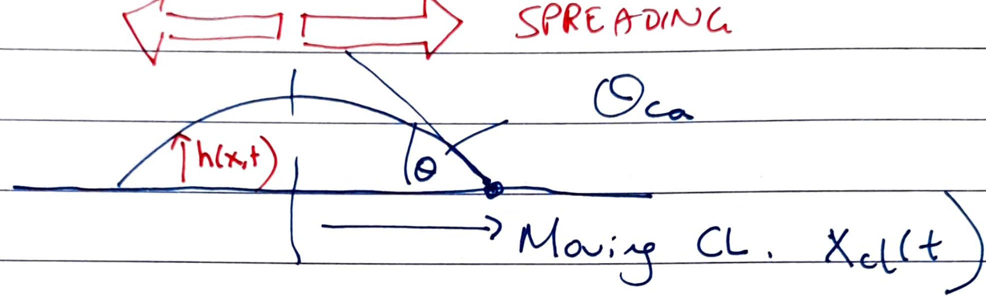
Title: New regularization of the contact-line singularity in droplet spreading

Joint work with K.E.P.

Date: Wed 24/07/2024 U.W.

1. Introduction – Theory of contact-line (CL) motion in the longwave / lubrication limit.



$\theta_{ca}(t)$ – dynamic contact angle (CA)

Lubrication Theory / Stokes flow: $\theta_{ca} << 1$.

N.S. equations simplify drastically:

$$(1) \quad \frac{\partial h}{\partial t} + \frac{\gamma}{3\mu}\frac{\partial}{\partial x}\left(h^3 \frac{\partial^3 h}{\partial x^3}\right) = 0.$$

$\frac{\gamma}{3\mu} \to 1$ in a new scaling; μ = dynamic viscosity.

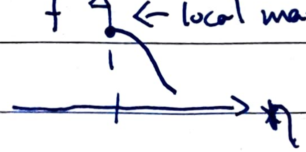
Moving BC: Attempt a similarity sl^{n} of (1) with n instead of 3: $h_t + \partial_x(h^n h_{xxx}) = 0$, and $n < 3$:

$$h(x,t) = t^a f\left(\frac{x}{t^a}\right) \qquad a = \frac{1}{n+4}$$

Obtain:

$$f^n f''' = \frac{nf}{n+4}$$

B.C. $f(0) = 1$, $f'(0) = 0$, $f''(0) = -\mu < 0$. different μ



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Rough Work

Contents of talk :

1. Introduction
2. Physics of small-param regularization.
3. Singular Solutions
4. Characterization of Solutions
   - Numerical
   - Existence theory
5. Partial Wetting
6. Conclusions

Adjust μ such that $f = f' = 0$ @ $\eta = \eta_0$.
This gives
$$x_0 = \eta_0 t^{\frac{1}{n+4}}$$
and hence, a moving C.L.

This works for $n \leq 3$

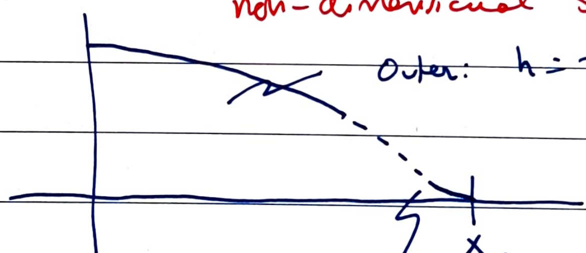
A problem arises when $n > 3$. Solutions (classical)

i) Navier slip length $u(x, y=0, t) = \lambda \left(\frac{\partial u}{\partial y}\right)_{y=0}$.
This gives a regularized TFE:

(2) $$\frac{\partial h}{\partial t} + \frac{\partial}{\partial x}\left[(h^3 + \lambda h^2)\frac{\partial^3 h}{\partial x^3}\right] = 0.$$

non-dimensional slip length

Sketch:



Inner: $\frac{\partial h}{\partial t} + \lambda \frac{\partial}{\partial x}\left[h^2 \frac{\partial^3 h}{\partial x^3}\right] = 0.$

Matching: $$\left(\frac{\partial h}{\partial x}\right)^3\Bigg|_{x=x_m} = \frac{dx_m}{dt} \ln\left(\frac{x_m}{\lambda b}\right)$$

b = constant.

