Generalized Phase Field Models with Anisotropy and Non-Local Potentials

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Introduction

- Classical Stefan problem (Lame and Clapeyron 1831, Stefan 1889)

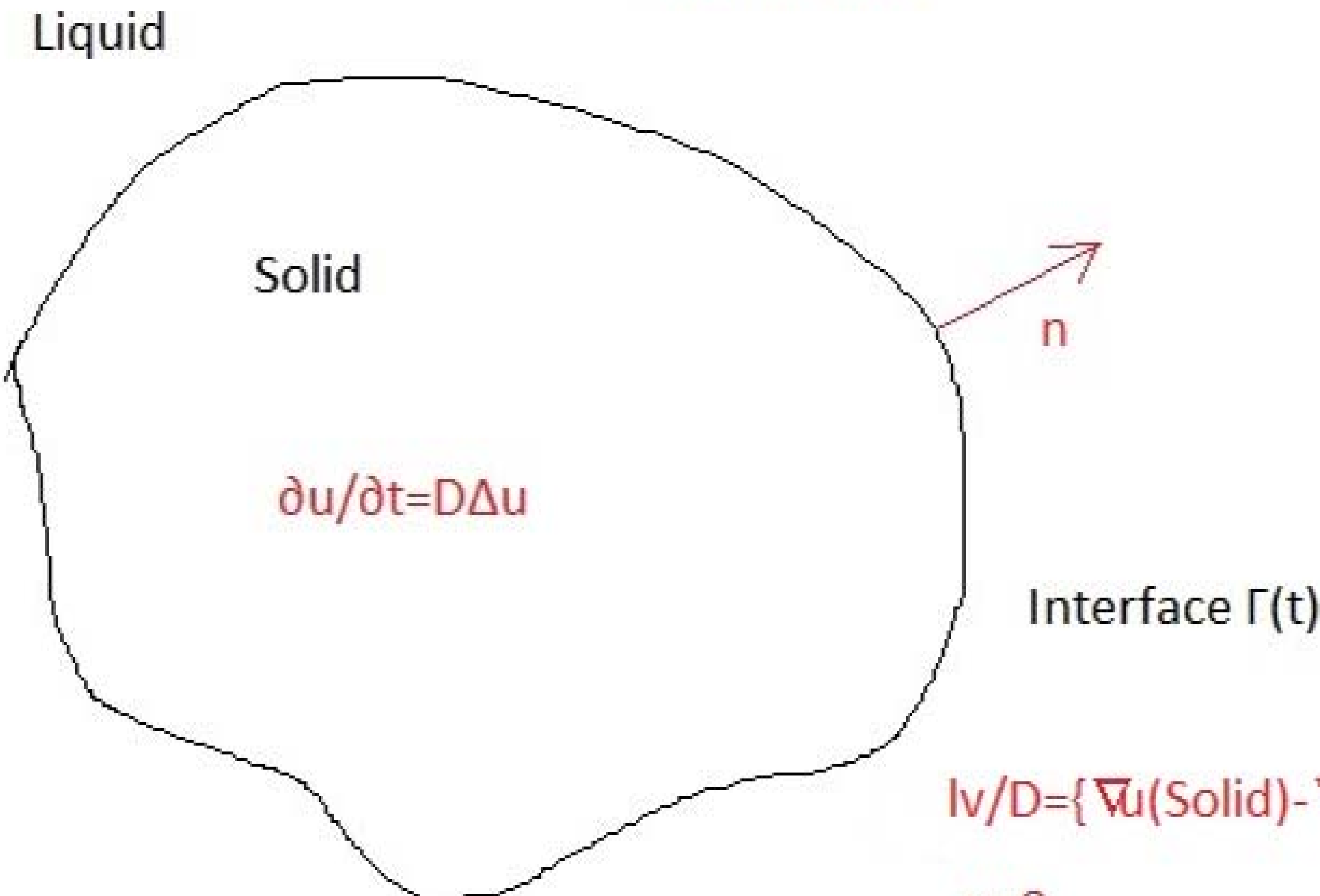
$$
\begin{aligned}
u_t &= D\Delta u \quad \text{in } \Omega \backslash \Gamma \\
lv_n &= D\left[\nabla u \cdot n\right]_+^- \quad \text{on } \Gamma \\
u &= 0 \quad ? \quad \text{on } \Gamma
\end{aligned}
$$

