How do degenerate mobilities determine singularity formation in Cahn-Hilliard equations?

CATALINA PESCE
Center for Doctoral Training in Partial Differential Equations
Mathematical Institute
University of Oxford

Joint work with Andreas Münch and Amy Novick-Cohen

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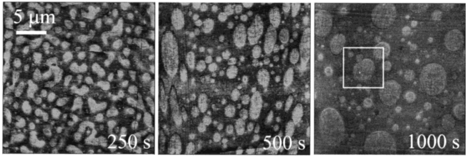
UNIVERSITY OF OXFORD
Mathematical Institute

Oxford Mathematics

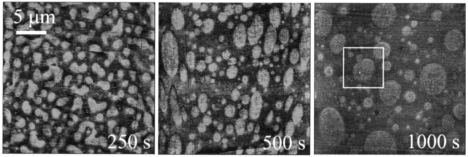
- Spinodal decomposition.
- Coarsening.



Polymer mixture at ratio 70/30. *Cabral, Higgins, Yerina, Magonov 2002*

Phase separation in binary alloys

- Spinodal decomposition.
- Coarsening.



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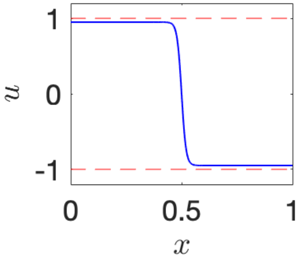
Phase-field models:

- Smooth phase field variable $u \approx \pm 1$ away from interface.
- u transitions between $+1$ and -1 across interface region of width $O(\varepsilon)$, $\varepsilon \ll 1$.



Let $\Omega \subset \mathbb{R}^N$, $N \geq 1$, a bounded and convex domain, $\partial\Omega \in C^{1,1}$, $T > 0$ and $0 < \varepsilon \ll 1$, $u = u(x,t)$,

$$\begin{aligned} \partial_t u &= -\nabla \cdot \mathbf{j}, \qquad \text{in } \Omega \times (0,T), \\ \mathbf{j} &= -M(u)\nabla\mu, \\ \mu &= -\varepsilon^2 \Delta u + f'(u), \end{aligned}$$

where $\mathbf{j}$ is the flux, $M \geq 0$ the mobility, μ the chemical potential and f the homogeneous free energy.

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Decaying energy $E[u](t) := \int_\Omega \left[\frac{\varepsilon^2}{2}|\nabla u|^2 + f(u)\right] dx$.

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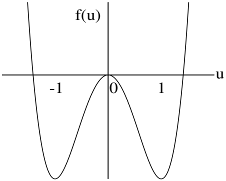
Applications of Cahn-Hilliard-type models

- Tumour growth models (e.g. Cristini, Lowengrub, Wise 2009; Oden et al. 2015)
- Motion of immiscible fluids with free boundaries (e.g. Ding, Spelt, Shu 2007; Abels, Garcke, Grün 2012)
- Polymer blends (e.g. De Gennes 1980, Castellano & Glotzer 1995)
- Surface diffusion and electromigration in crystals and alloys (e.g. Cahn, Elliott & Novick-Cohen 1996; Barrett, Garcke & Nürnberg 2007; Dziwnik, Münch, Wagner 2017)

Choice of f and M in $\partial_t u = \nabla \cdot (M(u)\nabla(-\varepsilon^2 \Delta u + f'(u)))$

Double well free energy:

$$f(u) := \frac{(1-u^2)^2}{2}$$



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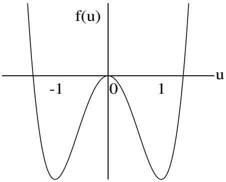

Constant and two-sided nonlinear mobilities:

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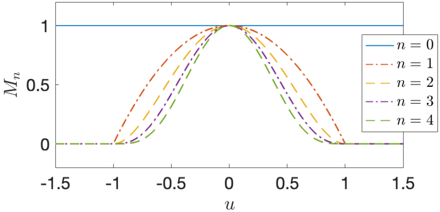
$n \in \mathbb{R}^+$. Note $M_n(\pm 1) = 0$.



