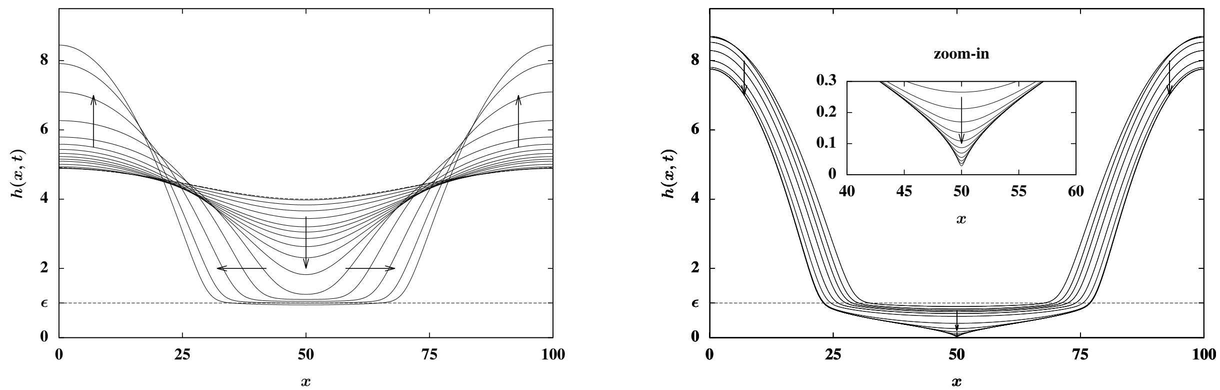
Finite-time rupture in thin films driven by non-conservative effects



Hangjie Ji (Duke Math → UCLA), Thomas Witelski (Duke Math)

- Self-similar rupture in unstable thin film equations for viscous flows
- Finite-time singularity formation in higher-order nonlinear PDEs
- Non-conservative models: physical motivation and mathematical generalizations
- Regimes for different classes of rupture dynamics
  – asymptotically self-similar and non-self-similar solutions

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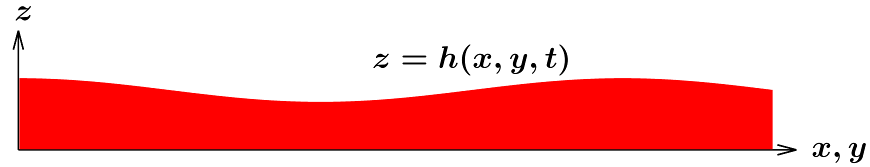
H. Ji and T. Witelski, Finite-time thin film rupture driven by modified evaporative loss, Physica D 342 (2017)

Classical lubrication models for thin viscous films



Fluid volume: $\quad 0 \le x, y \le L \qquad 0 \le z \le h(x, y, t) < H$

- Navier-Stokes eqns: $\{\vec{\mathbf{u}}, p\}$ for viscous incompressible flow
- Stokes eqns: Low Reynolds number flow limit, $\mathbf{Re} \to 0$
- Slender limit – aspect ratio $\delta = H/L \to 0$: $\{\vec{\mathbf{u}}, p\} \to h(x, y, t)$
- Boundary conditions at $z = 0$ (substrate) and $z = h(x, y, t)$ (free surface)

The Reynolds lubrication equation

$$\boxed{\frac{\partial h}{\partial t} = \nabla \cdot (m \nabla p)}$$

$h = h(x, y, t)$:	film height
$m = m(h)$:	mobility coeff
$p = p[h]$:	dynamic pressure
$\vec{\mathbf{J}} = -m\nabla p$:	mass flux

- $m(h) \sim h^n$: slippage effects, no-slip BC – $m(h) = h^3$
- $p = \Pi(h) - \nabla^2 h$: substrate wettability and surface tension

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[Oron, Davis, Bankoff 1997, Ockendon and Ockendon 1995, Craster and Matar 2009, ...]

Representing substrate wettability: The disjoining pressure

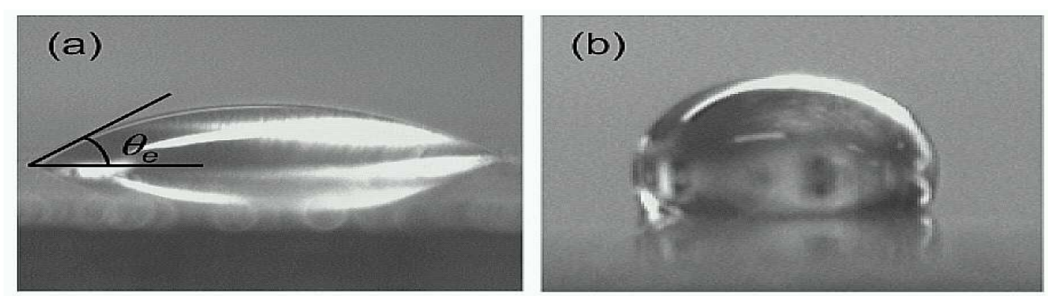
Fluid-solid intermolecular forces – physico-chemical properties of the solid and fluid. Wetting/non-wetting interactions described by a potential $U(h)$

$$p = \Pi(h) \equiv \frac{dU}{dh} \qquad \rightarrow \qquad \boxed{\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(h^3 \frac{\partial}{\partial x}\left[\Pi(h) - \frac{\partial^2 h}{\partial x^2}\right]\right)}$$

All $\Pi = O(h^{-3}) \to 0$ as $h \to 0$, weak influence for thicker films

(a) Hydrophilic materials: $\Pi \sim -1/h^3$
Wetting behavior – diffusive spreading of drops $\forall t \geq 0$

(b) Hydrophobic materials: $\Pi \sim +1/h^3$
Partially wetting – finite spreading of drops (finite support solns)
(*Non-wetting – large contact angle, strong repulsion, non-slender regime...*)



Dewetting: Instability of uniform coatings of viscous fluids on solid surfaces, Undesirable for many applications (painting, ...). Rich and complex dynamics...