- In Classical Stefan model temperature plays dual role. Around 1900 it became clear to materials scientists that $u \neq 0$ at interface. But the Stefan problem dominated mathematics of interfaces separating phases.
- If temperature does not distinguish phases, we need a new variable, ϕ (order parameter).

The Classical Stefan Problem

Find $\Gamma(t)$ and $u(x,t)$

$\partial u/\partial t = D\Delta u$



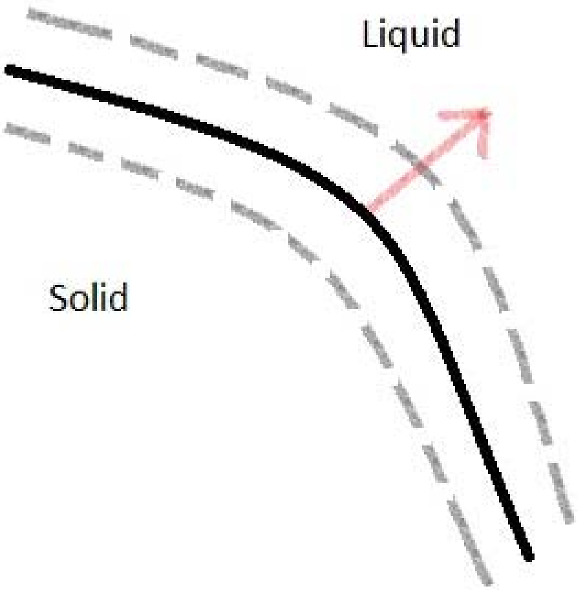
$lv/D = \{\nabla u(\text{Solid}) - \nabla u(\text{Liquid})\} \cdot n$

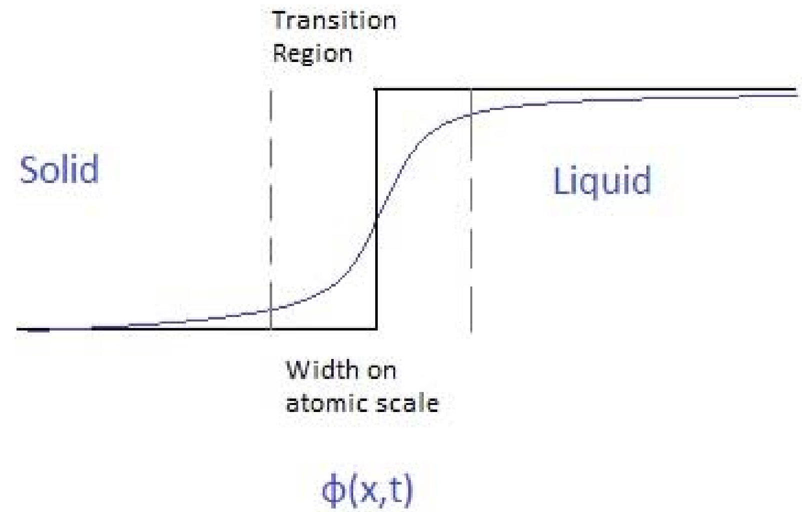
$u=0$

- Oleinik formulation consolidates first two eqs:

$$u_t + \frac{l}{2}\phi_t = D\Delta u$$

  where ϕ is just a step function.
- How do we obtain the second variable ϕ ?


Liquid
Solid


Transition
Region
Solid
Liquid
Width on
atomic scale
ϕ(x,t)

Idea of "order parameter" in statistical mechanics

Originally proposed by Landau in 1940's for critical phenomena. Review article by Hohenberg and Halpern 1977 on "Dynamics of critical phenomena" Model A, B... Cahn-Hilliard model etc.