Check: $h = t^{-a} h\left(\frac{x}{t^a}\right)$ in LHS, $a = 1/7$

$$\left(\frac{\partial h}{\partial x}\right)^3 = t^{-6/7} h'(x/t^a)$$

(3) $$\left|h'\left(\frac{x_m}{t^a}\right)\right|^3 = C t^{6/7} \frac{dx_m}{dt} + \text{log. correction}$$

constant.

$x_m \sim t^{1/7}$, $\frac{dx_m}{dt} = t^{-6/7}$

$$t^{6/7}\frac{dx_m}{dt} = \text{const.}$$

Const. = const. $\Rightarrow$ Eq. (3) is satisfied ∎

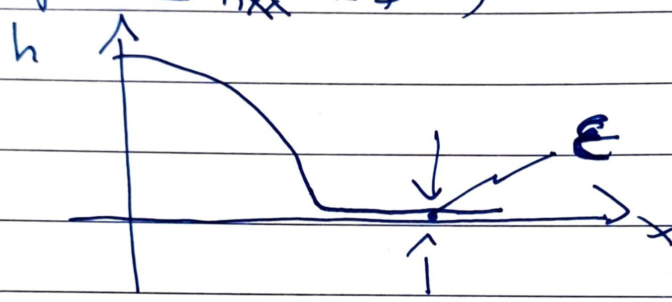
$$\boxed{x_m \sim t^{1/7}} \quad \text{TANNER'S LAW (2D)} \qquad (4)$$

Remark $x_m \sim t^{1/10}$ in 3D axisymmetric.

ii) Precursor-Film Modelling $h_t = -\partial_x(h^3 \partial_x P)$,
where

$$P = -h_{xx} + \Phi(h)$$

Van der Waals Potential



Drawbacks:

i) has a stress singularity @ x_m: h and h' are Ok @ $x = x_m$ but h'' is not Ok.

ii) Precursor film... miles out ??

New Solution:

Introduce a smoothened height:

$$\bar{h}(x,t) = \int_{-\infty}^{\infty} K(x-y,\alpha)\, h(y,t)\, dy$$

Taxonomy of different methods:

Method	Lengthscale
Navier slip	Slip length λ
Potential f$^{\underline{N}}$	Precursor film thickness $\mathcal{E}$
New	α

Use $\bar{h}$

Idea (somehow): $\mathcal{E}[\bar{h}] = \gamma \int_{-s/2}^{s/2} \sqrt{1+\bar{h}_x^2}\, dx$ is the interfacial energy. Go with small gradients (valid in lubrication theory):

$$\mathcal{E}[\bar{h}] = \frac{\gamma}{2} \int_{-s/2}^{s/2} |\partial_x \bar{h}|^2 dx$$

Take $S \to \infty$. Identity $\begin{cases} h = \text{"true height"} \\ \bar{h} = \text{"fuzzy height"} \end{cases}$

$$L[h, \bar{h}] = \frac{\gamma}{2} \int_{-\infty}^{\infty} |\partial_x \bar{h}|^2 dx + \text{PENALTY}$$

$$\text{PENALTY} = \frac{\gamma}{2\alpha^2} \int_{-\infty}^{\infty} |h - \bar{h}|^2 dx$$

Require $\frac{\delta L}{\delta \bar{h}} = 0 \Rightarrow -\gamma \bar{h}_{xx} - \frac{\gamma}{\alpha^2}(h - \bar{h}) = 0$

$$\Longrightarrow \quad (1 - \alpha^2 \partial_{xx})\bar{h} = h \qquad (5)$$

GRADIENT DESCENT DYNAMICS:

$$\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(h M(h, \bar{h}) \frac{\partial}{\partial x} \frac{\delta L}{\delta h} \right);$$