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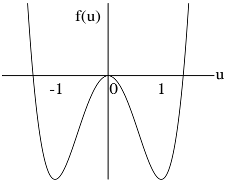

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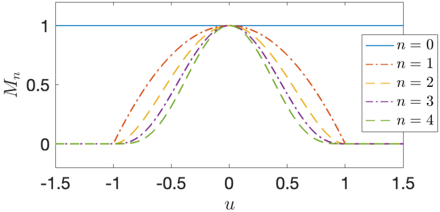

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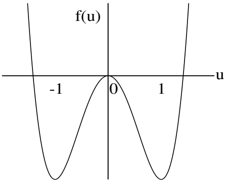

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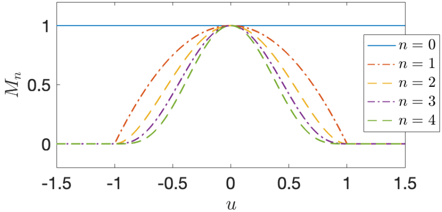

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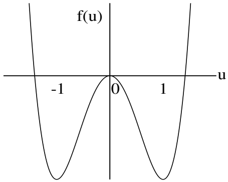

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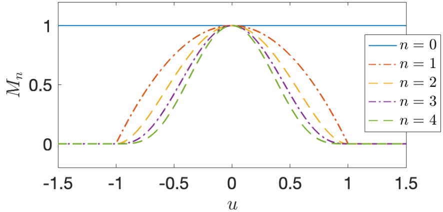

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Are there $n > 0$ that ensure $|u| < 1$? What happens when $|u| \to 1$?

Cahn-Hilliard equation in one dimension, $\Omega \subset \mathbb{R}$,

$$\partial_t u = \partial_x \big[M(u) \big(-\varepsilon^2 \partial_{xxx} u + \partial_x f'(u) \big) \big].$$

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Constantin, Elgindi, Nguyen, Vicol 2018: $n = 1$. Pressure b.c. with $p > 2$. The solution must pinch off in either finite or infinite time, i.e.

$$\inf_{[-1,1]\times[0,T)} h = 0,$$

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Bertozzi, Brenner, Dupont and Kadanoff 1994: $\Omega = (-1, 1)$. Pressure b.c. with $p > 2$. Infinite time pinch-off is possible for $n > 1/2$. Two different leading order profiles for cases $1/2 < n < 2$ and $n > 2$.

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Bernis and Friedman 1990: $\Omega = (-1, 1)$. Neumann b.c. $h_0 \geq 0$ plus assumptions on entropy of initial data.

- If $1 < n < 2$, then $h \geq 0$.
- If $2 \leq n < 4$, then $h \geq 0$ and $\{h = 0\}$ has zero measure.
- If $n \geq 4$, then $h > 0$ and the solution is unique.

Solution $u(x,t)$ is expected to converge to a stationary solution $U(x)$

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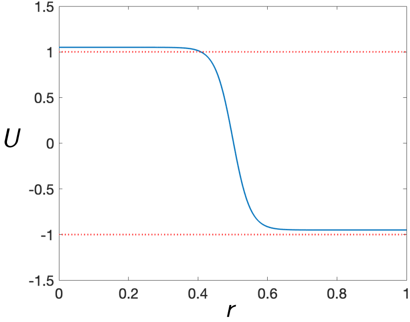

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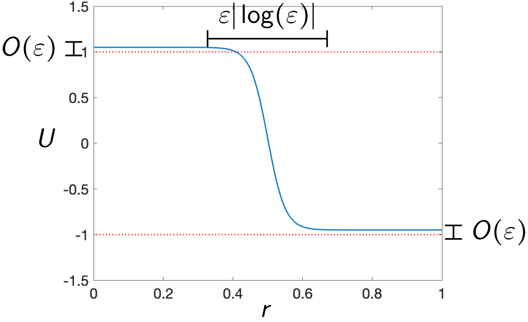
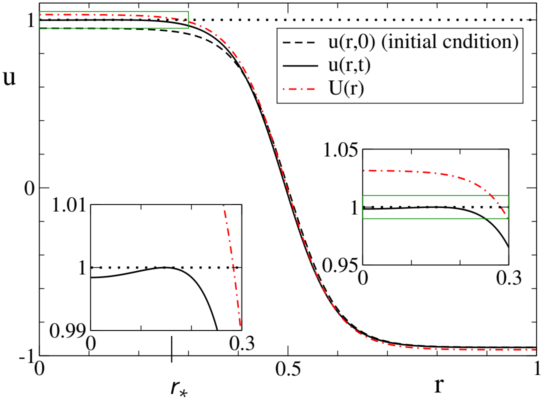


Time dependent 2D radial case with $M_2(u) = (1 - u^2)_+^2$

Lee, Münch, Süli 2016; Pesce, Münch 2021: For $|u_0| \leq 1$, numerical solution u develops a maximum less but close to 1 near interface, where $M_2(u) \sim 0$.