Physical issues

1. Landau "order parameter" based on idea that "correlation length" diverges to infinity near critical point.
2. It was shown to be wrong in that region.
3. For an ordinary phase transition, the correlation length is very small, not infinite.
4. For an ordinary phase transition, we "cannot hide behind 'universality." We need to obtain exact answers with exact physical parameters.
5. Even if all of this is OK how to compute with an interface thickness $\varepsilon = 10^{-8}$?

Is it possible that the idea could work well for the opposite region (atomic correlation length) when it does not work for the intended region (divergent correlation length)?

Basic ideas

- Write a free energy $\mathcal{F}[\phi, u] := \int_\Omega \left\{ (\nabla\phi)^2 + w(\phi) + uh(\phi) \right\}$ with w double well and e.g., $h'(\phi) = \left(1-\phi^2\right)^2$ or $h'(\phi) = 1$.
- Dynamics $\partial\phi/\partial t = -\delta\mathcal{F}/\delta\phi$ coupled with heat equation

$$\begin{aligned} \alpha\varepsilon^2\phi_t &= \varepsilon^2\Delta\phi + \frac{1}{2}\left(\phi-\phi^3\right) + \frac{5\varepsilon}{8d_0}h'(\phi)u \\ (u+\frac{1}{2}\phi)_t &= \Delta u \end{aligned}$$

$$u := \frac{T-T_E}{l/c}, \quad D := \frac{K}{\rho c}, \quad d_0 := \frac{\sigma}{[s]_E l/c}.$$

As $\varepsilon \to 0$ does this system converge to the sharp interface problem below?

$$\begin{aligned} u_t &= D\Delta u && \text{in } \Omega(t)\backslash\Gamma(t) \\ v_n &= D\hat{n}\cdot\nabla u]_+^-, && \text{on } \Gamma(t) \\ u &= -d_0\left(\kappa+\alpha v_n\right) && \text{on } \Gamma(t) \end{aligned}$$

Sketch of formal asymptotics

Let r be the signed distance from the interface, $\rho := r/\varepsilon$

$$\begin{aligned}\phi(x,t;\varepsilon) &= \phi^0(x,t) + \varepsilon\phi^1(x,t) + \ldots \\ &\approx \Phi(\rho,t;\varepsilon) = \Phi^0(\rho,t) + \varepsilon\Phi^1(\rho,t) + \varepsilon^2\Phi^2(\rho,t) + \ldots\end{aligned}$$

$$-\frac{\partial\phi(x,t;\varepsilon)}{\partial t} = \varepsilon v \Phi^0_\rho(\rho,t), \qquad \varepsilon^2\Delta\phi = \Phi^0_{\rho\rho} + \varepsilon\kappa\Phi^0_\rho + \ldots$$

So the phase equation is roughly

$$\begin{aligned}-\varepsilon v\Phi^0_\rho(\rho,t) &= \Phi^0_{\rho\rho} + \varepsilon\Phi^1_{\rho\rho} + \varepsilon\kappa\Phi^0_\rho \\ &\quad + \frac{1}{2}\left\{\Phi^0 + \varepsilon\Phi^1 - \left(\Phi^0 + \varepsilon\Phi^1\right)^3\right\} + \frac{c}{d_0}\varepsilon u\end{aligned}$$

$O(1)$ balance

$$\Phi^0_{\rho\rho} + \frac{1}{2}\left\{\Phi^0 - \left(\Phi^0\right)^3\right\} = 0 \qquad \Rightarrow \qquad \Phi^0(\rho) = \tanh(\rho/2) \qquad (1)$$

$O(\varepsilon)$ balance

$$\mathcal{L}\Phi^1 := \Phi^1_{\rho\rho} + \frac{1}{2}\left\{1 - 3\left(\Phi^0\right)^2\right\}\Phi^1 = v\Phi^0_\rho + \kappa\Phi^0_\rho + \frac{c}{d_0}u =: F \qquad (2)$$