$M(h, \bar{h})$ is the mobility. This fulfils:

$$\frac{d\mathcal{E}}{dt} \leq 0, \quad \frac{d}{dt} \int h\, dx = 0.$$

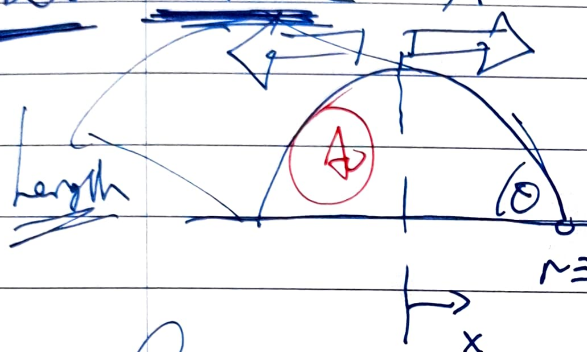
Note: $\frac{\delta L}{\delta h} = \frac{\gamma}{\sigma^2}(h - \bar{h}) \overset{Eq(5)}{=} -\gamma \bar{h}_{xx}$

So the PDE of interest is:

$$(6) \quad \frac{\partial h}{\partial t} + \frac{\partial}{\partial x}\left(h M(h,\bar{h}) \, \gamma \frac{\partial}{\partial x} \bar{h}_{xx} \right) = 0$$

Eq (6) is the Geometric Thin Film Equation.

2. Interlude: A note about the small lengthscale



- Slow spreading
- Quasi-static approx

Constant area is A_0. Quasi-static approx: treat droplet as spherical cap:

$$h_*(x) = \frac{3A_0}{4r^3}(r^2 - x^2).$$

Curvature: $\kappa = h_*'' = -\frac{3}{2}\frac{A_0}{r^3}$

Contact angle: $\tan\theta = -h_*'\big|_{x=r}$

$$\boxed{\tan\theta \simeq \theta = \frac{3}{2} A_0/r^2}$$

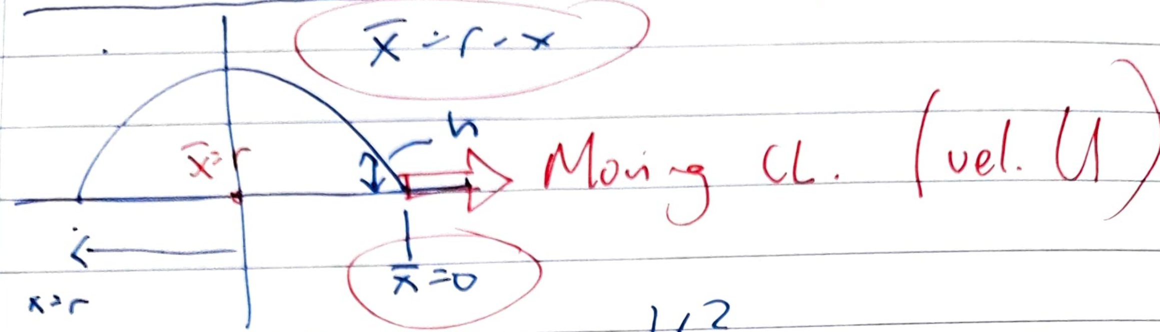
Surface energy: $p = -\gamma\kappa = \frac{3}{2}\frac{\gamma A_0}{r^3}$

$p = \text{Energy}/\text{Vol.} = \frac{\text{Energy}}{A_0 \cdot \text{Length}}$

$$\frac{d}{dt}\left(\frac{\text{Energy}}{\text{Length}}\right) = \frac{3}{2}\gamma A_0^2 \frac{d}{dt} r^{-3}$$

$$= -{}_5\,\frac{9}{2}\gamma\left(A_0^2/r^4\right)\dot{r}$$

Viscous dissipations — needed for the energy balance.



$$\varepsilon = \eta \left(\frac{\partial u}{\partial z}\right)^2 = \eta \frac{U^2}{h^2}$$

$$\frac{d}{dt}\left(\frac{\text{Energy}}{\text{Length}}\right) = 2\int_{\cancel{\bar{x}=0}\ L_*}^{r} \varepsilon\, h(\bar{x})\, d\bar{x}$$

$$= 2\eta U^2 \int_{L_*}^{r} \frac{1}{h^2}\, h\, d\bar{x}$$

$$= 2\eta U^2 \int_{L_*}^{r} \frac{1}{h}\, d\bar{x}$$

$h \simeq \theta \bar{x}$ near the C.L. (not the outer sl^n).