[de Gennes 1985, Oron et al 1997, de Gennes et al book 2004, Craster and Matar 2009, Bonn et al 2009]

Simplest model for unstable films with hydrophobic effects

$$\Pi(h) = \frac{1}{3h^3} \qquad \Longrightarrow \qquad \frac{\partial h}{\partial t} = -\frac{\partial}{\partial x}\left(h^{-1}\frac{\partial h}{\partial x} + h^3\frac{\partial^3 h}{\partial x^3}\right)$$

Linear instability of flat films: $h(x,t) \sim \bar{h} + \delta \cos(\frac{k\pi x}{L})e^{\lambda t}$

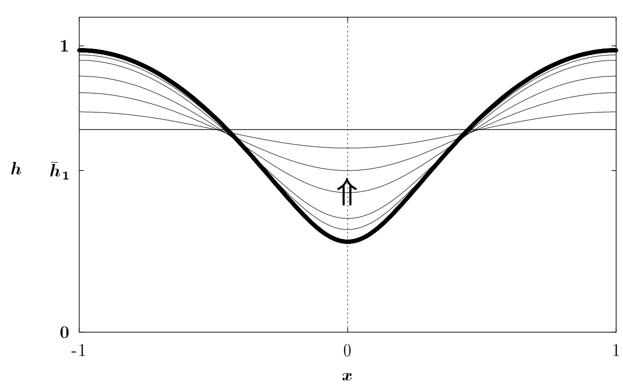
$$\lambda_k = \frac{1}{h_c^2}\left(\frac{1}{\bar{h}}k^2 - \frac{\bar{h}^3}{h_c^2}k^4\right) \qquad h_c = \sqrt{\frac{L}{\pi}} \quad \text{(critical thickness)}$$

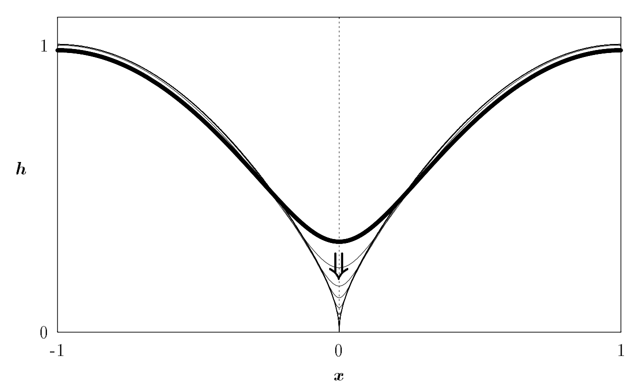
Bifurcation mean-thickness $\bar{h}$

$$\begin{cases} \bar{h} < \bar{h}_c & \text{Thin films are unstable} \\ \bar{h} > \bar{h}_c & \text{Thicker films stable to infinitesimal perturbations} \end{cases}$$

Bi-stable dynamics for $\bar{h} > \bar{h}_c$: IC $h_0(x) = $ (unstable equilibrium) $\pm\, \epsilon$

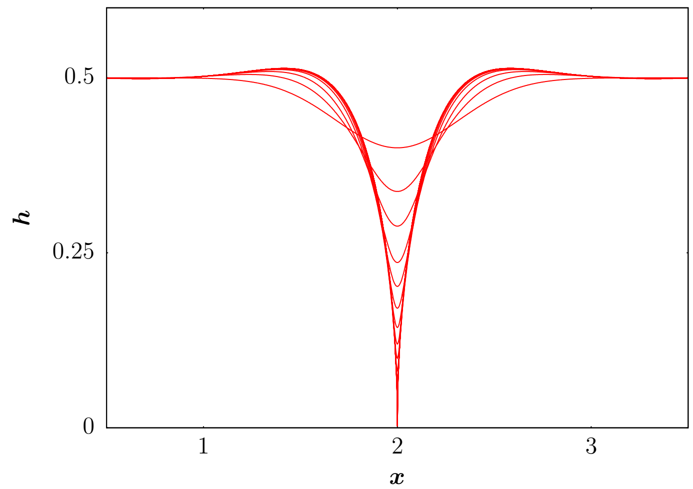
Relaxation: $h \to \bar{h}$ or Rupture: $h \to 0$





[Vrij 1970, Williams & Davis 1982, Laugesen & Pugh 2000]

Van der Waals driven thin film rupture: Finite-time rupture at position x_c



$$h(x_c, t) \to 0 \qquad \text{as} \quad t \to t_c$$

Scaling analysis of rupture in the PDE: let $\tau = t_c - t$

$$h = O(\tau^{1/5}) \to 0 \qquad x = O(\tau^{2/5}) \to 0 \qquad \text{as } \tau \to 0$$

1st-kind self-similar dynamics for formation of a localized singularity, $\Pi \to \infty$

$$h(x,t) = \tau^{1/5} H(\eta) \qquad \eta = (x - x_c)/\tau^{2/5}$$

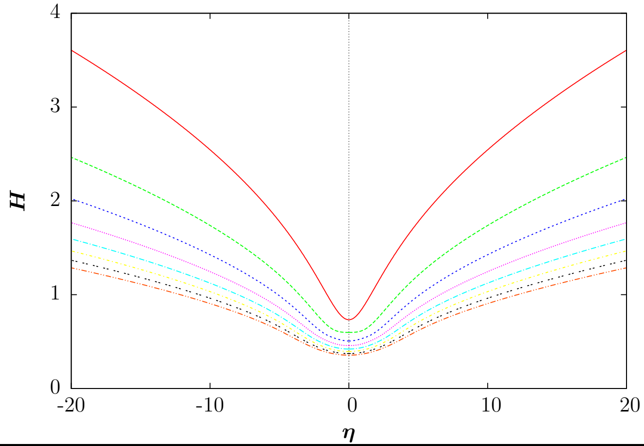
Similarity solution satisfies nonlinear ODE BVP

$$-\tfrac{1}{5}(H - 2\eta H') = -(H^{-1}H')' - (H^3 H''')' \qquad H(|\eta| \to \infty) \sim C|\eta|^{1/2}$$