Note that Φ^0_ρ solves the homogenous equation, $\mathcal{L}\Phi^0_\rho = 0$, so Fredholm alternative them implies, $\mathcal{L}\Phi^1 = F$ has a solution only if $\left(F, \Phi^0_\rho\right)_{L^2} = 0$. This means

$$\begin{aligned} \int_{-\infty}^{\infty}\left(v\Phi^0_\rho + \kappa\Phi^0_\rho + \frac{c}{d_0}u\right)\Phi^0_\rho d\rho &= 0, \quad \text{so} \qquad (3) \\ u &\simeq c_1 d_0 \kappa + c_2 v. \end{aligned}$$

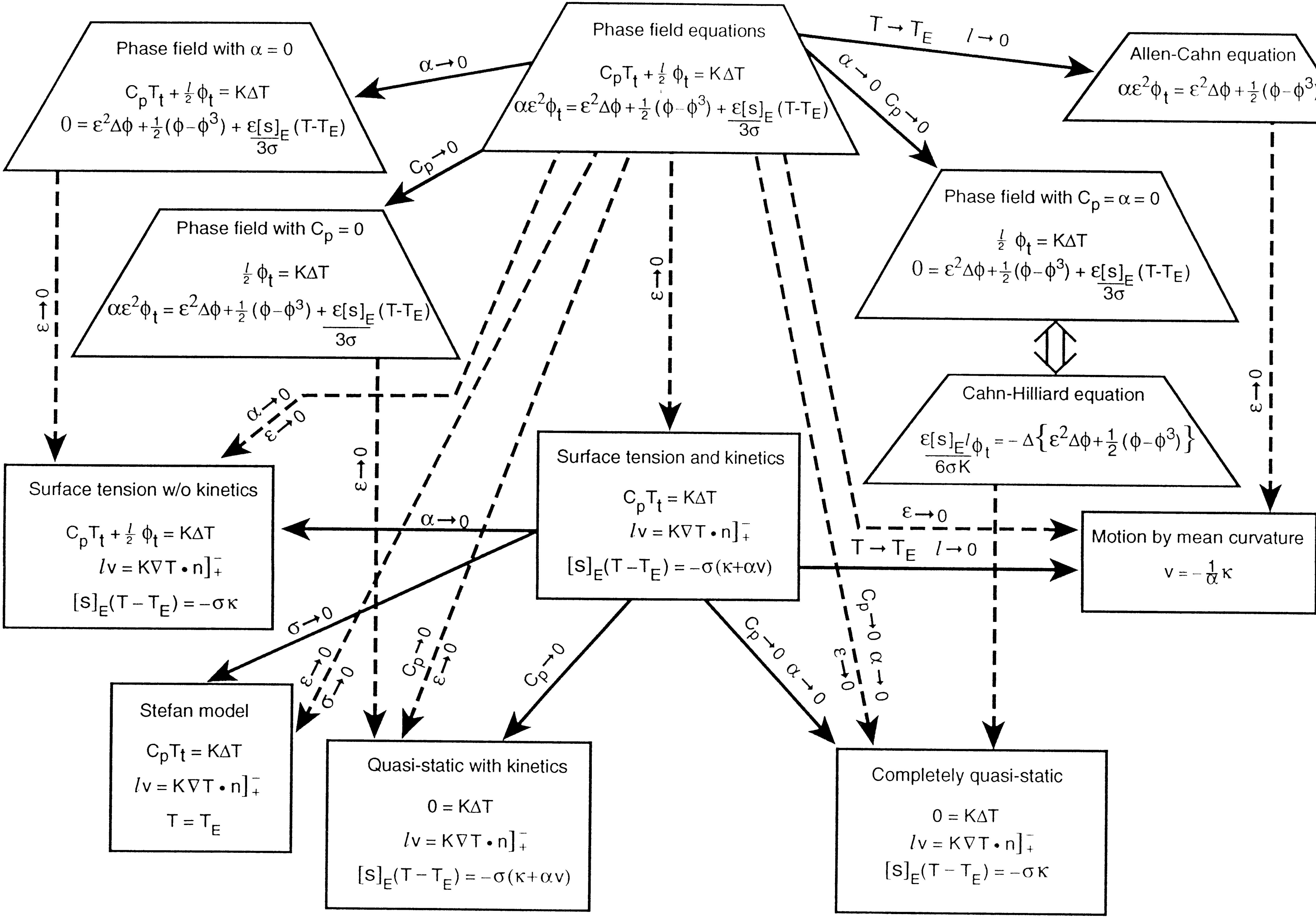
Match "inner solution" Φ with "outer solution" ϕ.