$$\Rightarrow h = \frac{3}{2}\frac{A_0}{r^2}\bar{x}$$

$$\Rightarrow \frac{d}{dt}\left(\frac{\text{Energy}}{\text{Length}}\right) = \frac{2\eta U^2 \cdot 2r^2}{3A_0}\int_{L_*}^{r} \frac{1}{\bar{x}}\, d\bar{x}$$

$$= \frac{4}{3}\frac{\eta}{A_0} U^2 r^2 \ln\left(\frac{r}{L_*}\right)$$

Equate expressions: $(U = \dot{r})$

$$-\cancel{\gamma}\dot{r}r^{-4} \propto \eta r^2 \dot{r}^{\cancel{2}}\left[-\ln L_* + \ln r\right]$$

$$\Rightarrow \quad \left| -r^{-6} \propto \frac{\eta}{\gamma}\dot{r}\ln\left(\frac{r}{L_*}\right)\right.$$

If I re-write this as.

$r^{-6} \propto \eta \dot{r} \ln L_x$ — log. correction

I recover Tanner's Law.

Back to our regularized Thin-Film Equation, which I now call the Geometric Thin Film Equation because of its connections with

3. Differential Geometry. Trivially, we can identify $h\,dx$ as a one-form density, and the Thin-film Equation can be written as:

$$(\partial_t + \mathcal{L}_u)\, h\,dx = 0,$$

where $u = -h M(h,\bar{h}) \frac{\partial}{\partial x}\frac{\delta L}{\delta h}$. This is a simple example of a more general equation.

Most general case:

$$(\partial_t + \mathcal{L}_u)\, T = 0,$$

where

$$T : M \longrightarrow V^{\otimes p} \otimes (V^*)^{\otimes q}$$

- M = manifold/configuration space
- TM = tangent bundle

Examples

i) $T = \underline{m}\cdot d\underline{x} \otimes dV$

$$\frac{\partial \underline{m}}{\partial t} + \underline{u}\cdot\underline{\nabla}\,\underline{m} + (\nabla \underline{u})^T\cdot \underline{m} + (\nabla\cdot\underline{u})\,\underline{m} = 0$$

EP Diff Equation.

ii) $\underline{M} = (m(x,t), 0, 0)$ gives $m_t + (um)_x + u_x m = 0$

SINGULAR SOLUTIONS

With $m = (1-\alpha^2\partial_{xx})u$ we get the Camassa–Holm (CH) equation. Why bring this up? CH equation admits "singular" or "particle" solutions:

$$m^{(N)}(x,t) = \sum_{i=1}^{N} p_i(t)\,\delta(x - X_i(t))$$

$$u^N(x,t) = \sum p_i(t)\, G(x - X_i(t))$$

Helmholtz kernel

Positions

Momenta

- Set of ODEs for $X_i(t)$'s and $p_i(t)$'s
- PDE $\longrightarrow$ ODE (Hamiltonian system).

Question: Can we get singular solutions for the Geometric Thin Film Equation G-TFE?

Yes – But we need a new kernel function.

Higher-order smoothing:

$$\ell(h) = \frac{1}{2}\gamma \int_{-\infty}^{\infty} \partial_x h \cdot \partial_x \bar{h}\, dx$$

$$\bar{h} = K * K * h \quad (\text{Two applications of Helmholtz smoothing})$$

$$\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(h M \frac{\partial}{\partial x}\frac{\delta \ell}{\delta h}\right)$$

$$\Rightarrow \boxed{\frac{\partial h}{\partial t} = -\frac{\partial}{\partial x}\left(h M \frac{\partial}{\partial x}\partial_{xx}\bar{h}\right)} \quad (7)$$

Another key trick: Make M a function of $\bar{h}$ and not h.

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First open question — Can we derive (7) directly from Physics — without introducing smoothing in an ad-hoc fashion?

More on singular solutions:

It's helpful to view the singular solutions as an approximation to the $s^{\underline{n}}$ of the PDE.

