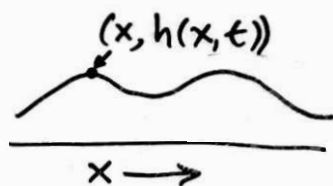
Note: the model can be derived for 2-d but the numerics take much longer because the observed phenomena occur on a very long time scale. The 2-d PDE → ODE reduction is currently being worked on by Glasner + Otto + Rump + Slepcev

Consider

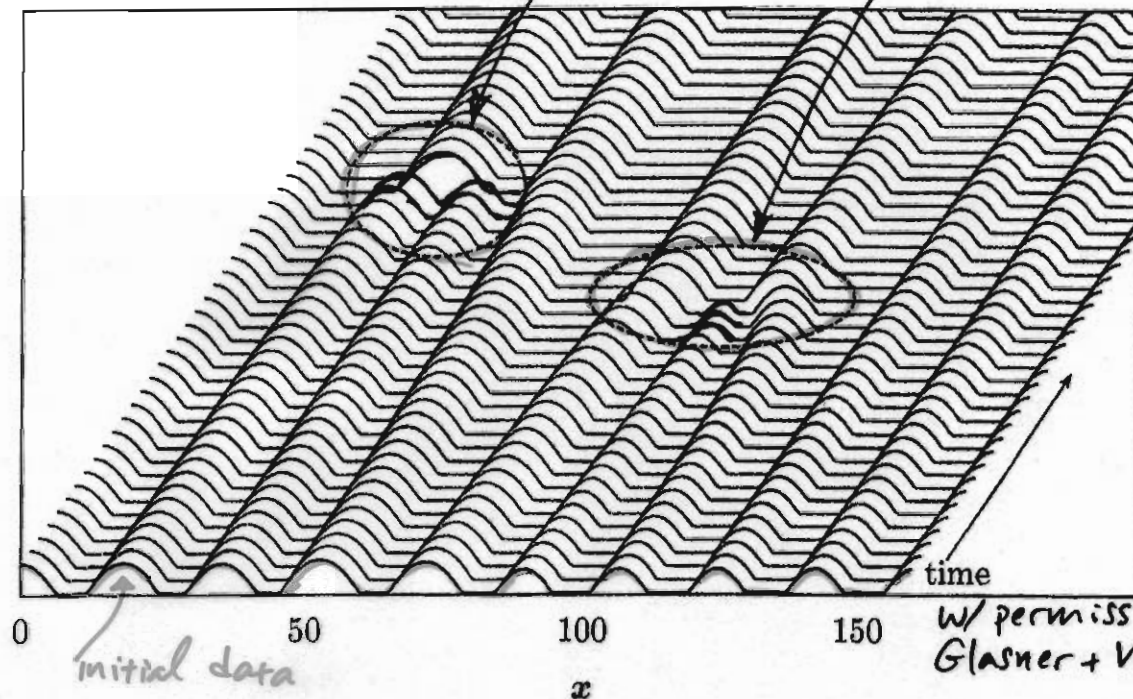$$\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(h^3 \frac{\partial}{\partial x} P\right)$$

$(x, h(x,t))$

$x \longrightarrow$

where

$$P = \frac{1}{\varepsilon}\left(\frac{\varepsilon}{h}\right)^3\left[1-\left(\frac{\varepsilon}{h}\right)\right] - h_{xx}$$

$\uparrow$ a Lennard-Jones potential

two droplets merged
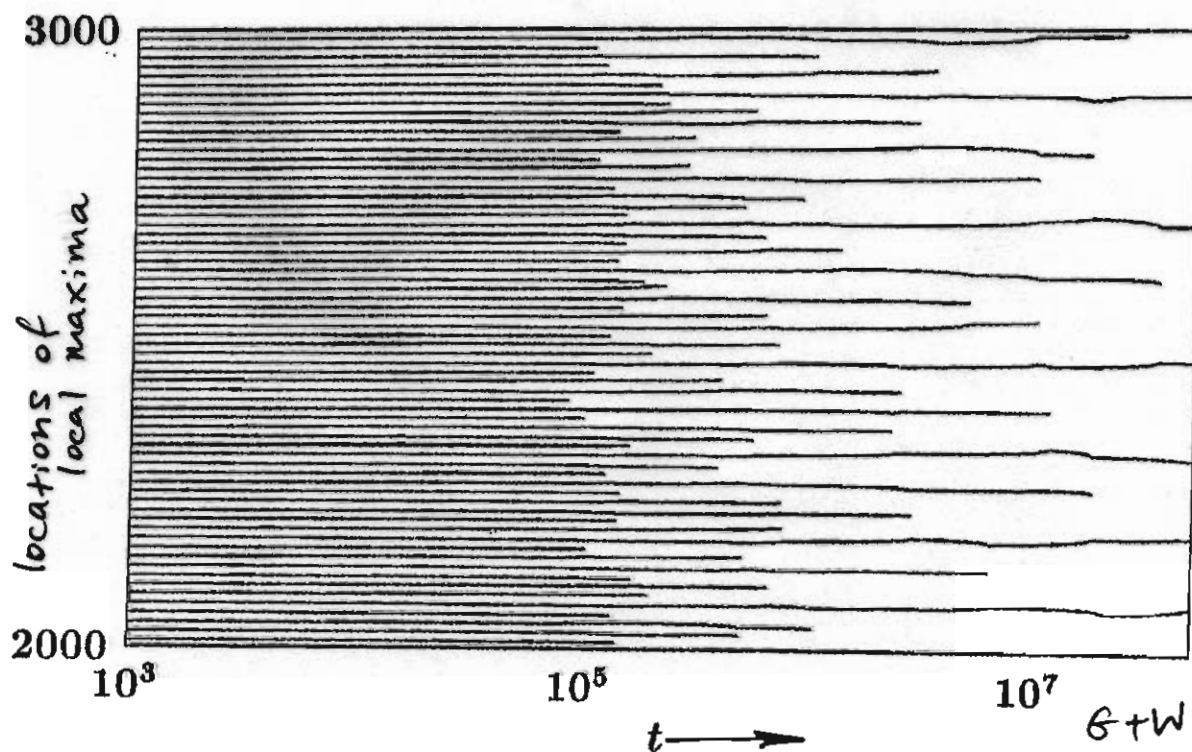
a droplet collapsed

time

reprod. w/ permission of Glasner + Witelski (2003)

0   50   100   150

initial data

x

$$h_t = \frac{\partial}{\partial x}\left(h^3 \frac{\partial}{\partial x}\left(\pi(h) - h_{xx}\right)\right) \text{ where } \pi(h) = \frac{1}{\varepsilon}\left(\frac{\varepsilon}{h}\right)^3\left[1 - \left(\frac{\varepsilon}{h}\right)\right]$$

3000
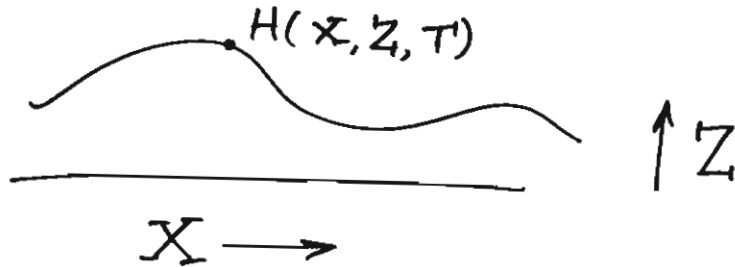
locations of local maxima

2000

10^3 10^5 10^7

$t \longrightarrow$

G+W 2003

plot the <u>locations</u> of the local maxima as a function of time

see <u>coarsening</u> as well as <u>drift</u>.

derivation of PDE model.

- Will do the derivation in 2d but same method works in 3d.

$H(X, Z, T)$

$\uparrow Z$

$X \longrightarrow$

Navier-Stokes in $\quad X \in (-\infty, \infty)$

$Z \in (0, H(X, Z, T))$

$$\begin{cases} \rho(\vec{U}_t + \vec{U} \cdot \nabla \vec{U}) = -\nabla(P - F(H)) + \mu \Delta \vec{U} \\ \nabla \cdot \vec{U} = 0 \end{cases}$$

↑ contr. due to intermolecular forces van der Waals attraction, Born repulsion ...

$\vec{U} = U\hat{i} + W\hat{k}$

at free boundary $Z = H(X, T)$:

$\vec{n}^T \Sigma \vec{n}$ = surface tension × curvature ← normal stress

$\vec{t}^T \Sigma \vec{n} = 0$ ← tangential stress

$ kinematic boundary condition

at the liquid/solid interface:

$W = 0 \qquad$ at $Z = 0$

$U = B \dfrac{\partial U}{\partial Z} \qquad$ " $\qquad$ " ← Navier slip condition, B = slip length

step 1 : nondimensionalize

notation : capital letters ⇒ dimensional quantity
$$X, Z, U, W \text{ etc}$$
\bbf font ⇒ length scales
lower case letters ⇒ dimensionless &
order 1

$$U = \mathbb{U} u \longleftarrow \text{dimensionless}$$

↗ dimensional   ↖ speed scale

$$Z = \mathbb{H} z \qquad X = \mathbb{L} x$$
$$H = \mathbb{H} h \qquad B = \mathbb{H} b$$

(length scales)

velocity scales : $U = \mathbb{U} u, \quad W = \mathbb{W} w$

time scale : $T = \dfrac{\mathbb{H}}{\mathbb{W}} t$

pressure scale : $P - F(h) = \mathbb{P}(p - \pi(h))$

¡¡ keep an eye out for how
the pressure scales !!