[Zhang & Lister 1999, Witelski & Bernoff 2000] **[Barenblatt 1996, Eggers & Fontelos 2009, 2015]**

Van der Waals driven thin film rupture: solns of NL similarity ODE BVP

$$-\frac{1}{5}(H - 2\eta H') = -(H^{-1}H')' - (H^3 H''')' \qquad H(|\eta|\to \infty) \sim C|\eta|^{1/2}$$



Using numerical methods,
an ∞-sequence of solns found
$k = 1, 2, \cdots$: $C_k \searrow$

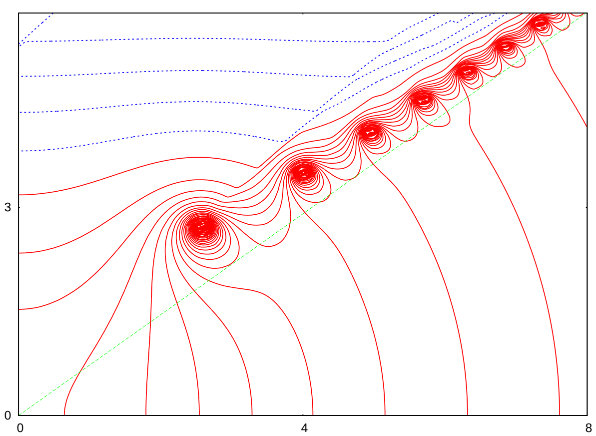
[Zhang & Lister 1999, Dallaston et al 2016]

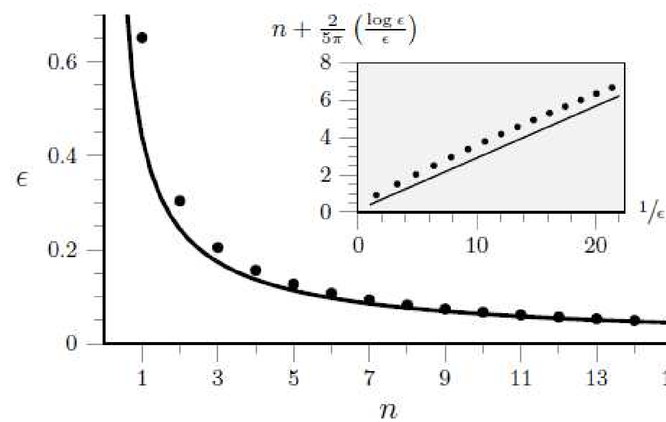
What determines the C_k's? **Exponential asymptotics** **[Chapman et al 2013]**

Let $H(\eta) = \epsilon^{2/5}\phi(z)$ with $\eta = \epsilon^{-1/5}z$ and $\epsilon = C^2 \to 0$

$$\frac{1}{5}(\phi - 2z\phi') - (\phi^{-1}\phi')' = \epsilon^2(\phi^3\phi''')' \qquad \phi(|z|\to \infty) \sim z^{1/2}$$

Analysis of Stokes phenomena from singularities of $\phi_0(z)$ in the complex plane



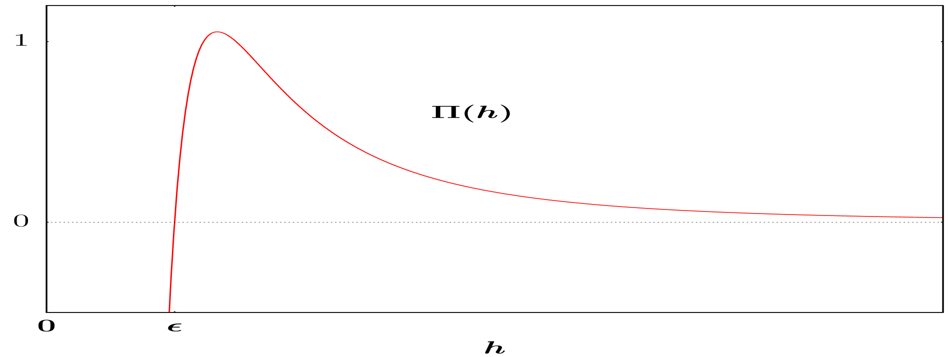


Numerical	Asymptotic
0.651071	0.437836
0.303993	0.243774
0.204949	0.173874
0.156492	0.136843
0.127355	0.113616
0.107764	0.097569
0.093626	0.085761
0.082911	0.076677
0.074422	0.069454
0.067625	0.063562
0.062005	0.058656
0.057287	0.054503
0.053277	0.050938
0.049800	0.047842
0.046760	0.045125

Continuation after rupture

- Solns with $\Pi = h^{-3}$ exist only up to first rupture, $0 \le t < t_c$.
- To continue solns to later times, must regularize the singularity and establish a uniform lower bound on h.
- Can be accomplished via a modified $\Pi(h)$ with balancing conjoining/disjoining effects **[Schwartz et al, Oron et al, ...]**

$$\Pi(h) = \frac{1}{\epsilon}\left(\frac{\epsilon}{h}\right)^3\left[1 - \frac{\epsilon}{h}\right]$$



  – $h(x,t) \ge h_{\min} = O(\epsilon) > 0$ ("precursor layer")
  – Ensures global existence of solns $\forall t \ge 0$ **[Bertozzi, Grün et al 2001]**
  – Widely-used, physically-motivated regularization