- Arbitrary I.C. $h^0(x)$, compactly supported on $(-L, L)$.
- $x_i(t=0) = x_i^0 = \left(i - \frac{N}{2}\right)\frac{2L}{N}$, $i = 1, 2, \ldots, N$ "Δx"
- Weights $w_i = h^0(x_i^0)\left(2L/N\right)$

Proposed approx. $s^{\underline{n}}$:

$$h^N(x,t) = \sum_{i=1}^{N} w_i\, \delta(x - x_i(t)) \quad t > 0.$$

__Exercise__: Sub into G-TFE / Eq. (7) with $M = h^2$.

Test w.r.t. smooth test function $\phi(x)$. __Result__:

$$\frac{dx_i}{dt} = V_i(x_1, \ldots, x_N), \qquad (8)$$

$$V_i(x_1, \ldots, x_N) = \left[h^2 \partial_{xxx} h\right]_{x = x_i}$$

→

Remarks about (8):

- "bar" means double Helmholtz
- $\partial_{xxxx} \bar{h}$ is a δ function.
- $\partial_{xxx} \bar{h}$ is a jump
- So the RHS of (8) is continuous except at ~~where~~ jumps.
- Jumps occur when $X_i(t) = X_j(t)$ for some i and j $(i \neq j)$.
- Try to stay away from such crossings.

A major result of our work so far is a no-crossing theorem, which was proved by KEP.

Theorem (No Crossing): If $X_1^0 < X_2^0 < \dots < X_N^0$, then $X_1(t) < X_2(t) < \dots < X_N(t)$ $\forall t > 0$.

Proof: Based on dynamical systems arguments. Eq. (8) can be re-written as:

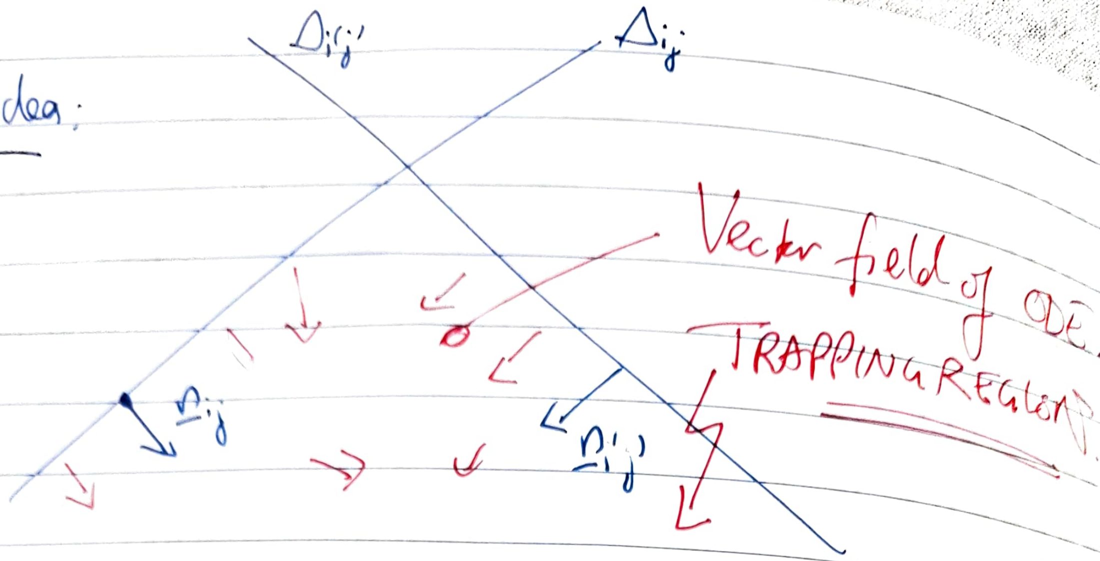
$$\frac{d}{dt}\begin{pmatrix} X_1 \\ \vdots \\ X_N \end{pmatrix} = \begin{pmatrix} V_1(X_1, \dots, X_N) \\ \vdots \\ V_N(X_1, \dots, X_N) \end{pmatrix} \leftarrow \text{vector field in } \mathbb{R}^n.$$

Let $\Delta_{ij} = \{ \underline{x} \in \mathbb{R}^n \mid X_i = X_j \}$ for some i and some j $(i \neq j)$

$\Delta = \bigcup_{i \neq j} \Delta_{ij}$ = set of all crossings.