Ultimately, we want a rigorous proof that in some norm $\|\cdot\|$ one has

$$\left\| True\ Solution\ \phi \ - \ \left(\phi^0 + \varepsilon\phi^1 + \ldots + \varepsilon^k\phi^k\right\| \leq C_{k+1}\varepsilon^{k+1}. \qquad (4)$$

Mathematical issues

Do solutions exist? Is ϕ even bounded? Does the interface remain at the same "thickness" etc. Can we establish (4) and (5) in some suitable norm? Main thrust of research in the 1980s.


Phase field equations
$C_p T_t + \frac{l}{2}\phi_t = K\Delta T$
$\alpha\varepsilon^2\phi_t = \varepsilon^2\Delta\phi + \frac{1}{2}(\phi-\phi^3) + \frac{\varepsilon[s]_E}{3\sigma}(T-T_E)$
Phase field with $\alpha = 0$
$C_p T_t + \frac{l}{2}\phi_t = K\Delta T$
$0 = \varepsilon^2\Delta\phi + \frac{1}{2}(\phi-\phi^3) + \frac{\varepsilon[s]_E}{3\sigma}(T-T_E)$
Allen-Cahn equation
$\alpha\varepsilon^2\phi_t = \varepsilon^2\Delta\phi + \frac{1}{2}(\phi-\phi^3)$
Phase field with $C_p = 0$
$\frac{l}{2}\phi_t = K\Delta T$
$\alpha\varepsilon^2\phi_t = \varepsilon^2\Delta\phi + \frac{1}{2}(\phi-\phi^3) + \frac{\varepsilon[s]_E}{3\sigma}(T-T_E)$
Phase field with $C_p = \alpha = 0$
$\frac{l}{2}\phi_t = K\Delta T$
$0 = \varepsilon^2\Delta\phi + \frac{1}{2}(\phi-\phi^3) + \frac{\varepsilon[s]_E}{3\sigma}(T-T_E)$
Cahn-Hilliard equation
$\frac{\varepsilon[s]_E l}{6\sigma K}\phi_t = -\Delta\left\{\varepsilon^2\Delta\phi + \frac{1}{2}(\phi-\phi^3)\right\}$
Surface tension w/o kinetics
$C_p T_t + \frac{l}{2}\phi_t = K\Delta T$
$lv = K\nabla T \bullet n]_+^-$
$[s]_E(T-T_E) = -\sigma\kappa$
Surface tension and kinetics
$C_p T_t = K\Delta T$
$lv = K\nabla T \bullet n]_+^-$
$[s]_E(T-T_E) = -\sigma(\kappa+\alpha v)$
Motion by mean curvature
$v = -\frac{1}{\alpha}\kappa$
Stefan model
$C_p T_t = K\Delta T$
$lv = K\nabla T \bullet n]_+^-$
$T = T_E$
Quasi-static with kinetics
$0 = K\Delta T$
$lv = K\nabla T \bullet n]_+^-$
$[s]_E(T-T_E) = -\sigma(\kappa+\alpha v)$
Completely quasi-static
$0 = K\Delta T$
$lv = K\nabla T \bullet n]_+^-$
$[s]_E(T-T_E) = -\sigma\kappa$
$\alpha \to 0$
$C_p \to 0$
$T \to T_E \quad l \to 0$
$\alpha \to 0 \quad C_p \to 0$
$\varepsilon \to 0$
$\alpha \to 0 \quad \varepsilon \to 0$
$\sigma \to 0$
$\varepsilon \to 0 \quad \sigma \to 0$
$C_p \to 0 \quad \varepsilon \to 0$
$C_p \to 0 \quad \alpha \to 0$
$C_p \to 0 \quad \alpha \to 0 \quad \varepsilon \to 0$