Step 2: seek an asymptotic model.

i.e. (U, W, P) solves the full problem
(Navier Stokes & boundary conditions)

then
$$U = \varepsilon^{\alpha}(u_0 + \varepsilon u_1 + \varepsilon^2 u_2 + \dots)$$
$$W = \varepsilon^{\beta}(w_0 + \varepsilon w_1 + \varepsilon^2 w_2 + \dots)$$
$$P = \varepsilon^{\gamma}(p_0 + \varepsilon p_1 + \varepsilon^2 p_2 + \dots)$$

where (u_0, w_0, p_0) solves an $O(1)$ approx of the full problem, (u_1, w_1, p_1) solves an $O(\varepsilon)$ approx. of the full problem, etc.

God willing, the approximate problems will be tractable and have solutions (u_i, w_i, p_i) that have nontrivial dynamics.

What is a natural choice for ε? The film is assumed to be <u>thin</u> so

$$\varepsilon := \frac{H}{L} \ll 1$$

What does this choice imply?

$$U_x + W_z = 0 \qquad \text{(divergence free cond)}$$

$$\Downarrow$$

$$\frac{U}{L} u_x + \frac{W}{\varepsilon L} w_z = 0$$

$$\frac{U}{L} u_x + \frac{W}{\varepsilon L} w_z = 0$$

if W is $O(\varepsilon)$ ($W = \varepsilon U$, for example)
then divergence-free condition becomes

$$\frac{U}{L} u_x + \frac{\varepsilon U}{\varepsilon L} w_z = 0 \implies u_x + w_z = 0$$

What if W isn't $O(\varepsilon)$? W is $O(1)$ for example.
then

$$\underbrace{\frac{U}{L}}_{\uparrow} u_x + \underbrace{\frac{W}{\varepsilon L}}_{\uparrow} w_z = 0$$

different orders of ε

$$\implies u_x = 0 \quad \text{and} \quad w_z = 0 \quad \text{in fluid domain}$$

- w indep of z and
  $w = 0$ at $z = 0 \implies W(x, z, t) \equiv 0$
- $w \equiv 0$ and u indep of x
  $\implies u_t = \text{const} + \mu u_{zz}$
  this $ \text{ boundary condition}$
  $u_z = 0$ at $z = h(x, t)$
  $\implies$ solvable only if $h(x, t) =$
  indep of x. 😟

concl: for interesting dynamics,
need W to be $O(\varepsilon)$. Assume $\underline{W = \varepsilon U}$.

We continue with the nondimensionalization now that we've settled on $H = \varepsilon L$ & $W = \varepsilon U$

• Still need to determine pressure scale P!

Navier Stokes:

$$\begin{cases} \varepsilon^2 \rho \dfrac{UL}{\mu}(u_t + uu_x + wu_z) = -\varepsilon^2 \dfrac{PL}{\mu U} p_x + \varepsilon^2 u_{xx} + u_{zz} \\[4mm] \varepsilon^2 \rho \dfrac{UL}{\mu}(w_t + uw_x + ww_z) = -\dfrac{PL}{\mu U} p_z + \varepsilon^2 w_{xx} + w_{zz} \end{cases}$$

$$u_x + w_z = 0$$

Boundary conditions at $z = h(x,t)$

tangential stress

$$\begin{cases} 2\varepsilon^2(u_x - w_z)h_x + (u_z + \varepsilon^2 w_x)(1 - \varepsilon^2 h_x^2) = 0 \\[4mm] p - \Pi(h) - 2\dfrac{\mu U}{L P}\left[w_z(1 - \varepsilon^2 h_x^2) - h_x(u_z + \varepsilon^2 w_x^2)\right]\Big/(1 + \varepsilon^2 h_x^2) \\[4mm] \qquad\qquad\qquad\qquad = -\varepsilon \dfrac{\sigma}{L P}\dfrac{h_{xx}}{(1 + \varepsilon^2 h_x^2)^{3/2}} \\[4mm] h_t = w - u h_x \end{cases}$$

R normal stress

Boundary conditions at $z = 0$:

$$\begin{cases} w = 0 \\ u = b u_z \end{cases}$$

option 1: $P = \dfrac{\mu U}{L} \Rightarrow p_z \sim w_{zz}$

option 2: $P = \dfrac{1}{\varepsilon^2}\dfrac{\mu U}{L} \Rightarrow p_x \sim u_{zz}$

Recall that we seek

$$u = u_0 + \varepsilon u_1 + \varepsilon^2 u_2 + \cdots$$
$$w = w_0 + \varepsilon w_1 + \varepsilon^2 w_2 + \cdots$$
$$p = p_0 + \varepsilon p_1 + \varepsilon^2 p_2 + \cdots .$$

where (u_i, w_i, p_i) solves a PDE + BC from $O(\varepsilon^i)$.

---

option 1: $\mathbb{P} = \dfrac{\mu U}{L}$ then the $O(1)$ system is

$$\begin{cases} 0 = u_{zz} \\ p_z = w_{zz} \\ u_x + w_z = 0 \end{cases} \quad \text{in} \quad 0 < z < h(x,t)$$

$$\begin{cases} u_z = 0 \\ p - \Pi(h) = 2[w_z - h_x u_z] \\ h_t = w - u h_x \end{cases} \quad \text{at } z = h(x,t)$$

↖ note: normal stress condition doesn't see surface tension to lowest order

$$\begin{cases} w = 0 \\ u = b u_z \end{cases} \quad \text{at } z = 0$$

the boundary conditions are such that they force $u_0 \equiv 0$ and $w_0 \equiv 0$ trivial solution. ☹

try option 2

option 2: $\mathbb{P} = \dfrac{1}{\varepsilon^2} \cdot \dfrac{\mu \mathbb{U}}{\mathbb{L}}$

Before proceeding, consider the normal stress condition at $z = h(x,t)$. The surface tension term is:

$$- \varepsilon \; \frac{\sigma}{\mathbb{L}\mathbb{P}} \; \frac{h_{xx}}{(1+\varepsilon^2 h_x^2)^{3/2}}$$

$$= -\varepsilon^3 \; \frac{\sigma}{\mu \mathbb{U}} \; \frac{h_{xx}}{(1+\varepsilon^2 h_x^2)^{3/2}}$$

$$= -\varepsilon^3 \; \frac{1}{Ca} \; \frac{h_{xx}}{(1+\varepsilon^2 h_x^2)^{3/2}}$$

This shows that the surface tension can be relevant at the lowest order only in situations where the capillary number, Ca, is <u>very</u> <u>small</u>:

$$Ca = \varepsilon^3 \qquad (or \quad \sigma = \frac{\mu \mathbb{U}}{\varepsilon^3})$$

We will assume the fluid flow is in this regime.

proceeding...

the first-order problem that
(u_0, w_0, p_0) satisfies is

$$\begin{cases} 0 = -p_x + u_{zz} \\ 0 = -p_z \\ u_x + w_z = 0 \end{cases} \quad \text{in} \quad 0 < z < h(x,t)$$

$$\begin{cases} u_z = 0 \\ p - \pi(h) = -h_{xx} \\ h_t = w - u h_x \end{cases} \quad \text{at} \quad z = h(x,t)$$

$$\begin{cases} w = 0 \\ u = b u_z \end{cases} \quad \text{at} \quad z = c$$
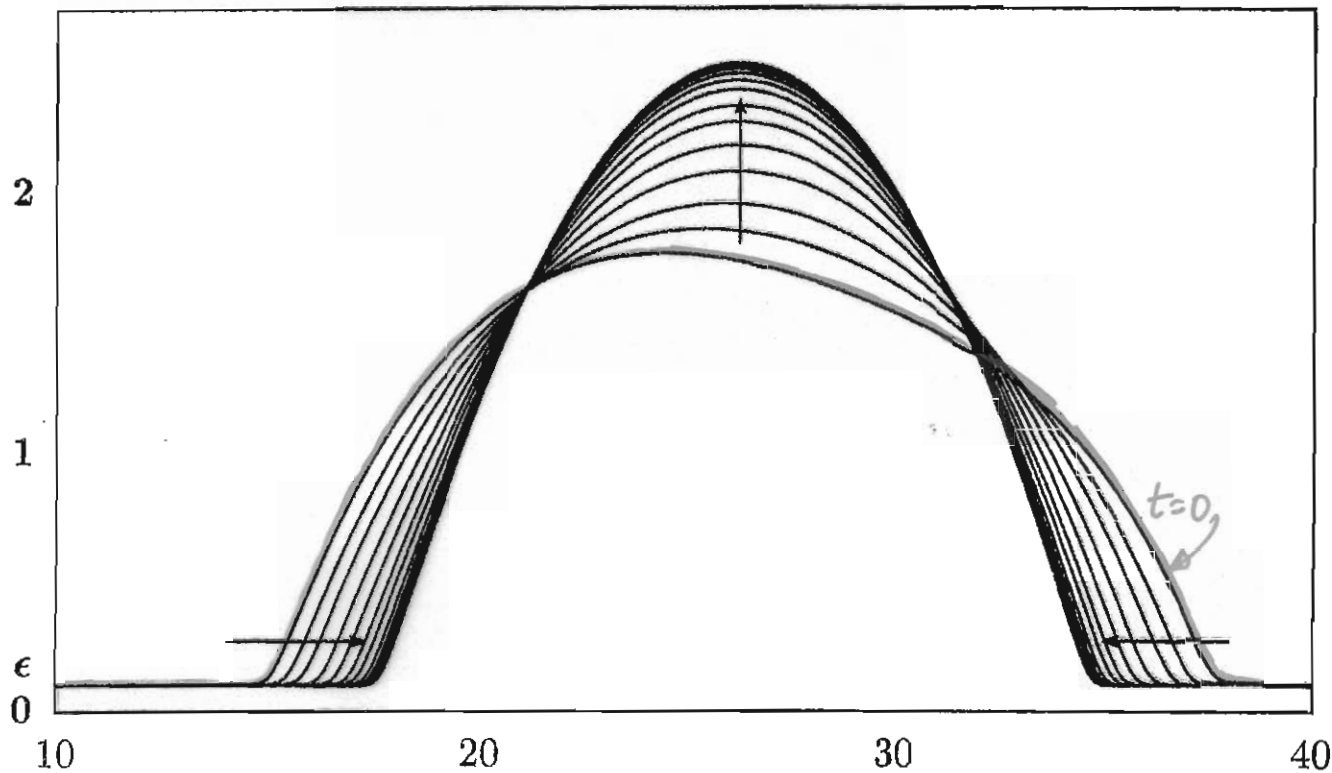
this system can be written all in one
equation:

$$h_t = -\frac{\partial}{\partial x} \left[\left(\tfrac{1}{3} h^3 + b h^2 \right) \frac{\partial}{\partial x} \left(h_{xx} - \pi(h) \right) \right]$$

$$= \frac{\partial}{\partial x} \left[\left(\tfrac{1}{3} h^3 + b h^2 \right) p_x \right]$$

where $p := \pi(h) - h_{xx}$

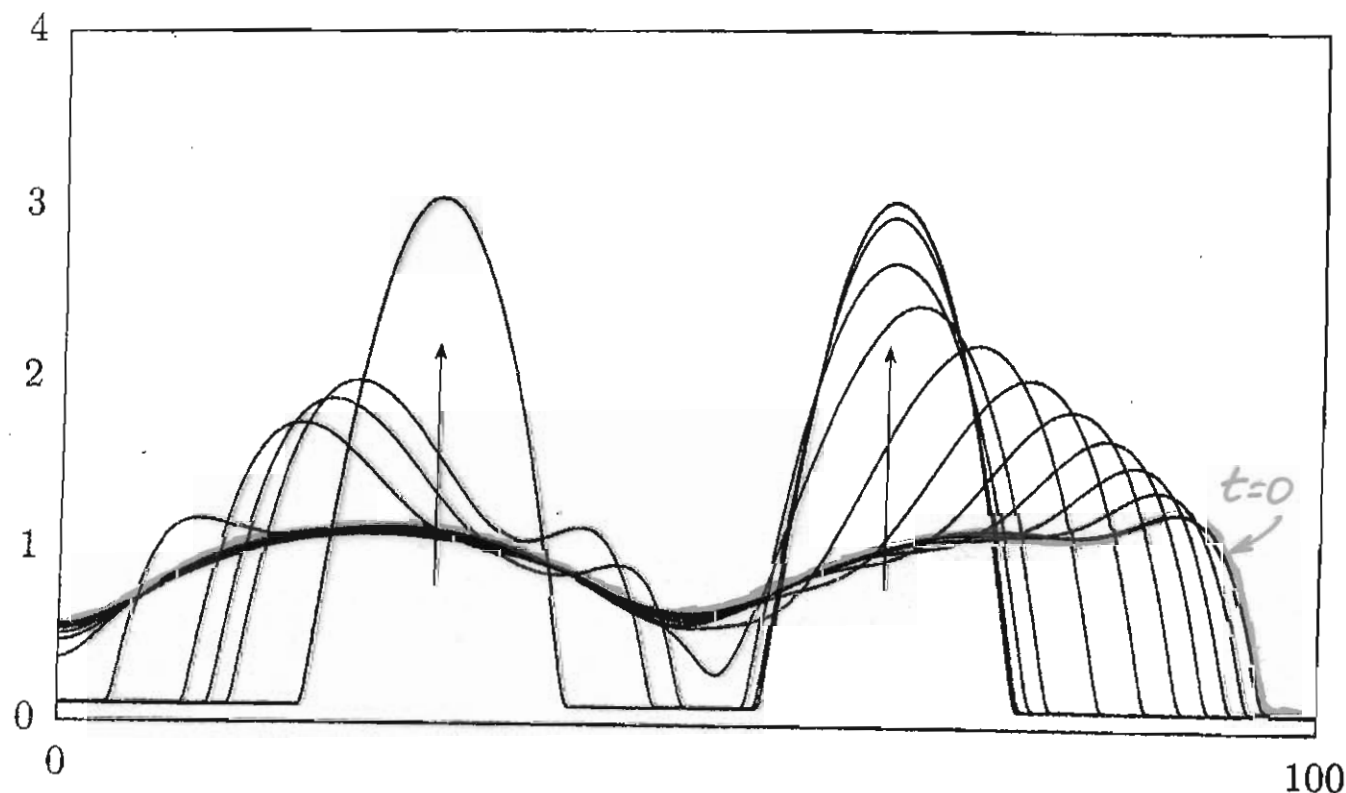Solving the $O(1)$ problem, we can return to the
original dimensional problem:

$$U = U [u_0 + \ldots]$$
$$W = \varepsilon U [w_0 + \ldots]$$
$$P = \frac{1}{\varepsilon^2} \frac{\mu U}{L} [p_0 + \ldots]$$

Observe: after a transient, solutions of the initial
    value problem appear to be "parabolas connected by flat films"

$t=0$,

ϵ

x
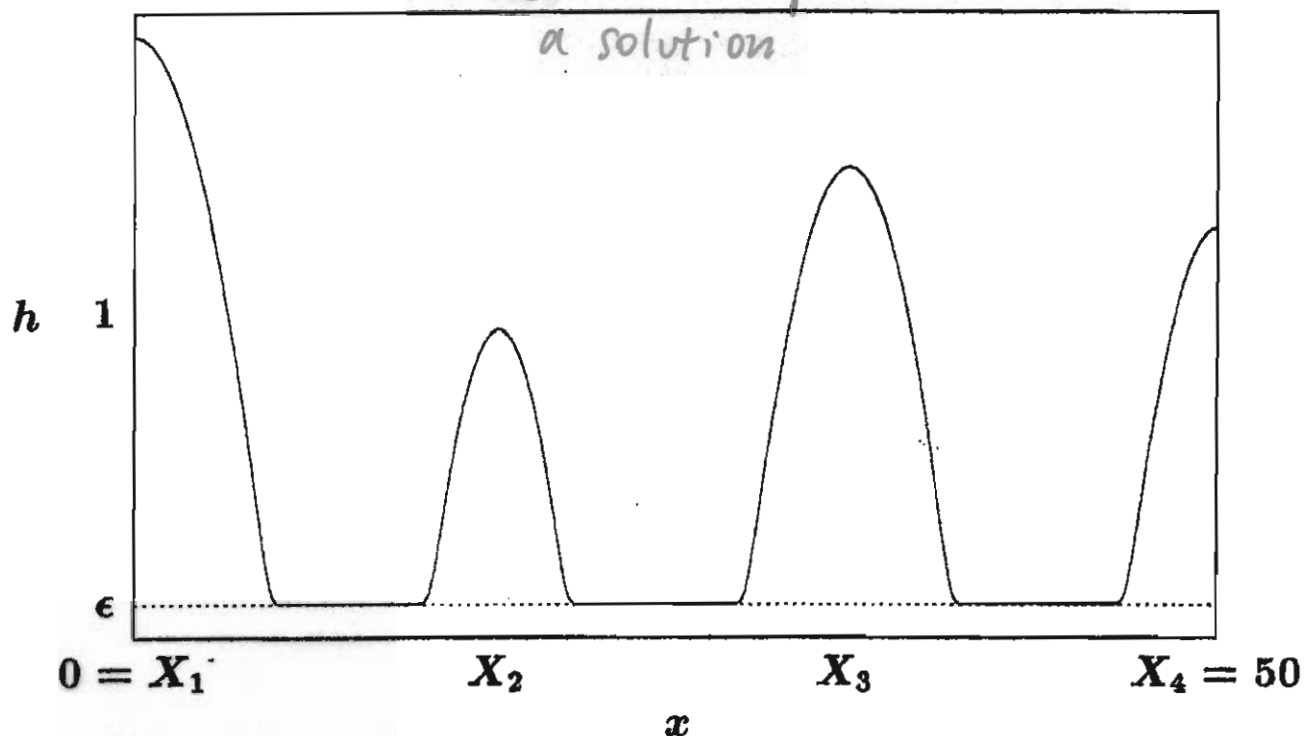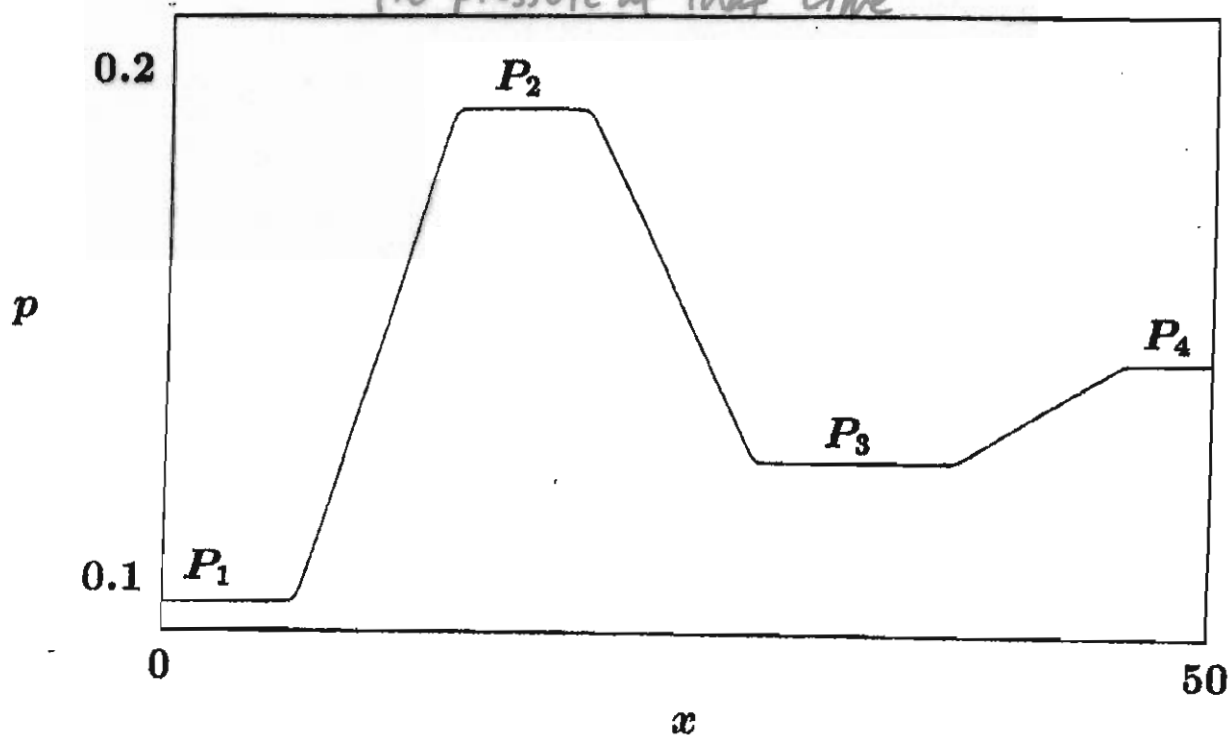
Glasner + Witelski '03