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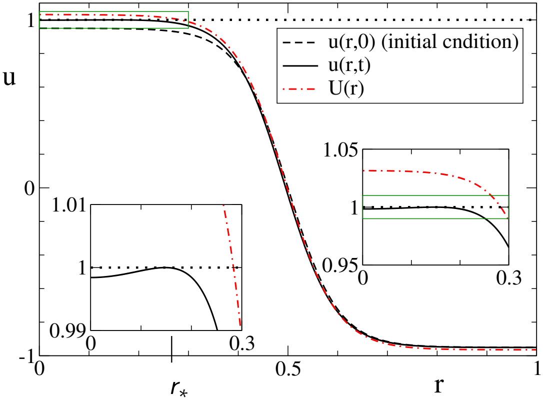

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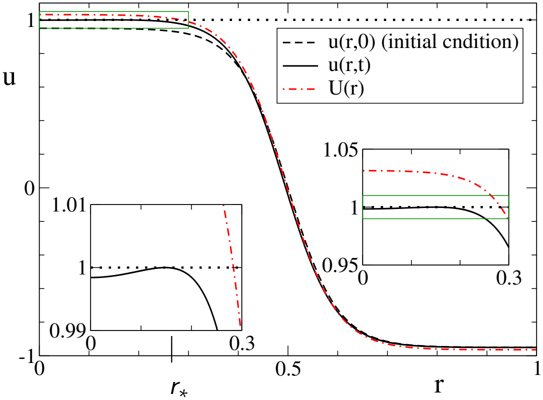

Does **touchdown** happen in finite or infinite time? Does it depend on n?

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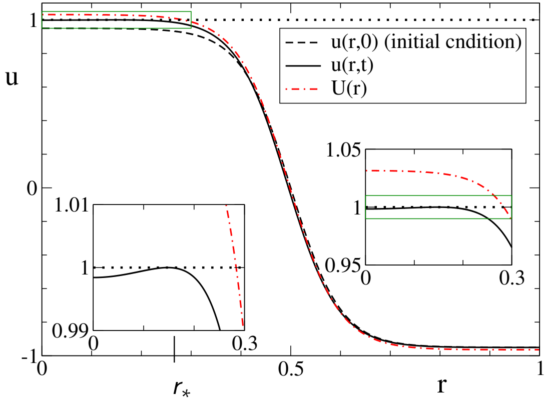

Does **touchdown** happen in finite or infinite time? Does it depend on n? Does it have some underlying structure?

Let $u = u(r,t)$,

$$\partial_t u = \frac{1}{r}\partial_r\left(rM(u)\partial_r\mu\right),$$
$$\mu = -\varepsilon^2\frac{1}{r}\partial_r\left(r\partial_r u\right) + f'(u),$$

for $(r,t) \in (0,1)\times(0,\infty)$, under boundary conditions

$$\partial_r u(1,t) = 0, \quad M(u(1,t))\partial_r\mu(1,t) = 0,$$
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Consider the Lebesgue and Sobolev spaces of radial functions $L^2_{\mathrm{rad}}(B)$, $H^p_{\mathrm{rad}}(B)$.

Theorem (Novick-Cohen and Pesce 2022+)

Let $u_0 \in H^1_{rad}(B)$ *with* $|u_0| \leq 1$ *plus assumptions on entropy of initial data. Then* $\exists u \in L^2([0,T]; H^2_{rad}(B)) \cap L^\infty(0,T; H^1_{rad}(B)) \cap C([0,T]; L^2_{rad}(B))$ *such that* $|u| \leq 1$

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$$\int_0^T \langle \zeta(t), \partial_t u(t) \rangle_{H^1, H^{-1}} \, dt = -\int_0^T \int_0^1 \mathbf{j} \, \partial_r \zeta \; r dr dt,$$

$$\int_0^T \int_0^1 \mathbf{j} \, \psi \; r dr dt = -\varepsilon^2 \int_0^T \int_0^1 \frac{1}{r} \partial_r \left(r \partial_r u \right) \partial_r (M(u) \psi) \; r dr dt + \int_0^T \int_0^1 (M f'')(u) \partial_r u \psi \; r dr dt,$$

for all $\zeta \in L^2(0,T; H^1_{rad}(B))$ *and* $\psi \in L^2(0,T; H^1_{rad}(B)) \cap L^\infty(B_T)$ *such that* $\frac{\psi}{r} \in L^2(0,T; L^2_{rad}(B))$ *which satisfy* $\psi = 0$ *on* $(0,T) \times \{0,1\}$.