Computational issues

- Real physical thickness of interface is 10^{-8} cm; capillarity length 10^{-6} or 10^{-7} cm; sample 1 cm; radius of curvature 10^{-4} cm.
- Computations would be impossible with these parameters.
- Ansatz: If we extract the surface tension from the interface thickness, then we can increase the interface thickness by a factor of 1000 without influencing motion of the interface (C & Socolovsky 1989, 1991).

Discuss three projects

- (with Christof Eck and Xinfu Chen) Second order asymptotics (in ε) on the PF eqs;
- (with Emre Esenturk) Anisotropy and higher order PF eqs;
- (with Xinfu Chen and Emre Esenturk) New perspective in PF: use potential with non-local interactions and anisotropy to obtain elegant expressions for interface from microscopic considerations

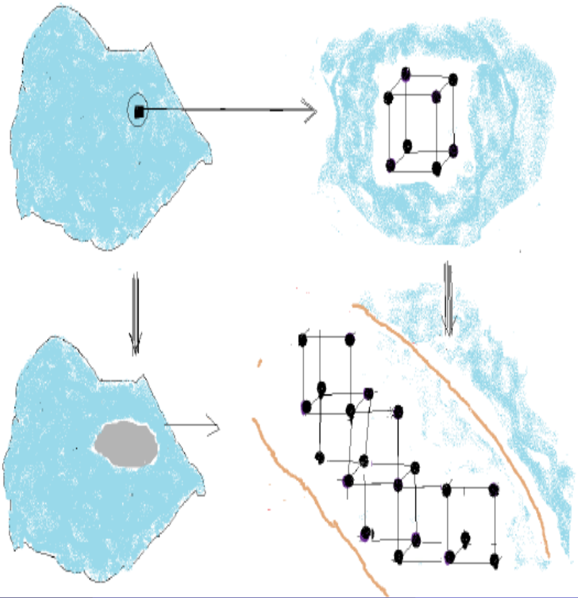
References

- (with C. Eck) "Rapidly converging phase field models via second order asymptotic" *Discrete and Continuous Dynamical Systems, Series B*, 142-152 (2005).
- (with X. Chen and C. Eck) "A rapidly converging phase field model," *Discrete and Continuous Dynamical Systems Series A*, 4, 1017-1034, 2006. Also,
  "Numerical tests of a phase field model with second order accuracy" *SIAM Applied Math* 68, 1518-1534 (2008).

References (continued)

- (with Emre Esenturk) "Anistropic Phase Field Equations of Arbitrary Order," to appear in *Discrete and Continuous Dynamical Systems, Series S 4, 311-350 (2011).*
- (with Xinfu Chen and E. Esenturk) "Interface condition for a phase field model with anisotropic and non-local interactions," *The Archive for Rational Mechanics and Analysis 202, 349-372 (2011).* Also, "A phase field model with non-local and anisotropic potential," *Modelling and Simulation in Materials Science and Engineering 19 (2011)*

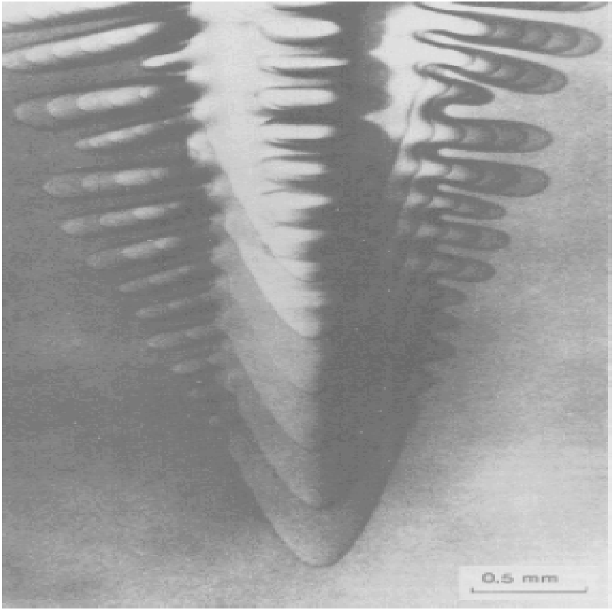
Microscopic interactions to macro behavior