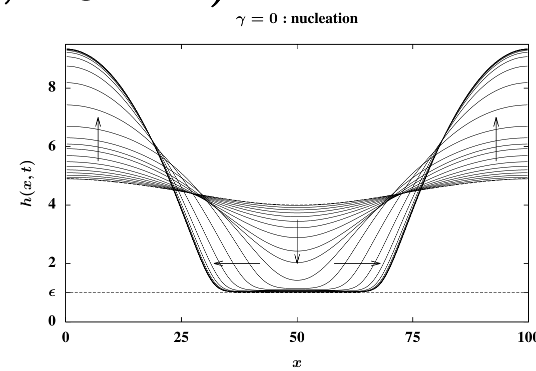
- Most studies of singularity formation and rupture in thin films are in the mass-conserving (non-volatile liquid) case
- Can lower-order non-conservative effects (e.g. evaporation) cause dramatic differences in the PDE dynamics?

Some non-conservative fourth-order PDE models

$$\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(\boxed{h^n}\frac{\partial}{\partial x}\left[\boxed{\Pi(h)} - \frac{\partial^2 h}{\partial x^2}\right]\right) - \boxed{J}$$

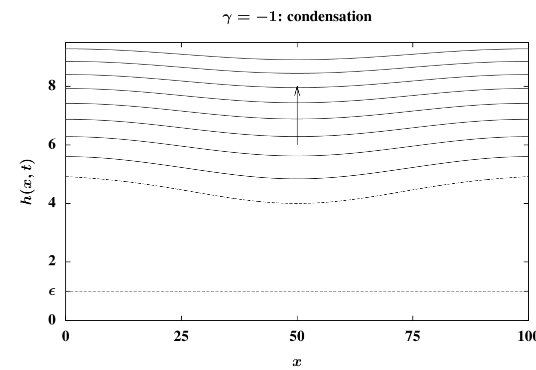
- **[Burelbach et al 1998, Oron et al 2001]** $(n = 3,$ full $\Pi, E_0 \lesseqgtr 0, K_0 > 0)$

$$J(h) = \frac{E_0}{h + K_0}$$



- **[Ajaev & Homsy 2001]** $(n = 3, \Pi = -1/h^3, \delta > 0)$

$$J(h) = \frac{E_0 - \delta(h_{xx} + h^{-3})}{h + K_0}$$



- **[Laugesen & Pugh 2000]** $(n, \Pi = h^m)$

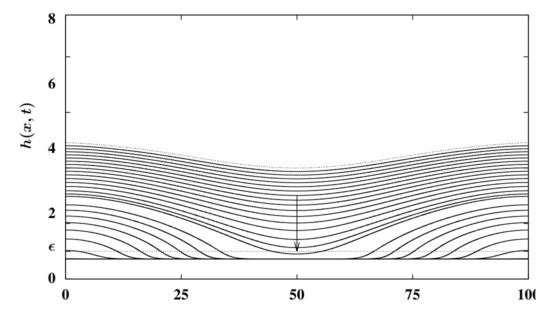
$$J(h) = \lambda h$$

- **[Galaktionov 2010]** $(n, \Pi = 0)$

$$J(h) = \lambda h^\rho$$

- **[Lindsay et al 2014+]** MEMS $(n = 0, \Pi = h)$

$$J(h) = \frac{\lambda}{h^2}\left(1 - \frac{\epsilon}{h}\right)$$



- Solid films, math biology, ...

If $|J|$ is small, yields a separation of timescales in dynamics...

Rupture in a generalized non-conservative Reynolds equation

$$\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(h^n \frac{\partial p}{\partial x}\right) + \frac{p}{h^m} \qquad p = -\left(\frac{1}{h^4} + \frac{\partial^2 h}{\partial x^2}\right)$$

- Pressure: surface tension and dominant hydrophilic term for $\Pi(h)$ for $h \to 0$ (should be stable and prevent rupture)
- Non-conservative flux: inspired by Ajaev's isothermal form, but with opposite sign (destabilizing). Params for physical form of evaporation are stabilizing.
- Generalized mobility coefficients h^n, h^m: inspired by **[Bertozzi and Pugh 2000]** – they studied finite-time blow-up ($h \to \infty$) in a long-wave unstable eqn

$$h_t = -(h^n h_{xxx})_x - (h^m h_x)_x$$

Destabilizing 2nd order term vs. regularizing 4th order term
Helpful for tracing/separating competing influences

- Here: explore if some form of lower order non-conservative effects can overcome conservative terms and drive finite-time free surface rupture.

Obtain a bifurcation diagram for dynamics with (n, m).

Global properties: conservative vs. non-conservative effects

$$\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(h^n \frac{\partial p}{\partial x}\right) + \frac{p}{h^m} \qquad p = -\left(\frac{1}{h^4} + \frac{\partial^2 h}{\partial x^2}\right)$$

- Evolution of fluid mass, $\mathcal{M} = \int_0^L h\,dx$

$$\frac{d\mathcal{M}}{dt} = \int_0^L \frac{p}{h^m}\,dx = m\int_0^L \frac{h_x^2}{h^{m+1}}\,dx + \int_0^L \frac{\Pi(h)}{h^m}\,dx$$

- Evolution of energy, $\mathcal{E} = \int_0^L \frac{1}{2}\left(\frac{\partial h}{\partial x}\right)^2 + U(h)\,dx \qquad \Pi(h) = \frac{dU}{dh}$

$$\frac{d\mathcal{E}}{dt} = -\int_0^L h^n \left(\frac{\partial p}{\partial x}\right)^2\,dx + \int_0^L \frac{p^2}{h^m}\,dx$$

  Not a monotone dissipating Lyapunov functional for this model (unlike the non-conservative/stabilizing [physical] case)