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- Based on proof by Elliott and Garcke 1996.

Theorem (Novick-Cohen and Pesce 2022+)

Let $u_0 \in H^1_{rad}(B)$ *with* $|u_0| \le 1$ *plus assumptions on entropy of initial data. Then* $\exists u \in L^2([0,T]; H^2_{rad}(B)) \cap L^\infty(0,T; H^1_{rad}(B)) \cap C([0,T]; L^2_{rad}(B))$ *such that* $|u| \le 1$ *and*

$$\int_0^T \langle \zeta(t), \partial_t u(t) \rangle_{H^1, H^{-1}} \, dt = -\int_0^T \int_0^1 \mathbf{j} \, \partial_r \zeta \; r dr dt,$$

$$\begin{aligned}\int_0^T \int_0^1 \mathbf{j} \, \psi \; r dr dt = &- \varepsilon^2 \int_0^T \int_0^1 \frac{1}{r} \partial_r \left(r \partial_r u \right) \partial_r (M(u) \psi) \; r dr dt \\ &+ \int_0^T \int_0^1 (M f'')(u) \partial_r u \psi \; r dr dt,\end{aligned}$$

for all $\zeta \in L^2(0,T; H^1_{rad}(B))$ *and* $\psi \in L^2(0,T; H^1_{rad}(B)) \cap L^\infty(B_T)$ *such that* $\frac{\psi}{r} \in L^2(0,T; L^2_{rad}(B))$ *which satisfy* $\psi = 0$ *on* $(0,T) \times \{0,1\}$.

- Based on proof by Elliott and Garcke 1996.
- Work in progress: Generalizations. For $n \ge 4$, $\{|u| = 1\}$ has zero measure.

What happens if $u \to 1$ ($v \to 0$) in finite time?

We will work from now on with $v(r,t) := 1 - u(r,t)$, which satisfies

$$\partial_t v = -\frac{1}{r}\partial_r \left[r v_+^n (2-v)_+^n \partial_r \left(\varepsilon^2 \frac{1}{r} \partial_r \left(r \partial_r v \right) + 2(-v^3 + 3v^2 - 2v) \right) \right].$$

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Proposition

Let $1 \le n < \infty$ and $v(r,t) > 0$ for all $(r,t) \in (0,1) \times (0,t^*)$ be a smooth solution. If there exists $t^* < \infty$ such that

$$\lim_{t \to t^*} \min_{r \in (0,1)} v(r,t) =: \lim_{t \to t^*} v(\bar{r}(t), t) = 0.$$

Then v becomes singular at that point in the following sense:

$$\int_0^{t^*} \left[\partial_{rrrr} v(r,t) + \partial_{rrr} v(r,t) + \partial_{rr} v(r,t) \right]_{r=\bar{r}(t)} dt = +\infty.$$

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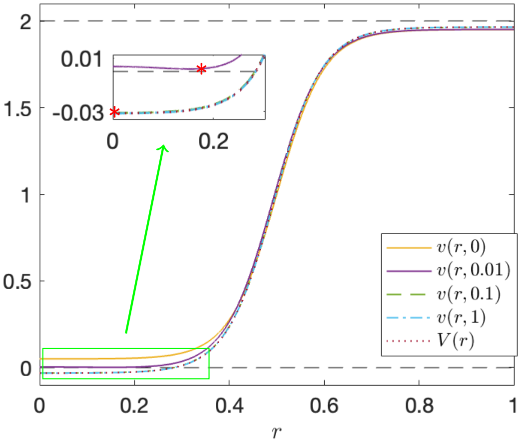
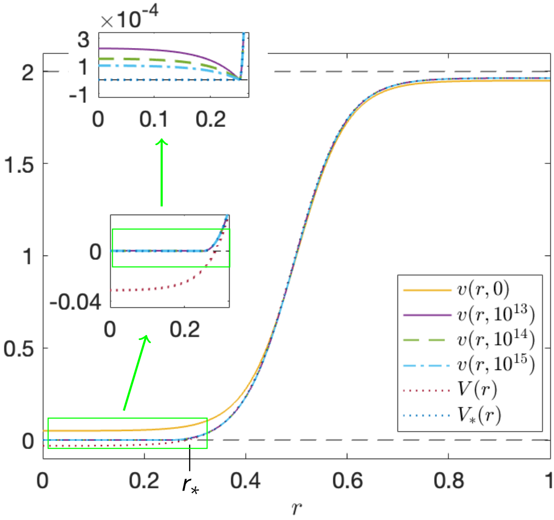
- Following similar thin-film results by Constantin et. al. 2018 and Bertozzi et. al. 1994.