Motivations

- Interest in the materials community in refined computations as computing advances.
- Better understanding of detailed anisotropy needed
- Understand relationships between molecular anisotropy, surface tension, equil shapes and dynamics

- Rubinstein & M. Glicksman (1991); and other experiments



Conditions on the interface

- Isotropic: Gibbs-Thomson relation

$$u[s]_E = -\sigma\kappa$$

σ is the surface tension,
$[s]_E$ is entropy difference between the phase per unit volume,
κ is the sum of principal curvatures, c is heat capacity and l is latent heat,
$u := (T - T_m)c/l$ is the reduced temperature,
T_m is the equilibrium melting temperature). When there is anisotropy, surface tension can be written as a function of surface normal, i.e. $\sigma(\hat{n})$. In this case, the equation above needs to be modified.

Generalization of Phase Field for second order convergence

$$u := \frac{T - T_E}{l/c}, \qquad D := \frac{K}{\rho c}, \qquad d_0 := \frac{\sigma}{[s]_E l/c}.$$

the sharp interface problem has the form

$$\begin{aligned} u_t &= D\Delta u && \text{in } \Omega(t)\backslash\Gamma(t) \\ v_n &= D\hat{n}\cdot\nabla u]_{+}^{-}, && \text{on } \Gamma(t) \\ u &= -\,d_0\left(\kappa + \alpha v_n\right) && \text{on } \Gamma(t) \end{aligned}$$

Gibbs-Thomson-Herring Condition (see also Kinderlehrer, Lee, Livshits, Ta'asan 2004).

Let

$$
\begin{aligned}
W(\pm 1) &= 0 < W(s) \quad \text{for all } s \neq \pm 1, \quad W''(\pm 1) > 0, \\
G'(\pm 1) &= 0, \qquad G(1) - G(-1) = \int_{-1}^{1} \sqrt{2W(s)}ds.
\end{aligned}
$$

The phase field equations corresponding are

$$
\begin{aligned}
\varepsilon^2 \left(\alpha_\varepsilon \phi_t - \Delta\phi \right) + W'(\phi) &= \varepsilon \frac{1}{d_0} G'(\phi) u \\
(u + \frac{1}{2}\phi)_t &= \Delta u
\end{aligned}
$$

where $\alpha_\varepsilon := \alpha + \varepsilon\alpha_1$ and α_1 is defined by

$$
\alpha_1 := \frac{\frac{1}{d_0} \int_{\mathbb{R}} \{ G(1) - G(\Phi(s)\} \left(1 + \Phi(s)\right) ds}{2 \int_{\mathbb{R}} \dot{\Phi}^2(s) ds}
$$

and Φ is the (unique) solution to

$$
\ddot{\Phi} - W'(\Phi) = 0 \quad \text{on} \quad \mathbb{R}, \quad \Phi(\pm\infty) = \pm 1, \quad \int_{\mathbb{R}} s\dot{\Phi}(s)ds = 0.
$$

Key Ideas

- Previous works used distance from the level set
  $\Gamma_\varepsilon(t) := \{x : \phi_\varepsilon(x,t) = 0\}$
  We used reference frame the level set corresponding to $\varepsilon = 0$, i.e.,$\Gamma_0(t)$.
- THEOREM. With the conditions above, there exists $\varepsilon_0 > 0$ and $C > 0$ such that solutions $(u_\varepsilon, \phi_\varepsilon)$ to the Phase Field equations satisfy

$$\text{distance}\{\Gamma_\varepsilon, \Gamma_0\} \le C\varepsilon^2 \quad \text{for all } 0 < \varepsilon < \varepsilon_0 .$$