- Use local properties at $h_{\min}(t) = h(x_c, t) = \min_x h(x,t)$ to characterize the dynamics $\{\partial_{xx} h(x_c,t), \partial_t h(x_c,t)\}$

[U. Thiele, Thin film evolution from evaporating ... to epitaxial growth, J. Phys. Condens. Matter 2010]

1. Linear stability: perturbed flat films $h(x,t) = \bar{h}(t) + \delta e^{ikx} e^{\sigma(t)} + O(\delta^2)$

$$\boxed{\frac{\partial h}{\partial t} = -\frac{\partial}{\partial x}\left(h^n \frac{\partial}{\partial x}\left[\frac{1}{h^4} + \frac{\partial^2 h}{\partial x^2}\right]\right) - \frac{1}{h^m}\left[\frac{1}{h^4} + \frac{\partial^2 h}{\partial x^2}\right]}$$

$$O(1): \quad \frac{d\bar{h}}{dt} = -\bar{h}^{-(4+m)}$$

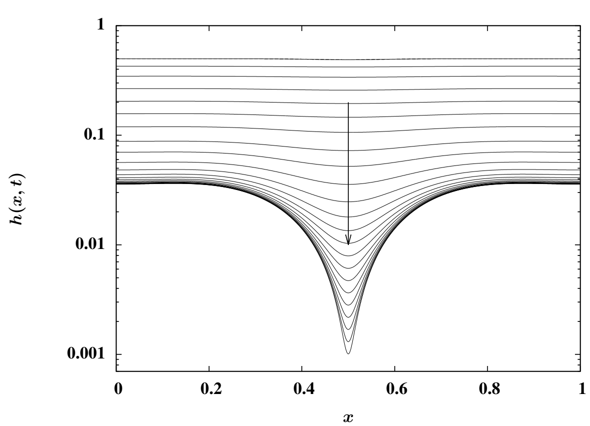
$$O(\delta): \quad \frac{d\sigma}{dt} = \left(k^2 \bar{h}^{-m} + (m+4)\bar{h}^{-(m+5)}\right) - \left(k^4 \bar{h}^n + 4k^2 \bar{h}^{n-5}\right)$$

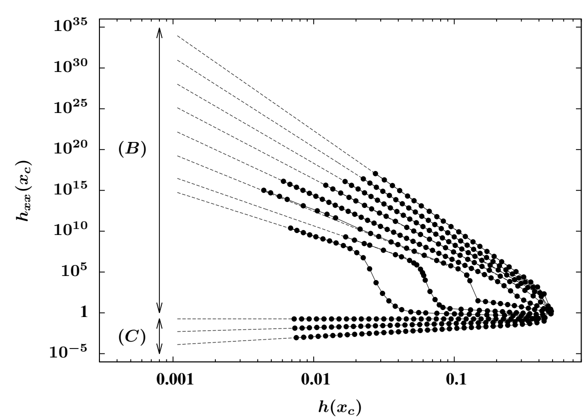
Flat film extinction $\bar{h}(t) \to 0$: finite time $(m > -5)$ vs. infinite time (exp/alg)

Growth of spatial perturbations: $\frac{d\sigma}{dt} > 0$ if $m > -4$ and $m + n > 0$

$$\begin{cases} h_{xx}(x_c, t) \sim C \exp\left(\frac{4k^2 \bar{h}^{m+n}}{m+n}\right) \bar{h}^{-(m+4)} \to 0 & m + n < 0 \\ h_{xx}(x_c, t) \sim C \bar{h}^{-(m+4)} \to \infty & m + n > 0 \end{cases}$$

For m near $m \geq -4$ perturbations grow slowly vs $\frac{d\bar{h}}{dt}$ before eventual transition





2. Localized rupture at (x_c, t_c): Observing finite-time self-similar solns?

$$h(x,t) \sim \tau^{\alpha} H(\eta) \qquad \tau = t_c - t \qquad \eta = \frac{x - x_c}{\tau^{\beta}}$$

Scaling behavior for observables at $h_{\min}(t)$ for $\tau \to 0$

$$\begin{aligned} h_{\min}(t) &= \tau^{\alpha} H(0) \\ \partial_t h_{\min}(t) &= -\alpha \tau^{\alpha-1} H(0) \\ \partial_{xx} h_{\min}(t) &= \tau^{\alpha-2\beta} H''(0) \end{aligned}$$

yields

$$|h_{\min,t}| = \alpha h_{\min}^{\mu} \qquad \mu = 1 - \frac{1}{\alpha}$$

$$\boxed{h_{\min,xx} = C h_{\min}^{\nu} \qquad \nu = 1 - \frac{2\beta}{\alpha}}$$

- A compact way for characterizing the dynamics
- Power-law scaling relation $\to$ self-similar behavior
- $\nu < 0 \implies$ curvature singularity at rupture, $h_{xx} \to \infty$ as $h \to 0$

The importance of numerical simulations...

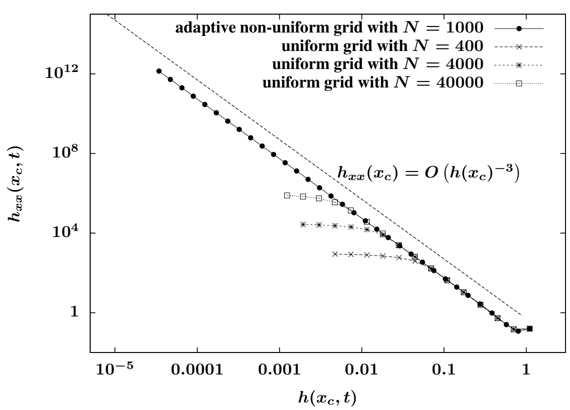
- In the absence of rigorous proofs, and expts, accurate numerical computations are essential for supporting conclusions from formal calculations
- Approach to singular behavior should be sustainable over a convincingly long dynamical regime to be distinguishable other transients
- Adaptive time-stepping and spatial regridding becomes necessary
- Splitting higher order PDE into first order systems is very useful