What happens as $t \to \infty$? Numerical solution for $n = 0$



Here $V = 1 - U$, U is the solution to the constant mobility stationary problem.

What happens as $t \to \infty$? Numerical solution for $n = 4$



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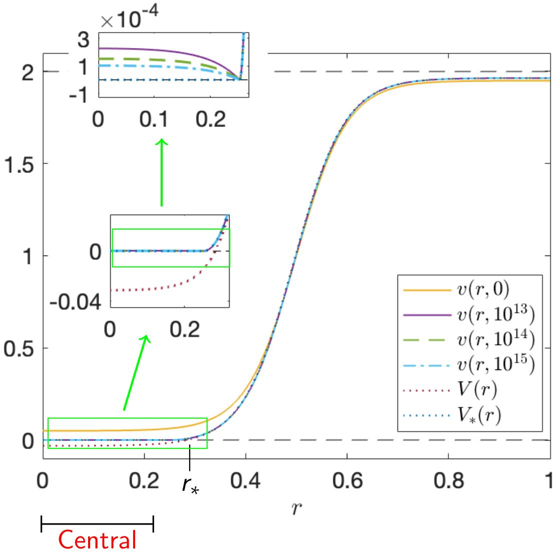

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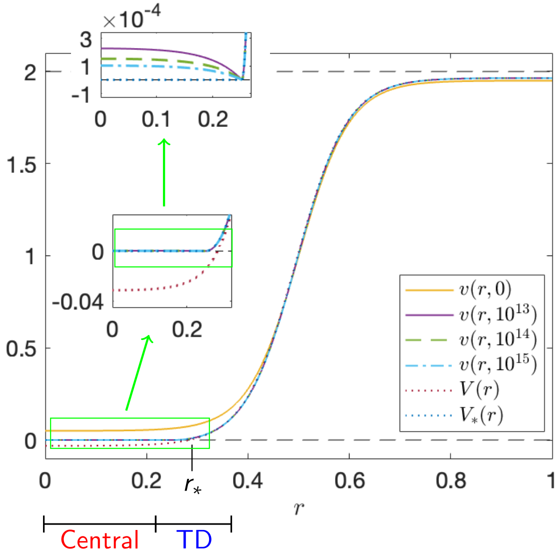

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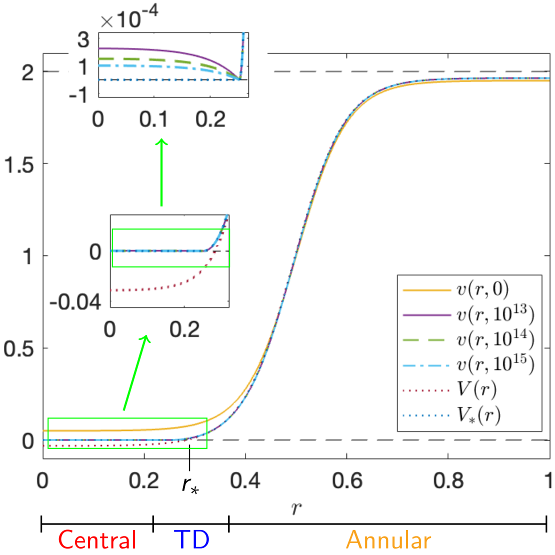

Pesce and Münch 2021: We can use **matched asymptotics** to obtain an asymptotic composite expansion with infinite time touchdown, namely

$$\begin{aligned} v_{comp}(r,t) :=& v_{central}(r,t) + v_{touchdown}(r,t) + v_{annular}(r,t) \\ & - A_- t^{-\frac{1}{2(n-1)}} (r - r_*)_- - A_+ (r - r_*)_+^2, \end{aligned}$$

where A_-, A_+ are constants fixed by matching.

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where A_-, A_+ are constants fixed by matching.

Matching at leading order gives

$$\begin{aligned} v_{central} &\sim t^{-\frac{1}{2(n-1)}}\psi_0(r), && && r \in (0, r_*), \\ v_{touchdown} &\sim t^{-\frac{1}{n-1}}\varphi_0(\eta), && \eta := \frac{r - r_*}{t^{-\frac{1}{2(n-1)}}}, && \eta \in (-\infty, +\infty), \\ v_{annular} &\sim 1 - U_*(r), && && r \in (r_*, 1), \end{aligned}$$

where ψ_0, φ_0 and U_* solve ODEs.