To show: $\underline{X}(t) \notin \Delta$ $\forall t > 0$.

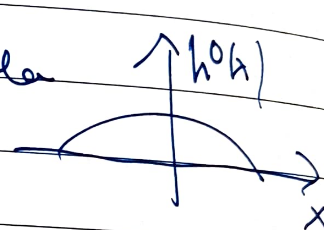
Idea:



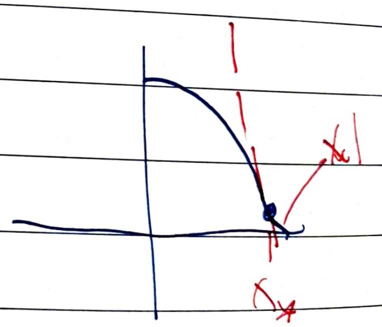
4. Characterization of Solutions
- Numerical
- Existence Theory

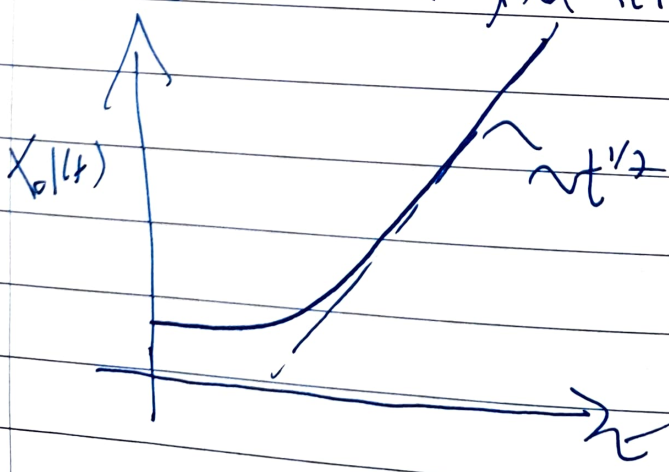
Numerical Solutions
- Implicit Euler, Central Differences
- Particle Solutions, Large N.

Initial condition: Spherical ~~cap~~ parabola



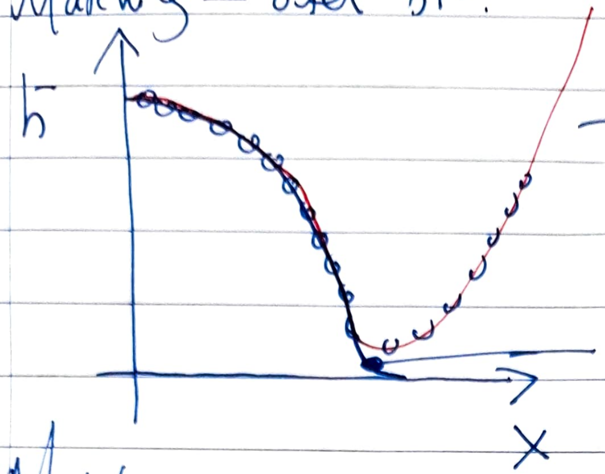
- Spreading well captured
- $x_*(t) = \arg\max_x \left[-\bar{h}(x,t)\right]$
- Track back and find x_{cl}





Tanner's law is recovered from the numerics.

Matching — outer sl^n.

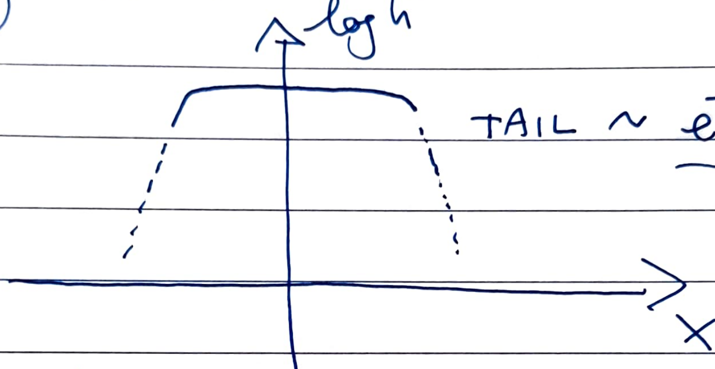


— $f(\eta)$ from $f^2 f''' = \frac{\eta f}{7}$.