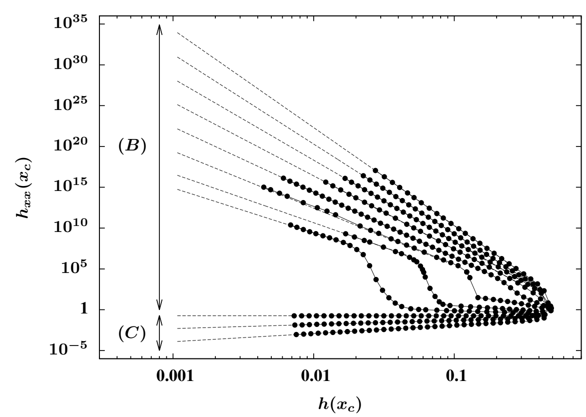
$$h_t = -(h^n(h^{-4} + h_{xx})_x)_x - h^{-m}(h^{-4} + h_{xx})$$

becomes

$$h_t + (h^n q)_x + h^{-m} p = 0, \qquad q = p_x, \qquad p = h^{-4} + s_x, \qquad s = h_x.$$

Keller box scheme, second order accurate in space...





[H.B. Keller, A new difference scheme for parabolic problems, 1971]

2. Seeking self-similar solns: Substitute $h = \tau^{\alpha} H(x/\tau^{\beta})$ into PDE

$$\frac{\partial h}{\partial t} = -\frac{\partial}{\partial x}\left(h^n \frac{\partial}{\partial x}\left[\frac{1}{h^4} + \frac{\partial^2 h}{\partial x^2}\right]\right) - \frac{1}{h^m}\left[\frac{1}{h^4} + \frac{\partial^2 h}{\partial x^2}\right]$$

becomes

$$\begin{aligned}\tau^{\alpha-1}\left(-\alpha H + \beta\eta H_\eta\right) = -\Big(&-4\tau^{(n-4)\alpha-2\beta}\left(H^{n-5}H_\eta\right)_\eta \\ &+ \tau^{(n+1)\alpha-4\beta}\left(H^n H_{\eta\eta\eta}\right)_\eta\Big) \\ &- \left(\tau^{-(4+m)\alpha}\frac{1}{H^{4+m}} + \tau^{(1-m)\alpha-2\beta}\frac{H_{\eta\eta}}{H^m}\right)\end{aligned}$$

- Not possible to balance all terms at once (no exact similarity solns)
- For $\tau \to 0$ use method of dominant balance[a] to determine distinguished limits giving ODEs for *asymptotically self-similar solns*
- Looks like lots of combinations possible, but there are only **two** *feasible distinguished limits* for finite-time rupture solns after eliminating ill-posed and spurious cases

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[a] Balance largest terms and confirm rest of terms are asymptotically smaller for $\tau \to 0$

2(a) Second-order similarity solutions: For $0 < m + n < 5$ and $m > -4$

The dominant balance is

$$\alpha H - \beta \eta H_\eta + 4\left(H^{n-5} H_\eta\right)_\eta - \frac{1}{H^{4+m}} = 0$$

with scaling parameters

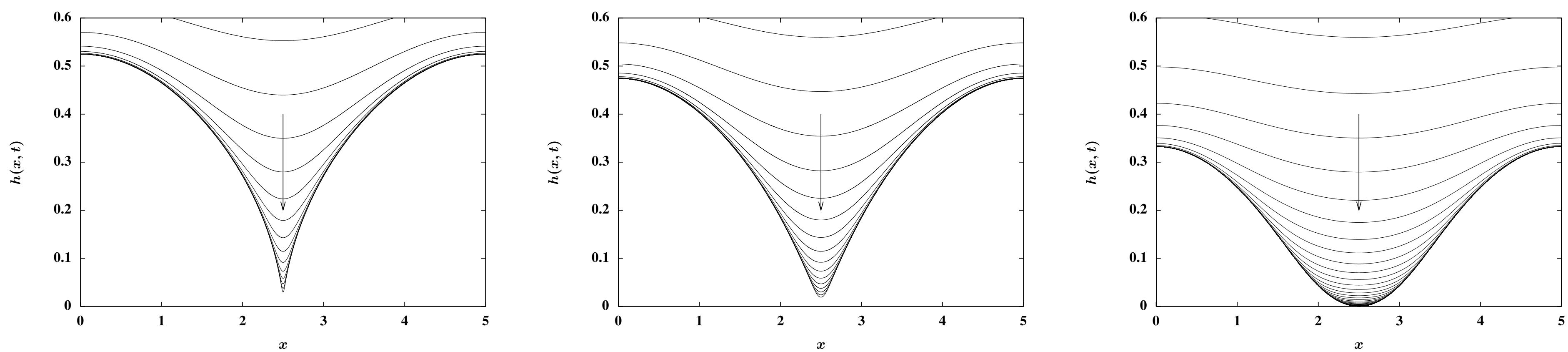
$$\alpha = \frac{1}{m+5} \qquad \beta = \frac{n+m}{2(m+5)}$$

Leading order reduced model: second-order diffusion eqn with singular absorption

$$\frac{\partial h}{\partial t} = 4\frac{\partial}{\partial x}\left(h^{n-5}\frac{\partial h}{\partial x}\right) - \frac{1}{h^{m+4}}$$

$h_{\mathbf{min},xx} = C h_{\mathbf{min}}^{\nu}$ with $\nu = 1 - n - m$

$-4 < \nu < 1 \implies$ can have rupture without a singularity in the curvature!