PhD Thesis, Pesce 2022: We can find consistent asymptotic expansions only for $1/2 < n \leq 2$. Similar to the previous case but now

$$\begin{aligned} v_{comp}(r,t) :=& v_{central}(r,t) + v_{touchdown}(r,t) + v_{annular}(r,t) \\ & - A_- t^{-\frac{1}{n}} (r - r_*)_-^{\frac{3}{n+1}} - A_+ (r - r_*)_+^2, \end{aligned}$$

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Matching at leading order gives

$$\begin{aligned} v_{central} &\sim t^{-\frac{1}{n}} \psi_0(r), && && r \in (0, r_*), \\ v_{touchdown} &\sim t^{-\frac{2(n+1)}{n(2n-1)}} \varphi_0(\eta), && \eta := \frac{r - r_*}{t^{-\frac{(n+1)}{n(2n-1)}}}, && \eta \in (-\infty, +\infty), \\ v_{annular} &\sim 1 - U_*(r), && && r \in (r_*, 1), \end{aligned}$$

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In the setting of radial solutions in 2D unitary ball:

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Conclusion

In the setting of radial solutions in 2D unitary ball:

- For $n > 0$, **existence and regularity** of bounded radially symmetric weak solutions.
- For $n \geq 1$, **finite time touchdown** implies singularity formation.
- For $n > 1/2$ there is a numerical solution that converges in long time to an asymptotic approximation with **infinite time touchdown**. Different leading order expansions for $1/2 < n \leq 2$ and $2 < n$.
- Informed by research on **thin-film equations**.

How do degenerate mobilities determine singularity formation in Cahn-Hilliard equations?

CATALINA PESCE
Center for Doctoral Training in Partial Differential Equations
Mathematical Institute
University of Oxford

Joint work with Andreas Münch and Amy Novick-Cohen

Oxbridge PDE Conference, April 2022

UNIVERSITY OF OXFORD
Mathematical Institute

Oxford Mathematics

Theorem (Rellich-Kondrachov Compactness Theorem)

Assume U is a bounded open subset in $\mathbb{R}^N$, ∂U is C^1 and let $N > mp \geq 1$. If $1 \leq q < \frac{pN}{N-mp}$, then the embedding

$$W^{m,p}(U) \hookrightarrow L^q(U)$$

is compact.

Theorem (Guedes et. al. 2011)

Let $N > mp$ and $\beta > 0$. If $1 \leq q < \frac{p(N+\beta)}{N-mp}$, then the embedding

$$W^{m,p}_{rad}(B) \hookrightarrow L^q(B, |x|^\beta)$$

is compact.

Proposition (PhD thesis, Pesce 2022)

Let $N = mp$ and $\beta \geq 0$. Then the embedding

$$W^{m,p}_{rad}(B) \hookrightarrow L^q(B, |x|^\beta)$$

is compact for all $1 \leq q < \infty$.

Taking $\beta = 1$, $m = 1$ and $p = 2$, we obtain

$$H^1_{\mathrm{rad}}(B) \hookrightarrow L^q_{\mathrm{rad}}(B)$$

is compact for all $1 \leq q < \infty$. In particular, we take $q = 2$.

Central region:

$$\varepsilon^2\left(\partial_{rr}\psi_0(r) + \frac{1}{r}\partial_r\psi_0(r)\right) - 4\psi_0(r) = c_1,$$
$$\partial_r\psi_0(0) = 0,$$
$$\psi_0(r_*) = 0,$$

where c_1 is a constant.

Annular region:

$$-\frac{\varepsilon^2}{r}\frac{d}{dr}\left(r\frac{dU_*}{dr}\right) + f'(U_*) = \sigma,$$
$$U_*'(1) = 0,$$
$$U_*(r_*) = 1, \quad U_*'(r_*) = 0,$$

where σ is a constant.