red = initial data

$t=0$

x

Glasner + Witelski '03

A large-time snapshot of a solution

$0 = X_1$ $\quad X_2 \quad\quad X_3 \quad\quad X_4 = 50$

x

Glasner + Witelski '03

the pressure at that time

0 $\qquad\qquad\qquad\qquad\qquad\qquad 50$

x

Glasner + Witelski '03

observe: the pressure is nearly constant in the parabola-like regions ⇒ they're nearly steady states. the pressure is nearly linear in the ultra thin film regions ⇒ there's nearly constant flux in these regions.

These simulations suggest that the steady states of

$$h_t = \frac{\partial}{\partial x}\left[h^3 \frac{\partial}{\partial x}\left(\pi(h) - h_{xx}\right)\right]$$

will be very important. And so one starts by studying them.
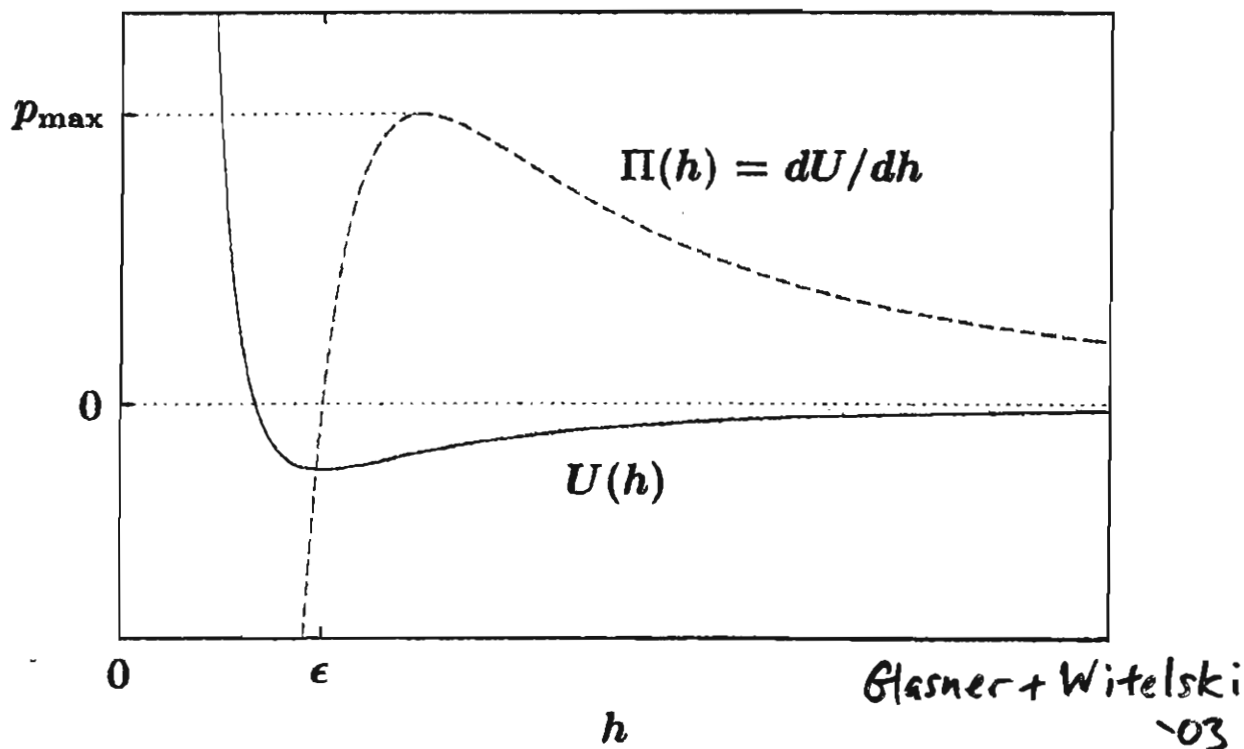
$$h_t = \frac{\partial}{\partial x}\left[h^3 p_x\right]$$

$$\Rightarrow p(x,t) = \bar{p} \quad \text{(constant)} \quad \text{for a steady state.}$$

That is $\quad \pi(h) - h_{xx} = \bar{p} \quad$ for a constant steady state.

Assumptions on $\pi(h)$: $\quad \pi(h) = U'(h)$
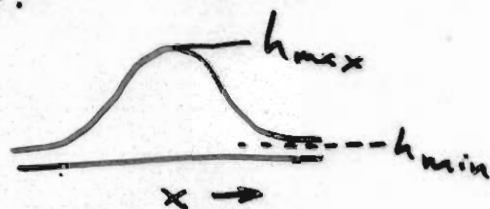where $U(h)$ is the potential

- $U(h)$ has a unique minimum at $h = \varepsilon$
  (a constant film $h \equiv \varepsilon$ is stable & ε is the length scale of the ultra-thin film)

- $\pi(h)$ has a unique maximum, p_{max}, at $h_{peak} > \varepsilon$
  (stable steady states that look like ⌢ exist)

- $\pi(h)$ is $o(\frac{1}{h})$ and $U(h) \to 0$ as $h \to \infty$
  (disjoining pressure negligible where film thick)

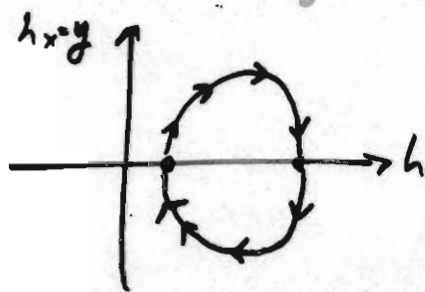- $\lim_{h \downarrow 0} U(h) = \infty$ (intermolecular forces dominate, where film thin)

p_{max}

0

$\Pi(h) = dU/dh$

$U(h)$

0   ϵ

h

Glasner + Witelski
'03

the four conditions are satisfied.

to find a steady state $\bar{h}(x; \bar{p})$ one seeks
h so that $\qquad h_{xx} = \Pi(h) - \bar{p}.$

$$\begin{cases} h_x = y \\ y_x = \Pi(h) - \bar{p} \end{cases}$$
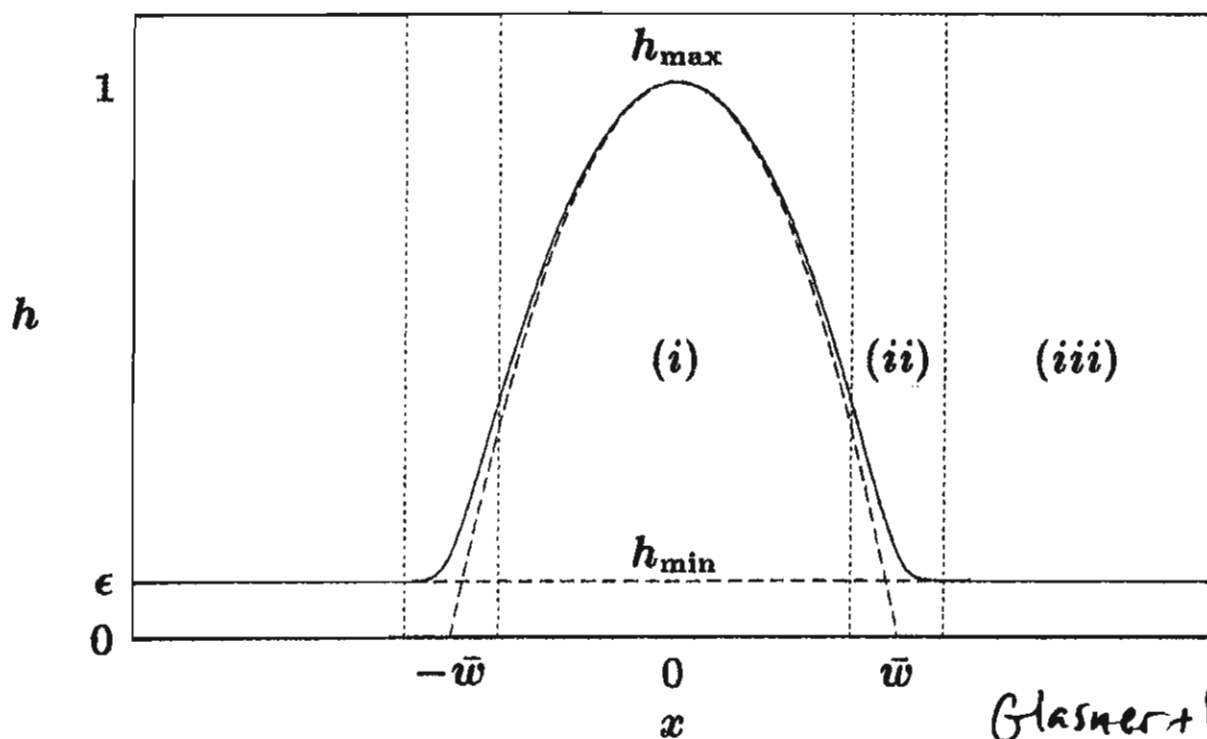

h_{max}

h_{min}

$x \rightarrow$

seek orbit connecting h_{min} to h_{min}

$h_x = y$

h

orbit parametrised
by x

$\Pi(h)$

p_{max}

$\bar{p}$

h_{min}

h

Glasner + Witelski '03

We see that ∃ droplet-shaped steady
states for all pressures $\bar{p} \in (0, p_{max})$
and as $\bar{p} \uparrow p_{max}$ $h_{max} - h_{min} \downarrow 0$