Rupture with various $H = O(|\eta|^{\alpha/\beta})$ far-fields ($m = 0$, n varies)

2(b) Fourth-order similarity solutions: For $m + n > 5$ and $m > -4$

The dominant balance is

$$-\alpha H + \beta \eta H_\eta + \frac{H_{\eta\eta}}{H^m} + (H^n H_{\eta\eta\eta})_\eta = 0$$

with scaling parameters

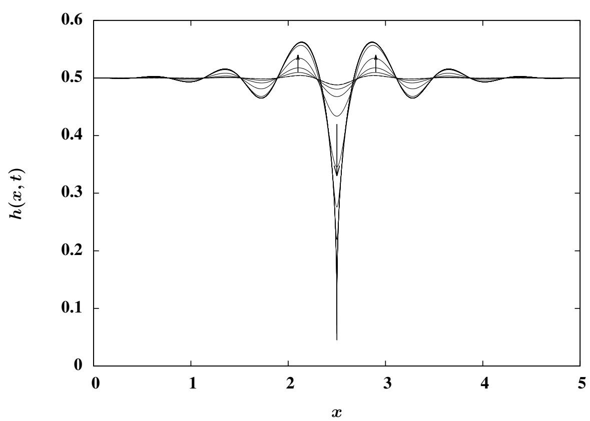
$$\alpha = \frac{1}{n + 2m} \qquad \beta = \frac{n + m}{2(n + 2m)}$$

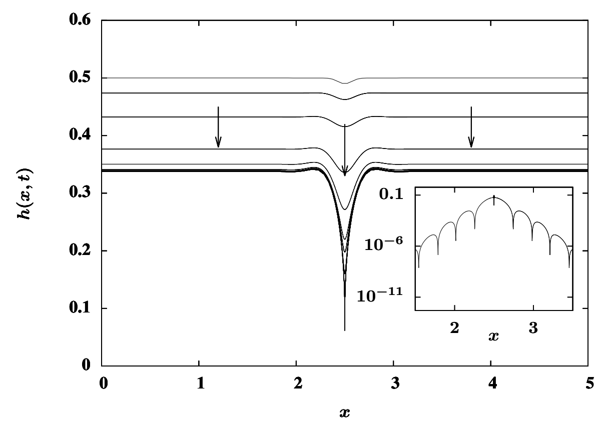
Leading order reduced model: non-conservative unstable 4th order

$$\frac{\partial h}{\partial t} = -\frac{\partial}{\partial x}\left(h^n \frac{\partial^3 h}{\partial x^3}\right) - \frac{1}{h^m}\frac{\partial^2 h}{\partial x^2},$$

$h_{\mathbf{min},xx} = C h_{\mathbf{min}}^{\nu}$ with $\nu = 1 - n - m$

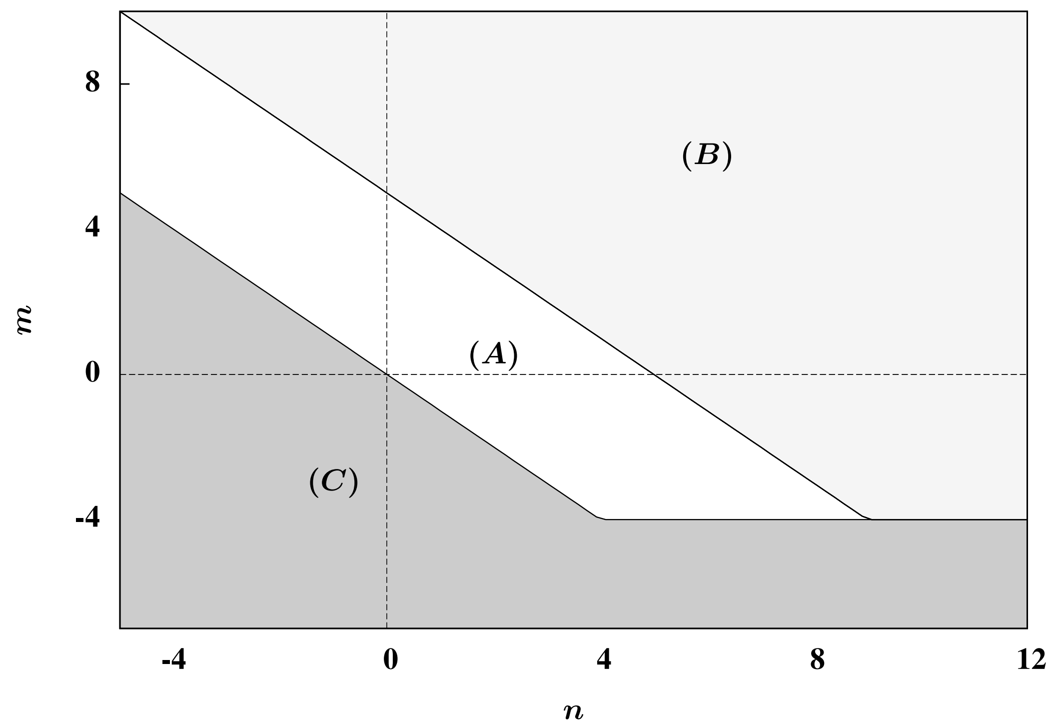
$\implies \nu < -4$ always have a curvature singularity





Notes: (1) locally nearly-conservative, (2) usual discrete family of $H(\eta)$ solns (first one is stable), and (3) can rupture for $n > 4$ despite **[Bernis & Friedman 1990]**

Bifurcation diagram (v1.0)



(A) Localized second-order self-similar rupture

(B) Localized fourth-order self-similar rupture

(C) Uniform-film thinning

But.... numerical simulations suggest region (A) is not quite right....