Touchdown region:

$$\varphi_0^n(\eta)\partial_{\eta\eta\eta}\varphi_0(\eta) = J, \quad \eta \in (-\infty, \infty),$$

$$\varphi_0(\eta) = \begin{cases} A_-\eta + \frac{JA_-^{-n}(-\eta)^{3-n}}{(n-1)(n-2)(n-3)} + B_- + h.o.t. & \text{if } n < 3, \\ A_-\eta + \frac{J}{2A_-^3}\ln(-\eta) + B_- + h.o.t. & \text{if } n = 3, \\ A_-\eta + B_- + h.o.t. & \text{if } n > 3, \end{cases} \text{ as } \eta \to -\infty,$$

$$\varphi_0(\eta) = A_+\eta^2 + B_+\eta + C_+ + h.o.t. \text{ as } \eta \to \infty$$

where $A_\pm$, $B_\pm$, C_+, J are constants.

Case $n \leq 2$

Central region:

$$
\begin{aligned}
-\frac{1}{n}\psi_0 =& -\frac{2^n}{r}\partial_r\left[r\psi_0^n\partial_r\left(\varepsilon^2\left(\partial_{rr}\psi_0+\frac{1}{r}\partial_r\psi_0\right)-4\psi_0\right)\right] \text{ in } (0,r_*),\\
\psi_0(r) =& a_0^- + a_2^- r^2 + h.o.t., \qquad \text{as } r\to 0,\\
\psi_0(r) =& a_0^+(r_*-r)^{\frac{3}{n+1}} + a_1^+(r_*-r)^{\frac{4n+1+\sqrt{-8n^2+20n+1}}{2(n+1)}} + h.o.t., \qquad \text{as } r\to r_*,
\end{aligned}
$$

where a_0^-, a_2^-, a_0^+, a_1^+ are constants.

Touchdown region:

$$\varphi_0^n(\eta)\partial_{\eta\eta\eta}\varphi_0(\eta) = J, \quad \eta \in (-\infty, \infty),$$

as $\eta \to +\infty$, let $n_* := \frac{7+3\sqrt{3}}{11}$ we have

$$\varphi_0(\eta) = \begin{cases} A_-(-\eta)^{\frac{3}{(n+1)}} + B_-(-\eta)^{\frac{2-n}{n+1}} + C_-(-\eta)^{\frac{4n+1-\sqrt{-8n^2+20n+1}}{2(n+1)}} + h.o.t. & \frac{1}{2} < n < n_*, \\ A_-(-\eta)^{2-\frac{\sqrt{3}}{3}} + B_- x^{1-\frac{\sqrt{3}}{3}} \ln\left(\frac{1}{x}\right) + C_- x^{1-\frac{\sqrt{3}}{3}} + h.o.t. & n = n_*, \\ A_-(-\eta)^{\frac{3}{(n+1)}} + B_-(-\eta)^{\frac{4n+1-\sqrt{-8n^2+20n+1}}{2(n+1)}} + C_-(-\eta)^{\frac{2-n}{n+1}} + h.o.t. & n_* < n < 2, \\ ? & n = 2, \end{cases}$$

where

$$A_- = \left| \frac{-J(n+1)^3}{3(1-2n)(2-n)} \right|^{\frac{1}{n+1}}.$$

On the other hand, as $\eta \to +\infty$, we have

$$\varphi_0 = \begin{cases} A_+\eta^2 + \frac{-J\eta^{3-2n}}{A_+^n(2n-1)(2n-2)(2n-3)} + B_+\eta + C_+, & \frac{1}{2} < n < 1, \\ A_+\eta^2 + \frac{-J}{A_+}\eta(\ln(\eta)+1) + B_+\eta + C_+, & n = 1, \\ A_+\eta^2 + B_+\eta + \frac{-J\eta^{3-2n}}{A_+^n(2n-1)(2n-2)(2n-3)} + C_+, & 1 < n < \frac{3}{2}, \\ A_+\eta^2 + B_+\eta + \frac{J}{2A_+^{3/2}}\ln(\eta) + C_+, & n = \frac{3}{2}, \\ A_+\eta^2 + B_+\eta + C_+ + \frac{-J\eta^{3-2n}}{A_+^n(2n-1)(2n-2)(2n-3)}, & \frac{3}{2} < n \le 2, \end{cases}$$

where $A_\pm$, $B_\pm$, C_+, J are constants.

In the central region, we specifically make the ansatz

$$v(r,t) \sim t^{\alpha}\psi(r)$$

with some $\alpha < 0$.

This assumption can be tested by plotting $v(r,t)/v(0,t)$ for different times, we expect all curves to collapse near $r = 0$.