$\eta = x/t^a$.

o — TPE (numerics)

Matching — inner



TAIL $\sim e^{-|x-x_c|/a}$.

Same sl^{n}s can be generated using particle method.

- No finite-difference grid required
- "Particles" tend to accumulate in regions of high interfacial curvature, reflecting tendency of method to mimic AMR, without the comp. overhead of that method.
- Error of F.D. method: $\mathcal{E}(\Delta x) = \|\bar{h}_{\Delta x} - \bar{h}_{\Delta x/2}\|_{L^1}$ with $\mathcal{E}(\Delta x) \le C \cdot \Delta x^2$.
- If we let $\Delta x = 2L/N$ in the particle method, then $\mathcal{E}(\Delta x)$ is $O(\Delta x^2)$ in the particle method also. $\longrightarrow$

- Intriguingly, the particle is $O(N^2)$ in terms of its complexity as a numerical algorithm.
- But by using the no-crossing theorem, a fast particle method can be created, which is $O(N \log N)$. This idea was first introduced by Camassa for the CH equation.

We also look at the rigorous convergence of the particle sl^ns (with R. Smith).

The starting-point here is to treat solutions of the G-TFE as elements of $M^+(\mathbb{R})$. This is the set of all positive Radon measures on $\mathbb{R}$.

Radon measures in this context are linear functionals on the space $C_0(\mathbb{R})$, that is, continuous functions that vanish at infinity

So, if $\mu \in M(\mathbb{R})$, it can be identified as a linear functional:

$$\mu(f) = \int f \, d\mu \quad \forall f \in C_0(\mathbb{R}).$$

In this way, we have the identification,

$$M(\mathbb{R}) = \left(C_0(\mathbb{R})\right)^*.$$

We obtain a norm on $M(\mathbb{R})$:

$$\|\mu\|_2 = \sup\left\{ \mu(f) \,\middle|\, f \in B_{C_0(\mathbb{R})} \right\}$$

Examples. $\mu = \sum_{i=1}^{N} w_i \delta_{x_i}$, or

$\mu = g(x)\,dx$, where g is itself in $C_0(\mathbb{R})$.
In the first case, if $w_i \geq 0$ for each i, then $\mu \in M^+(\mathbb{R})$.

In this way, we see that the particle solution

$$\mu_N = \sum_{i=1}^{N} w_i \delta_{x_i(t)}$$

of ~~the~~ g-TFE is in $M^+(\mathbb{R})$.

In the works with R. Smith, we have shown convergence: There exists a $\mu \in M^+(\mathbb{R})$ s.t.

$$\mu_N \xrightarrow{*} \mu \quad \text{as } N \to \infty$$

In other words,

$$\int f \, d\mu_N \to \int f \, d\mu$$

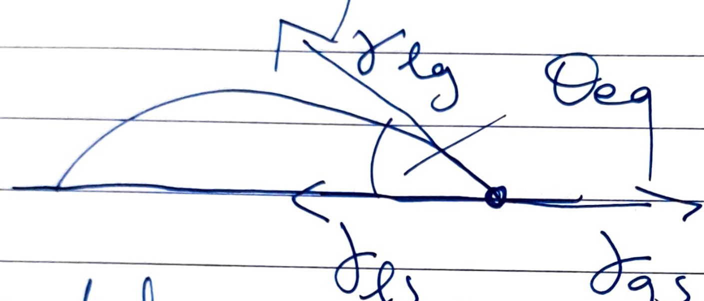
for all suitable test functions f.

This result is essentially a compactness result:
- μ_N bounded
- μ_N Lipschitz in the t-variable.

Hence, a convergent subsequence can be extracted.

5. Partial wetting. In the last part of the talk, I deal with partial wetting. It's a best effort, quite possibly incomplete.

Partial wetting: Spreading goes on and on and then... stops at equilibrium.