$$h_t = 4(h^{n-5}h_x)_x - h^{-m-4}$$

$n - 5 < 0$: fast diffusion case seems different than

$n - 5 > 0$: slow diffusion

2(d) Refined analysis: For Region (A) with $n > 5$

Restart the local analysis for (x_c, t_c) without the self-similar assumption.
Let $h(x,t) = ((m+5)v(x,\tau))^{1/(m+5)}$ then PDE becomes

$$\frac{\partial v}{\partial \tau} = \mathcal{N}[v]$$

Local expansion of $v(x,\tau)$

$$v(x,\tau) = v_0(\tau) + \tfrac{1}{2}v_2(\tau)X^2 + O(X^4) \qquad X = x - x_c$$

Solve coupled nonlinear ODEs for v_0, v_2 with $v_0 \to 0$ as $\tau \to 0$

$$\frac{dv_0}{d\tau} = 1 + E v_0^{2\beta-1} v_2 \qquad \frac{dv_2}{d\tau} = F v_0^{2\beta-2} v_2^2$$

Non-self-similar rupture solutions

For $n > 5$

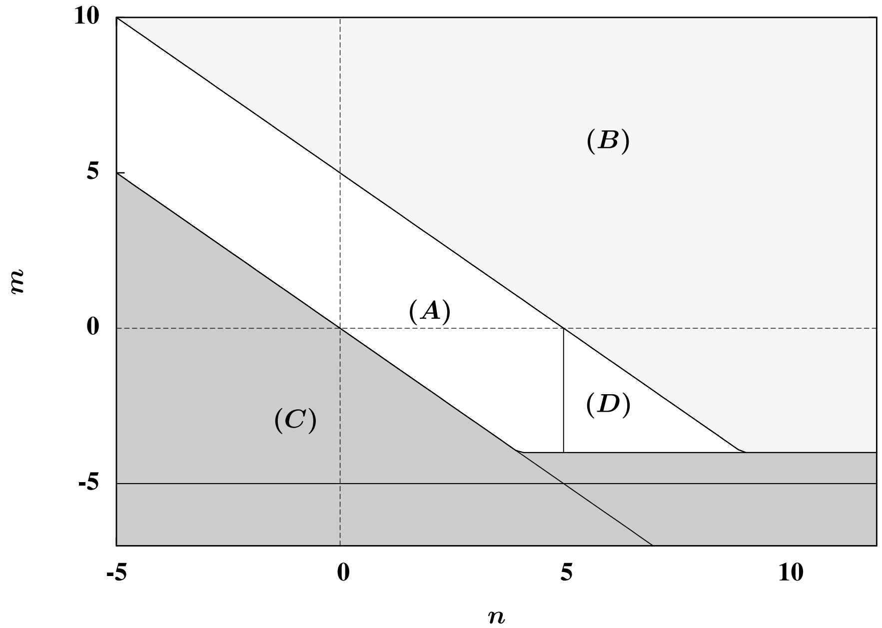
$$h(x,t) = \alpha^{-\alpha}(t_c - t)^{\alpha}\left(1 + D_2\frac{(x-x_c)^2}{(t_c-t)} + D_0(t_c-t)^{2\beta-1} + \cdots\right)$$

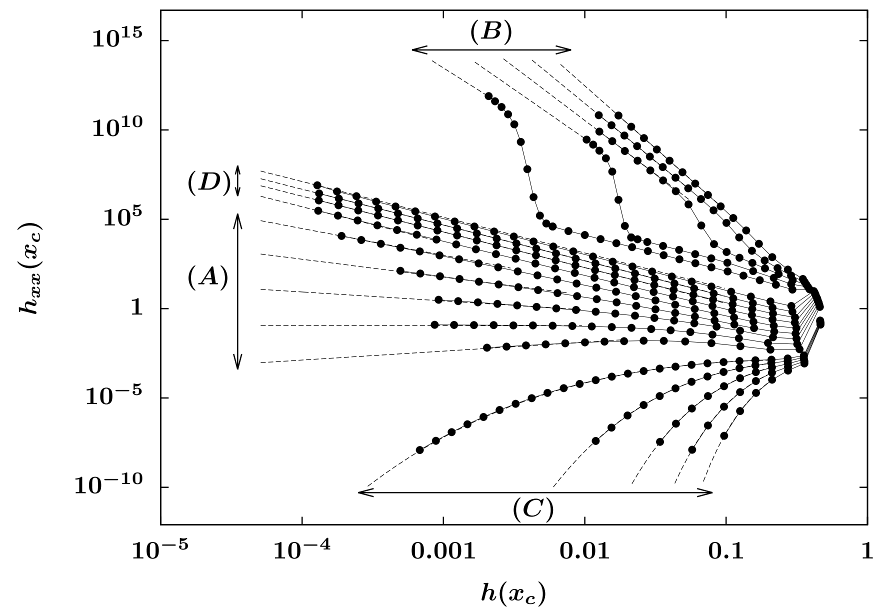
For $n = 5$

$$h(x,t) = \alpha^{-\alpha}(t_c - t)^{\alpha}\left(1 + \frac{\alpha E}{F|\ln{(t_c-t)}|} + \frac{\alpha(x-x_c)^2}{2F(t_c-t)|\ln{(t_c-t)}|} + \cdots\right)$$

[Guo, Pan, Ward, Touchdown... of a MEMS device, SIAM J. Appl. Math 2005]

Bifurcation diagram (refined)





$h_{\min,xx} = Ch_{\min}^{\nu}$ with $\nu = 1 - 2\beta/\alpha$

Series of numerical simulations with single IC, $m = -2$ fixed, range of n values

(A) Localized second-order self-similar rupture, $-2 < \nu < 1$

(B) Localized fourth-order self-similar rupture, $\nu < -2$

(C) Uniform-film thinning (finite-time or infinite time), $h_{\min,xx} \sim$ exp decay

(D) Non-self-similar, but looks "$\beta = \frac{1}{2}$"-ish, $\nu \sim -2$