The droplet steady states have three regions:

(i) droplet core. Contains bulk of fluid mass. Surface
 tension far more important than intermolecular
 forces. (transl: $\pi(h)$ small here.)

(iii) outer region. This is the ultrathin film. Here,
 intermolecular forces dominate surface tension

(ii) the "contact line". Both types of forces important.
 Here, the core is asymptotically matched to
 the outer region.

To proceed any further, one needs fine information about the steady states. This will be obtained via asymptotics.

Asymptotics in what? Natural choice is ε: the (approximate) thickness of the ultrathin film. [Note! This is the ε in $U(h)$ not the $H = \varepsilon \underline{L}$ in the model deriv.]

Caveat: If one wants to take $\varepsilon \downarrow 0$ one needs to make sure the potential $U(h; \varepsilon)$ behaves reasonably as $\varepsilon \downarrow 0$.

If $U(h; \varepsilon) = \mathcal{U}\left(\frac{h}{\varepsilon}\right)$ then the ultrathin film will have bounded energy as $\varepsilon \downarrow 0$. This then ensures that h_x is bounded for steady states & near steady states. (The lubrication approximation is valid as $\varepsilon \downarrow 0$.)

The potential will be assumed to have this form.

$$U(h;\varepsilon) = \mathcal{U}\left(\tfrac{h}{\varepsilon}\right) \implies \pi(h;\theta) = \tfrac{1}{\varepsilon}\mathcal{U}'\left(\tfrac{h}{\varepsilon}\right)$$

Back to the steady states.

$$h_{xx} = \pi(h) - \bar{p}$$

by assumption, $\pi(\varepsilon) = 0$. Also π is very steep near ε. $\implies h_{min}$, which satisfies

$$\pi(h_{min}) - \bar{p} = 0$$

will be $O(\varepsilon)$. Specifically, one can show

$$h_{min} \sim \varepsilon + \varepsilon^2 \frac{\bar{p}}{\mathcal{U}''(1)} + \dots$$

Once h_{min} is known, one finds h_{max} via the integral of $h_{xx} = \pi(h) - \bar{p}$.

$$h_{xx} = \pi(h) - \bar{p} \implies h_{xx}h_x = \pi(h)h_x - \bar{p}h_x$$

$$\implies \tfrac{1}{2}(h_x)^2 = U(h) - \bar{p}h + C_1$$

evaluate at h_{min} to find C_1.
Since $h_x = 0$ at h_{max}, we find

$$0 = U(h_{max}) - \bar{p}h_{max} - U(h_{min}) + \bar{p}h_{min}$$

Solve this ↑ to find h_{max}. Find $h_{max} \sim -\dfrac{\mathcal{U}(1)}{\bar{p}}$

In region (i) (the droplet core) $\varepsilon \ll h \leq h_{max}$
and (by assumption on $\Pi(h)$) one has
$\Pi(h)$ negligible.

$\Rightarrow$ in the core region

$$h(x;\bar{p}) \sim \tfrac{1}{2}\bar{p}(\bar{w}^2 - x^2) \Rightarrow h_{max} \sim \tfrac{1}{2}\bar{p}\bar{w}^2$$

$\bar{w}$ = effective width of droplet

By prior asymptotics, $h_{max} \sim -\dfrac{\mathcal{U}(1)}{\bar{p}}$

$$\Rightarrow \bar{w} \sim \dfrac{\sqrt{2|\mathcal{U}(1)|}}{\bar{p}}$$

Mass of droplet core $= \displaystyle\int_{-\bar{w}}^{\bar{w}} h(x;\bar{p}) \sim \dfrac{2}{3} \dfrac{(2|\mathcal{U}(1)|)^{3/2}}{\bar{p}^2}$

lesson: $\bar{p}$ <u>determines the height, width, and mass of droplet core.</u>

also, as droplet core vanishes, $\bar{p} \uparrow p_{max}$

What drives the coarsening process?

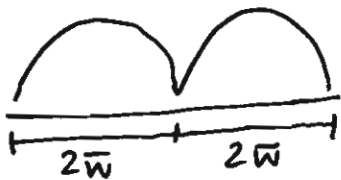$$h_t = \frac{\partial}{\partial x}\left(h^3 \frac{\partial}{\partial x} p\right)$$

is a gradient flow wrt a non-obvious inner product (Otto). The flow is minimizing the energy

$$E(h) := \int U(h) + \frac{1}{2}h_x^2 \, dx$$

Given no-flux boundary conditions,

$$\frac{dE}{dt} = -\int h^3 p_x^2 \, dx \leq 0$$

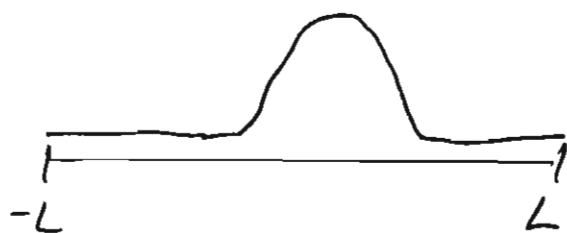Exercise: Compare the energy of 2 droplets to the energy after they merge.

$$2\bar{w} \qquad 2\bar{w} \qquad\qquad vs \qquad\qquad 4\bar{w} \qquad \leftarrow \text{ultra-thin film}$$

$$\text{energy} \sim 2 \int_{-\bar{w}}^{\bar{w}} \frac{1}{2}h_x^2 \, dx = \frac{2}{3}\frac{(2|U(0)|)^{3/2}}{\bar{p}}$$

$$= \frac{2}{3}\frac{A^3}{\bar{p}}$$

$$\text{energy} \sim \frac{\sqrt{2}|A^3}{3\bar{p}} + \frac{4-2\sqrt{2}}{\bar{p}} A U(\varepsilon)$$

where $A := \sqrt{2|U(0)|}$

note: not only is one drop lower energy than two but since $U(\varepsilon) < 0$ the ultrathin film decreases the energy further

To find approximating ODEs for the PDE dynamics, first start by studying a single drop

consider the PDE $\quad h_t = \frac{\partial}{\partial x}\left(h^3 \frac{\partial}{\partial x} P\right)$

subject to boundary conditions

$$\begin{cases} -h^3 P_x \big|_{x=-L} = \sigma \tilde{J}_- \\ -h^3 P_x \big|_{x=L} = \sigma \tilde{J}_+ \\ h_{xxx}(-L) = h_{xxx}(+L) = 0 \end{cases}$$

$\longrightarrow$ specify the fluid flux at the boundaries

The evolution is well-posed w/ these BC.

Initial data:

$$h_0(x) = \tilde{h}(x; P_0)$$

$\uparrow$ steady state w/ pressure P_0

the steady state will respond only
in response to the fluxes at the boundaries
so set the evolution time scale to be
the same as the flux scales

$$\tau = \sigma t$$

Assume the dynamics are quasistatic. That
is, the initial steady state

$$\overline{h}(x; P_0)$$

centered at $x=0$ will move to another
steady state, centered somewhere else and
with some other pressure.

Assume

$$h(x,t) \doteq \overline{h}(x - X(\tau); P(\tau)) + \sigma h_1(x,\tau) + O(\sigma^2)$$

put this ansatz into the evolution eqn

$$h_t = \partial_x (h^3 \partial_x P)$$

and find ...

$$-\frac{d\bar{h}}{dx}\frac{dX}{d\tau} + \frac{d\bar{h}}{dp}\frac{dP}{d\tau} = \mathcal{L}h_1$$

$$\text{where } \mathcal{L}\psi := \frac{\partial}{\partial x}\left(\bar{h}^3\frac{\partial}{\partial x}\left(\pi'(h)\psi - \psi_{xx}\right)\right)$$

our goal: separate ODEs for $\frac{dX}{d\tau}$ and $\frac{dP}{d\tau}$

$\mathcal{L}$ is a singular operator. If one wants to solve

$$\mathcal{L}h_1 = RHS.$$

then one will need to apply the Fredholm alternative to ensure there is a solution h_1.

Applying the Fredholm alternative will yield the ODEs for $\frac{dX}{d\tau}$ and $\frac{dP}{d\tau}$.