Force balance: $\gamma_{lg}\cos\theta + \gamma_{ls} = \gamma_{gs}$

$$\Rightarrow \boxed{\cos\theta_{eq} = \frac{\gamma_{gs}-\gamma_{ls}}{\gamma_{lg}}} \quad (9)$$

Laplace-Young

Idea for novel (regularized) treatment of partial wetting — go back to energy functional (prior to regularization):

$$\mathcal{E} = \gamma_{lg}\int_{-r}^{r}\sqrt{1+h_x^2}\,dx + \underbrace{2r}_{\text{droplet footprint}}\gamma_{ls} + \gamma_{gs}(S-2r)$$

$$\simeq \tfrac{1}{2}\gamma_{lg}\int_{-r}^{r} h_x^2 + 2r\left(\gamma_{lg}+\gamma_{ls}-\gamma_{gs}\right) +$$

$$\overset{\text{Eq.}(9)}{=} \tfrac{1}{2}\gamma_{lg}\int_{-r}^{r} h_x^2 + 2r\,\gamma_{lg}\left(1-\cos\theta_{eq}\right) +$$

Note: $w = 2r$ is the droplet footprint.

Idea:

$$w = \text{Const.}\,\frac{\|\bar{h}\|_1^{2}}{\langle h, \bar{h}\rangle} = c\,\frac{A_0^{2}}{\langle h, \bar{h}\rangle},$$

where $A_0 = \int h\,dx = \int \bar{h}\,dx$

Justification: If $h = \max\left\{0, \frac{3A_0}{4r}\left(1 - \left(\frac{x}{r}\right)^2\right)\right\}$, then

$$\frac{\|\bar{h}\|_1^{2}}{\langle h, \bar{h}\rangle} = \frac{5}{6}\cdot 2r + O(\alpha^2)$$

(10) G-TFE becomes:

$$\frac{\partial h}{\partial t} + \frac{\partial}{\partial x}\left[h M(\bar{h}) \frac{\partial}{\partial x}\left(-\overset{=1}{\gamma}\, \bar{h}_{xx} - 2\gamma \overset{c(1-\cos\theta_{eq})}{\chi} \frac{A_0}{\langle h, \bar{h}\rangle^2}\,\bar{h}\right)\right] = 0.$$

Note: (10) comes from

$$\frac{\partial h}{\partial t} + \frac{\partial}{\partial x}(hU) = 0, \text{ with}$$

$$U = \left[-\frac{\partial}{\partial x}\frac{\delta E}{\delta h}\right]\cdot M(\bar{h})$$

Const.

Const.

A cool property of (10) is the exact analytical sol^n @ eq^m:

$$h\bar{h}^2 \frac{\partial}{\partial x}\left(\partial_{xx}\bar{h} + \xi^2 \bar{h}\right) = 0, \qquad \xi^2 = \frac{2\lambda^2}{\langle h, \bar{h}\rangle^2}.$$

$$\bar{h} = \begin{cases} B_1 \cos(\xi x) + B_2 & |x| < r \\ C_1 e^{-|x|/\alpha} + C_2 |x| e^{|x|/\alpha} & |x| > r \end{cases}$$

Matching condition @ $|x| = r$: Continuity of $\bar{h}, \bar{h}_x, \bar{h}_{xx}$.
Also: $\int \bar{h}\,dx = A_0 \to 1$.

- Good transient results as well showing close agreement with Cox–Voinov model:

$$\left.\left(\frac{\partial h}{\partial x}\right)^3\right|_{x_m} = \theta_{eq}^3 + c \cdot \frac{dx_m}{dt} \cdot \log\left(\frac{x_m}{\alpha}\right)$$

$[\theta(t)]^3$ $\theta_{eq} = 1$ in our scaling   fitting constants

This reduces to Tanner's Law when $\theta_{eq} \to 0$.

- But I am still not sure about this approach:
  - Estimate of droplet footprint looks weird
  - Eq^m sol^n is very complicated.

- The correct treatment of the partial wetting case is for me an unsolved puzzle.

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6. Conclusions

g-TFE

- New CL model valid for lubrication theory
- Model nails the complete-wetting case.

Outstanding work / challenges

- Proper theoretical underpinning for g-TFE
- Proper description of partial wetting.