Similarly, in the touchdown region,

$$v(r,t) \sim t^{\beta}\varphi(\eta), \qquad \eta := \frac{r - r_*}{t^{\gamma}},$$

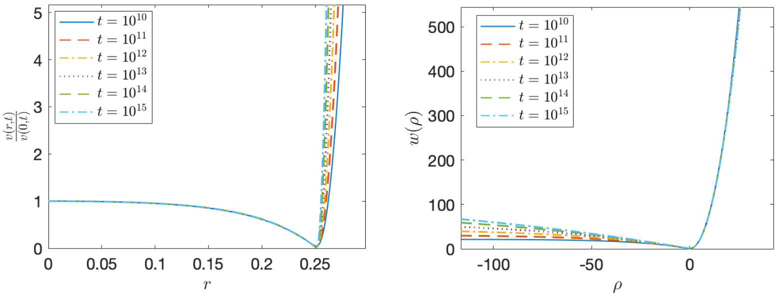
for some β, $\gamma < 0$. We test this ansatz by first scaling

$$w := \frac{v(r,t)}{\min\limits_{r\in[0,1]} v(t)}, \quad \rho := \left(\frac{\partial_{rr} v(r_*,t)}{v(r_*,t)}\right)^{1/2} (r - \overline{r}(t)).$$

Note that $\rho \sim \eta$ when t is large.

This assumption can be tested by plotting w as a function of ρ for different times, we expect all curves to collapse near $r = r_*$.

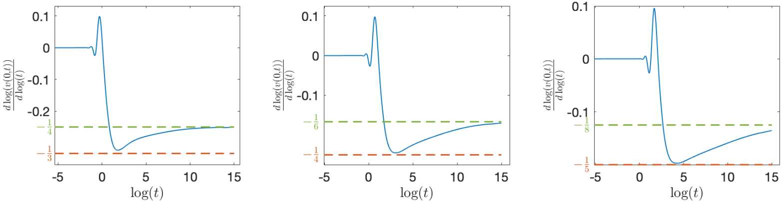
Case $n > 2$: Self-similarity



Left: Central region rescaled according to r vs. $v(r,t)/v(0,t)$ for different times. Right: Rescaled touchdown region, w vs ρ. For $n = 4$.

To obtain the coefficients we note that, for example in the central region,

$$\log(v(0,t)) \sim \log(\psi(0)) + \alpha \log(t).$$

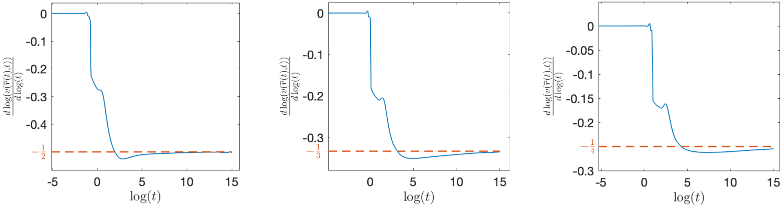


$\frac{d\log(v(0,t)))}{d\log(t)}$ vs $\log(t)$ for final time 10^{15} and (left) $n = 3$, (middle) $n = 4$, (right) $n = 5$.

$$\alpha \sim -\frac{1}{2(n-1)}$$

Case $n > 2$: Similarity coefficients

Same for β:



$\frac{d\log(v(\bar{r}(t),t)))}{d\log(t)}$ vs $\log(t)$ for final time 10^{15} and (left) $n = 3$, (middle) $n = 4$, (right) $n = 5$.

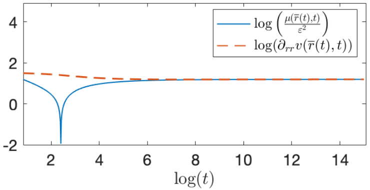
$$\beta \sim -\frac{1}{(n-1)}$$

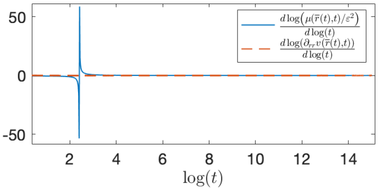
For γ note

$$\partial_{rr} v(r_*, t) \sim t^{\beta - 2\gamma} \partial_{\eta\eta} \varphi(\eta).$$

Moreover, when t is large

$$\mu(r, t) \sim \varepsilon^2 \partial_{rr} v(r, t).$$





Left: Log-log for $\mu(\bar{r}, t)/\varepsilon^2$ and $\partial_{rr} v(\bar{r}, t)$, Right: Derivative of (left) for $n = 4$ and $\varepsilon = 0.05$.

$$2\beta \sim \gamma \sim -\frac{1}{(n-1)}$$