<u>Fact</u>: we know there is a two parameter family of steady states of $h_t = \frac{\partial}{\partial x}(h^3 p_x)$

First parameter: translate in space.
$$\bar{h}(x;\bar{p}) \rightarrow \bar{h}(x-x_0;\bar{p})$$

Second parameter: change the pressure
$$\bar{h}(x;p) \rightarrow \bar{h}(x;p+p_0)$$

This two-parameter family will be used to deduce two null-vectors to be used in Fredholm alternative.

$$\mathcal{L}\psi = \frac{\partial}{\partial x}\left(\bar{h}^3 \frac{\partial}{\partial x}\left(\pi'(\bar{h})\psi - \psi_{xx}\right)\right)$$

is not self adjoint. The adjoint operator is

$$\mathcal{L}^*\psi = \left[\pi'(h) - \frac{\partial^2}{\partial x^2}\right]\left[\frac{\partial}{\partial x}\left(\bar{h}^3 \frac{\partial\psi}{\partial x}\right)\right]$$

$\mathcal{L}^*$ has 2-d null space, spanned by

$$\psi_1(x) = 1 \qquad \psi_2(x) = \int_0^x \frac{\bar{h}'(\tilde{x}) - h_{min}}{\bar{h}(\tilde{x})^3}\, d\tilde{x}$$

Fredholm alternative:
   take inner product of

$$\mathcal{L}h_1 = -\frac{\partial\bar{h}}{\partial x}\frac{dX}{d\tau} + \frac{\partial\bar{h}}{\partial p}\frac{dP}{d\tau}$$

with ψ_1 and then with ψ_2.

$$\langle \mathcal{L}h_1, \psi_1 \rangle = \langle h_1, \mathcal{L}^*\psi_1 \rangle = \tilde{J}_+ - \tilde{J}_-$$

$$\left\langle -\frac{\partial\bar{h}}{\partial x}\frac{dX}{d\tau} + \frac{\partial\bar{h}}{\partial p}\frac{dP}{d\tau}, \psi_1 \right\rangle = \int_{-L}^{L} -\frac{\partial\bar{h}}{\partial x}\frac{dX}{d\tau} + \frac{\partial\bar{h}}{\partial p}\frac{dP}{d\tau}$$

$$= \frac{dP}{d\tau}\int_{-L}^{L}\frac{\partial\bar{h}}{\partial p}$$

Hence

$$\frac{d P}{d \tau} = \frac{\tilde{J}_+ - \tilde{J}_-}{\int_{-L}^{L} \frac{\partial \bar{h}}{\partial p} dx}$$

Now take the inner product with ψ_2.

$$< \mathcal{L} h_1, \psi_2 > = \frac{1}{2} \left(\int_{-L}^{L} \frac{\bar{h} - h_{min}}{\bar{h}^3} dx \right) (\tilde{J}_+ + \tilde{J}_-)$$

$$< -\frac{\partial \bar{h}}{\partial x} \frac{dX}{d\tau} + \frac{d\bar{h}}{\partial p} \frac{dP}{d\tau}, \psi_2 > = \frac{dX}{d\tau} \int_{-L}^{L} \frac{(\bar{h} - h_{min})^2}{\bar{h}^3}$$

Hence

$$\frac{dX}{d\tau} = \frac{-\int_{-L}^{L} \frac{\bar{h} - h_{min}}{\bar{h}^3}}{2 \int_{-L}^{L} \frac{(\bar{h} - h_{min})^2}{h^3}} [\tilde{J}_+ + \tilde{J}_-]$$

Since σ was a dummy variable used to extract the linear portion of the problem, one can now set $\sigma = 1$ hence

$$\frac{dX}{dt} = - C_X(P, X)(J_+ + J_-)$$

$$\frac{dP}{dt} = C_P(P, X)(J_+ - J_-)$$

where $C_P(P, X) = \frac{1}{\int_{-L}^{L} \frac{\partial \bar{h}}{\partial p}}$ and C_X ✓ above.

So far, no asymptotics have been done yet. No ε-small arguments were involved in finding the ODEs for $\frac{dX}{dt}$ and $\frac{dP}{dt}$.

They will be used to approximate the coefficients $C_p(X,P)$ and $C_X(X,P)$

$$C_X(X,P) = \frac{\int_{-L}^{L} \frac{\bar{h}-h_{min}}{\bar{h}^3} dx}{2\int_{-L}^{L} \frac{(\bar{h}-h_{min})^2}{\bar{h}^3}}$$

outside the droplet core, $\bar{h}-h_{min}$ is exponentially small. $\Rightarrow$ although the integral is on $[-L,L]$ the integrals on $[-L,-\bar{w}]$ and $[\bar{w},L]$ will be very small. And so

$$C_X(X,P) \approx \frac{\int_{-\bar{w}}^{\bar{w}} \frac{\bar{h}-h_{min}}{\bar{h}^3} dx}{2\int_{-\bar{w}}^{\bar{w}} \frac{(\bar{h}-h_{min})^2}{\bar{h}^3} dx}$$

good news: in $[-\bar{w},\bar{w}]$ the steady state $\bar{h}$ is well approximated by $\frac{\bar{P}}{2}(\bar{w}^2-x^2)$ and so $C_X(X,P)$ is easy to approximate.

Approximating $C_p(x,p)$ isn't as simple.

$$C_p(x,p) = \left(\int_{-L}^{L} \frac{\partial \bar{h}}{\partial p} \, dx \right)^{-1}$$

if one considers $\int_{-L}^{L}$ as $\int_{-L}^{-\bar{w}} + \int_{-\bar{w}}^{\bar{w}} + \int_{\bar{w}}^{L}$

then the $\int_{-\bar{w}}^{\bar{w}}$ integral is tractable because we

know $\bar{h} \sim \frac{p}{2}(\bar{w}^2 - x^2)$ there. But, the $\int_{-L}^{-\bar{w}}$ & $\int_{\bar{w}}^{L}$

integrals require further thought. On $[-L, -\bar{w}]$,

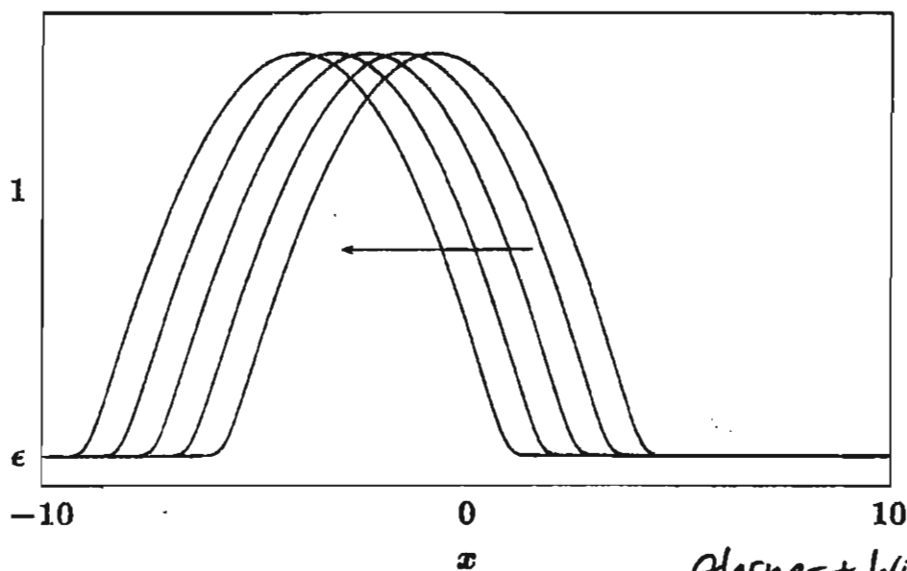$\bar{h}$ is approximately constant $\bar{h} \cong h_{min} \cong \varepsilon + \varepsilon^2 \frac{p}{u''(1)}$

$\Rightarrow \frac{\partial \bar{h}}{\partial p} \cong \frac{\varepsilon^2}{u''(1)}$ on $[-L, -\bar{w}] \Rightarrow \int_{-L}^{-\bar{w}} \frac{\partial \bar{h}}{\partial p} \, dx$ is $O(\varepsilon^2 L)$

<u>Assume</u> $\varepsilon^2 L \ll 1$ then $C_p(x,p) \cong \left(\int_{-\bar{w}}^{\bar{w}} \frac{\partial \bar{h}}{\partial p} \, dx \right)^{-1}$

again, this is something
easily computable given
the further approximation
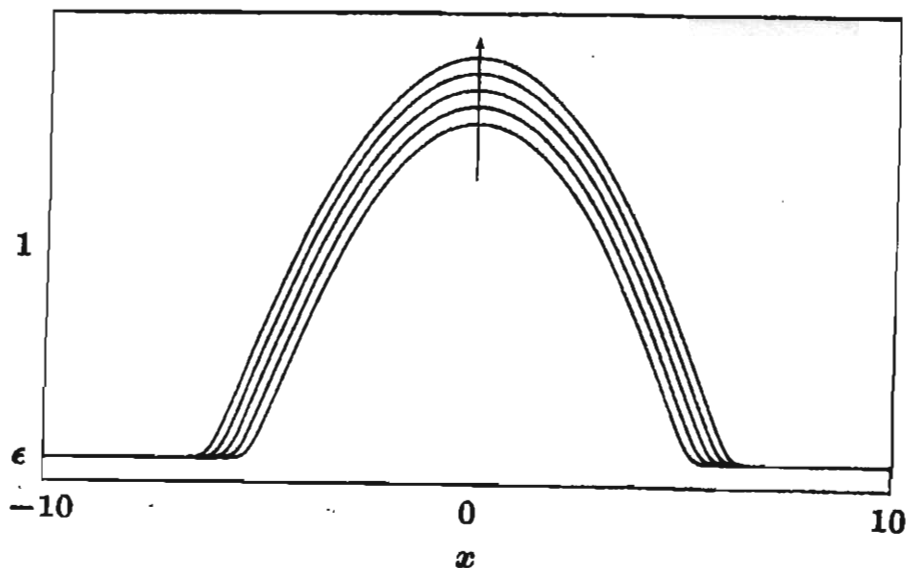$\bar{h} \approx \frac{p}{2}(\bar{w}^2 - x^2)$

Glasner + Witelski '03

example 1: $J_+ = J_-$ then $\frac{dP}{dt} = 0 \Rightarrow$ rigid translation
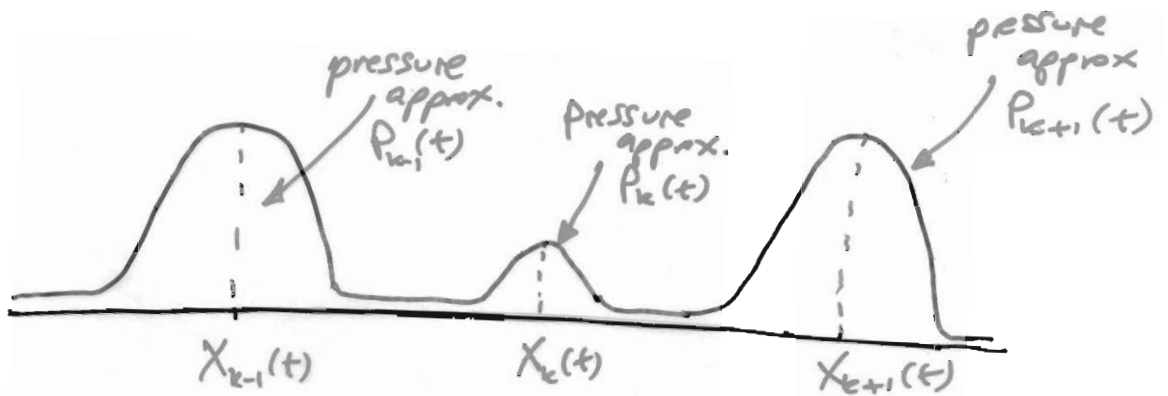

Glasner + Witelski '03

example 2: $J_+ = -J_- \Rightarrow \frac{dX}{dt} = 0$

pure change of mass (change of pressure).

Having found ODEs to model the dynamics of a single quasistatic droplet subject to fluxes, one now uses this to model an array of droplets

pressure approx. $P_{k-1}(t)$

pressure approx. $P_k(t)$

pressure approx $P_{k+1}(t)$

$X_{k-1}(t)$

$X_k(t)$

$X_{k+1}(t)$

droplets connected by an ultrathin film of thickness approx. ε

One can use the ODEs for $\frac{dX}{dt}$ and $\frac{dP}{dt}$ if one knew the flux between droplets. That is the flux within the ultrathin film. This information would provide $J_{k,k+1}$

the flux from droplet k to droplet $k+1$ which would then be used to give J_+^k for the $\left(\frac{dX_k}{dt}, \frac{dP_k}{dt}\right)$ ODEs and J_-^{k+1} for the $\left(\frac{dX_{k+1}}{dt}, \frac{dP_{k+1}}{dt}\right)$ ODEs

Let ε = approximate thickness of
the ultra thin film

l = distance between droplets

Scaling arguments show that

$$\text{if } \frac{\varepsilon}{l} \ll 1 \qquad *$$

then the ultra thin film evolves
quasistatically according to the PDE

$$\tilde{h}_t = -\frac{\partial}{\partial x}\left(\tilde{h}^3 \frac{\partial}{\partial x} \pi'(\tilde{h})\right)$$

(note this is the full evolution but with
the $-h_{xx}$ term due to surface tension
dropped.)

This means that for each ultrathin film one
needs to solve

$$\frac{\partial}{\partial x}\left(\tilde{h}^3 \frac{\partial}{\partial x} \pi'(\tilde{h})\right) = 0$$

subject to boundary conditions from
the flanking droplets

note that this fails when two droplets coalesce,

This will be best done by rewriting the PDE as

$$\tilde{h}_t = -\frac{\partial}{\partial x}\left(\tilde{h}^3 \frac{\partial}{\partial x} \pi(\tilde{h})\right) = -\frac{\partial}{\partial x}\left(h^3 \pi'(h) h_x\right)$$

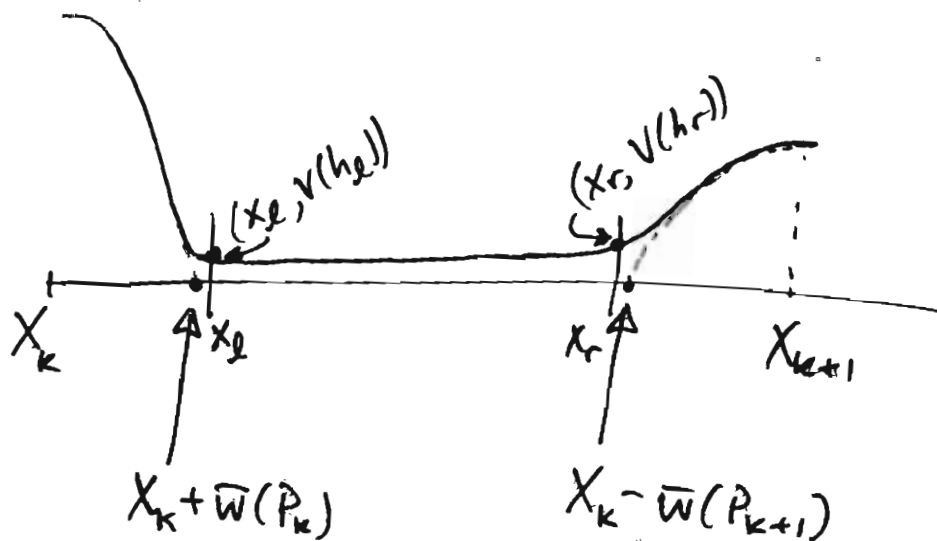$$= \frac{\partial^2}{\partial x^2}\left(V(\tilde{h})\right) = \frac{\partial}{\partial x}\left(V'(h) h_x\right)$$

where $V(\tilde{h})$ is determined up to a constant by

$$V'(h) = -h^3 \pi'(h)$$

The quasistatic problem for the ultrathin film then becomes

$$\frac{\partial^2}{\partial x^2}\left(V(h)\right) = 0 \quad \Rightarrow \quad V(h) \text{ is linear}$$

subject to boundary conditions from flanking droplets.

The flux is then constant $\left(flux = \frac{\partial}{\partial x} V(h)\right)$ so one needs simply to find the slope of $V(h(x))$ in the ultrathin film

$$(x_\ell, V(h_\ell))$$

$$(x_r, V(h_r))$$

$$X_k \qquad X_\ell \qquad X_r \qquad X_{k+1}$$

$$X_k + \overline{W}(P_k) \qquad\qquad X_k - \overline{W}(P_{k+1})$$

Using the asymptotics that gave information
about the droplet core, for each flanking
droplet one uses

$$P_k \text{ to determine } \overline{W}(P_k)$$

$$X_k \text{ is known}$$

$$\Rightarrow X_k + \overline{W}(P_k) \text{ is known}$$

Similarly $\quad X_{k+1} - \overline{W}(P_{k-1})$ is known

These are used to approximate the length
of the ultrathin film, needed for

$$\frac{d}{dx} V(h) = \frac{V(h_r) - V(h_\ell)}{x_\ell - x_r}$$

One now needs to approximate h_ℓ & h_r
the heights of the ultrathin film at each
end.

Again, this is done by invoking the asymptotics
for the droplet core.

$$h_\ell \sim h_{min}(P_k)$$
$$h_r \sim h_{min}(P_{k+1})$$

the flux in the ultrathin film is now
approximated!

$$\begin{array}{c} \text{flux from droplet } k \\ \text{to droplet } k+1 \end{array} \sim \frac{V(h_{min}(P_{k+1})) - V(h_{min}(P_k))}{[X_{k+1} - \bar{w}(P_{k+1})] - [X_k + \bar{w}(P_k)]}$$

this then gives J_+^k and J_-^{k+1}.

Once the values $\{J_+^k\}_{k=1}^N$ and $\{J_-^k\}_{k=1}^N$ are
known, the right hand sides for the 2N
ODEs
$$\frac{dX^k}{dt} = \ldots$$
are known and
the approximation
is done.
$$\frac{dP^k}{dt} = \ldots$$

• = positions $X_k(t)$ as computed from solution of PDE

— = positions as computed from system of ODEs
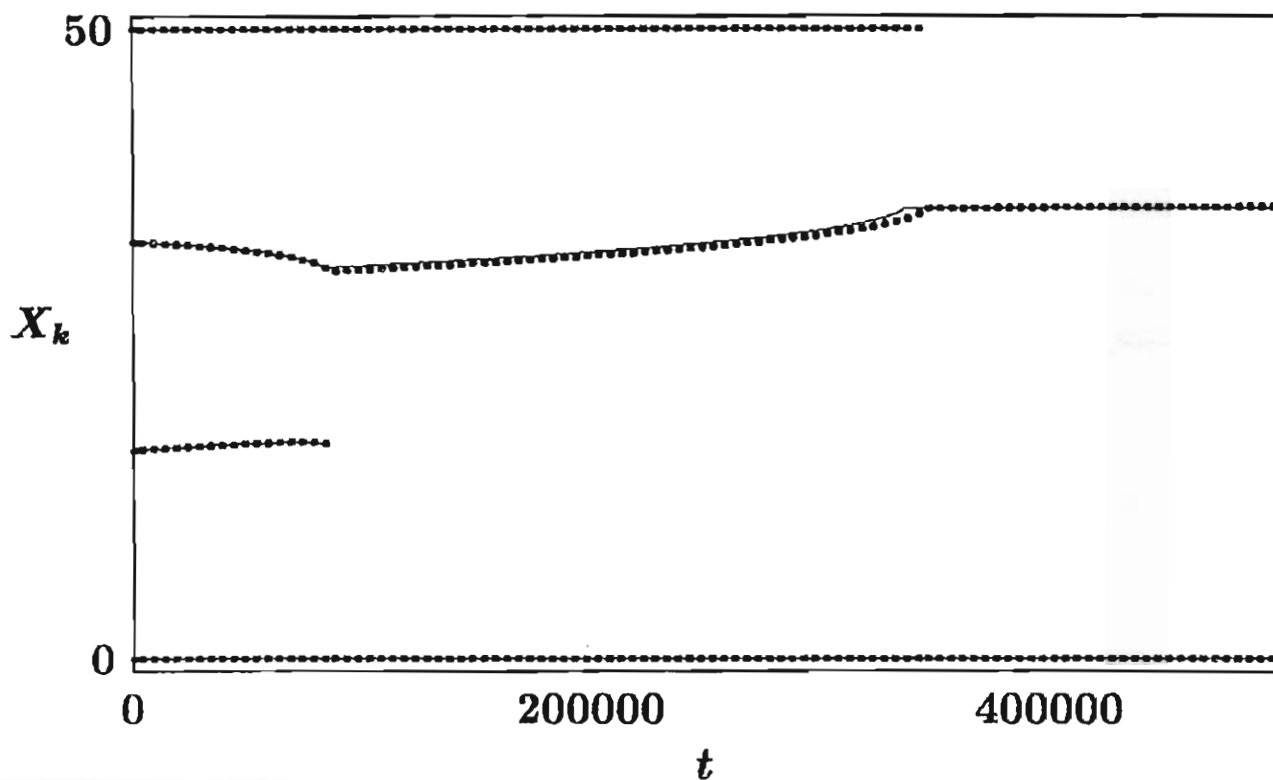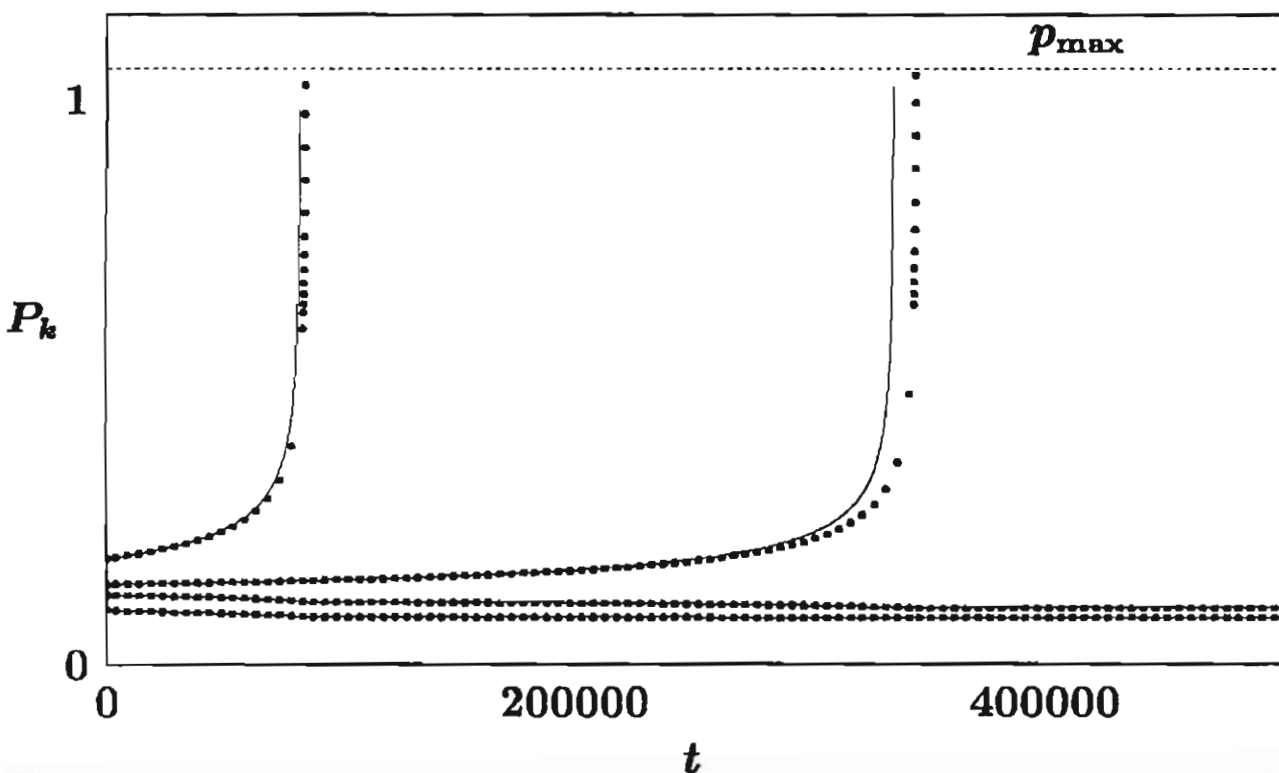
Glasner + Witelski '03

FIG. 11. Comparison of predictions for droplet positions $X_k(t)$ from the direct numerical solution of the PDE (1.11) (dots) and the ODE model of coarsening (5.9) (solid curves) for the problem shown in Fig. 8. The termination of the X_2 and X_4 branches occurs when those droplets collapse.

Glasner + Witelski '03

Note: The figure shows P_k on the vertical axis (with markings at 0 and 1, and a dashed line labeled p_{max}) versus t on the horizontal axis (0, 200000, 400000).
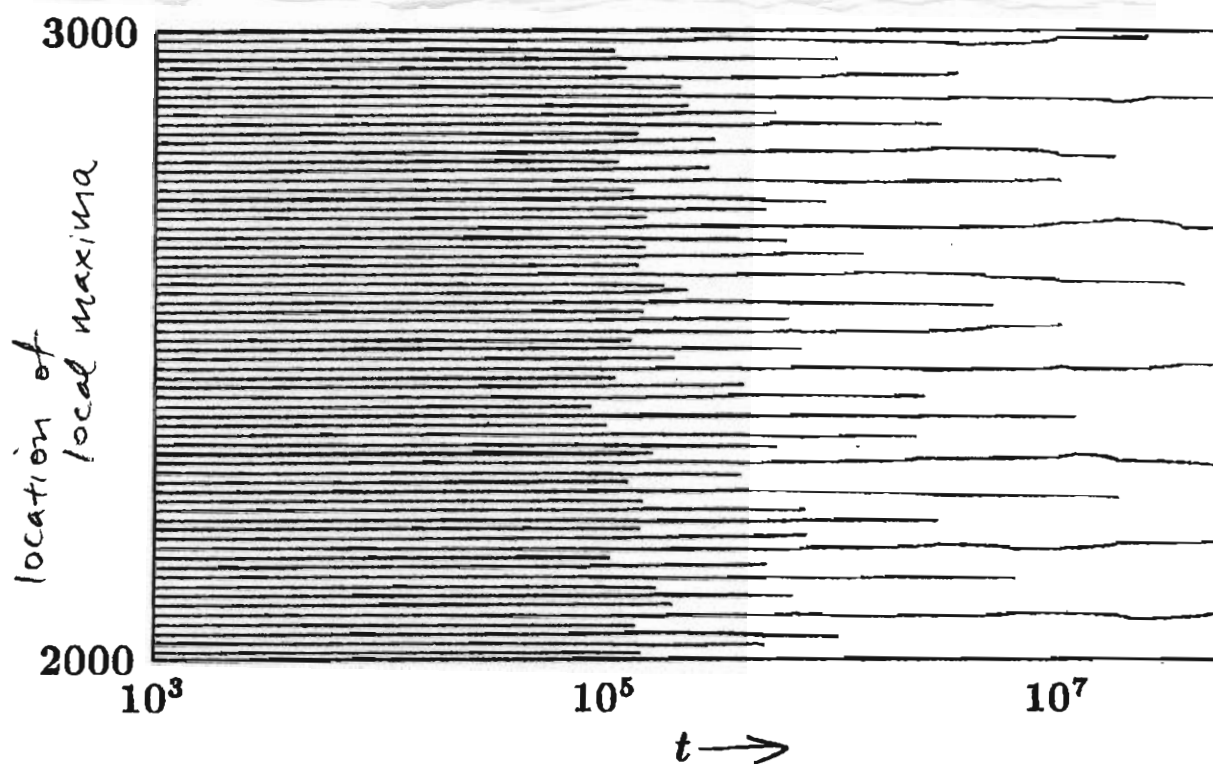
• = pressures of droplets as computed
from solutions of PDE

— = pressures as computed by system
of ODEs

Note: good agreement until pressures
large (i.e. until droplet in question
is small.)

coalescence $\Rightarrow \frac{\varepsilon}{l} \not\ll 1$ where $l =$ distance between
droplets.

$\Rightarrow$ PDE $\Rightarrow$ ODE reduction
fails.

The figure axes: vertical axis labeled "location of local maxima" ranging from 2000 to 3000; horizontal axis labeled $t \longrightarrow$ ranging from 10^3 to 10^7.

Glasner +
Witelski (2003)

Compute a solution of the PDE initial value
problem. From the solution, find the number
of droplets $N(t)$ at each time t.
Glasner + Witelski find

$$N(t) = O(t^{-2/5})$$

One can also find this $O(t^{-2/5})$ behaviour
from the reduced ODE model, further
demonstrating the usefulness of the
PDE $\Rightarrow$ ODE reduction.