$$
\begin{aligned}
\partial_t &= -v\partial_r + \partial_t^\Gamma, \quad \partial_t^\Gamma := \partial_t + \sum_{i=1}^{n-1} S_t^i \partial_{s^i}, \\
\nabla &= N\,\partial_r + \nabla^\Gamma, \quad \nabla^\Gamma := \sum_{i=1}^{n-1} \nabla S^i\,\partial_{s^i} \\
\Delta &= \partial_{rr} + \Delta R\,\partial_r + \Delta^\Gamma, \quad \Delta^\Gamma := \sum_{i=1}^{n-1} \Delta S^i \partial_{s^i} + \sum_{i,j=1}^{n-1} \nabla S^i \cdot \nabla S^j \partial_{s^i s^j}
\end{aligned}
$$

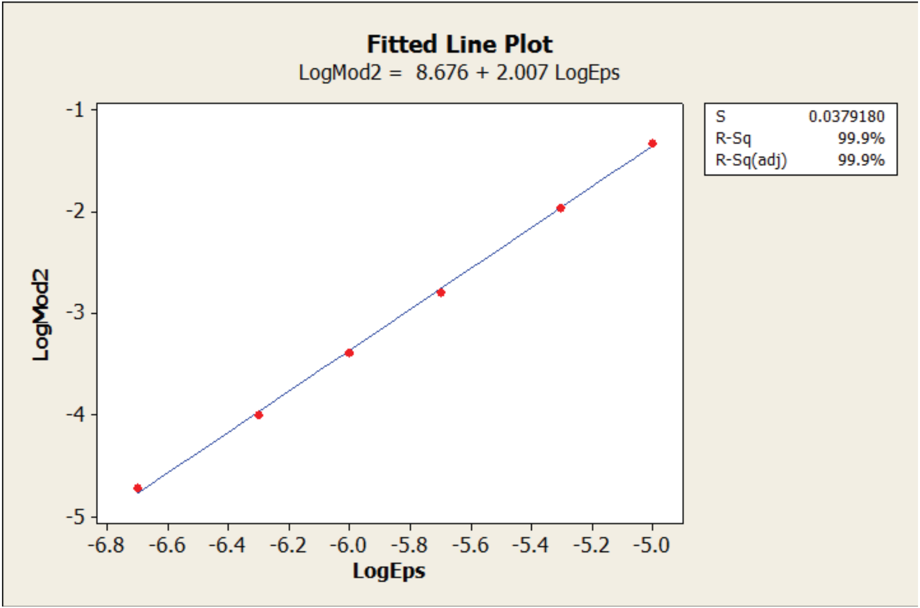
where $\nabla S^i(x,t), S_t^i(x,t), \Delta R(x,t), R_t(x,t)$ are evaluated at $x = X_0(s,t) + rN(s,t)$, and are regarded as functions of (r,s,t).

$$
\begin{aligned}
w_t &= \{-v_0\varepsilon^{-1} - \partial_t^\Gamma h_\varepsilon\} w_\rho + \partial_t^\Gamma w \\
\nabla w &= \{N\varepsilon^{-1} - \nabla^\Gamma h_\varepsilon\} w_\rho + \nabla^\Gamma w, \\
\Delta w &= \{\varepsilon^{-2} + |\nabla^\Gamma h_\varepsilon|^2\} w_{\rho\rho} + \{\Delta R\, \varepsilon^{-1} - \Delta^\Gamma h_\varepsilon\} w_\rho \\
&\quad -2\nabla^\Gamma h_\varepsilon \cdot \nabla^\Gamma w_\rho + \Delta^\Gamma w
\end{aligned}
$$

where $\nabla^\Gamma, \partial_t^\Gamma, \Delta^\Gamma$ are again differentiations with ρ fixed.

Numerical Studies

- Are C and ε_0 too big or small to be useful?
- Take specific W, G and α_1 that satisfy conditions.
- Relative difference between true soln and computed.
- Computations show difference goes as ε^2.
- Several sets of parameters, incuding dendritic.


Fitted Line Plot
LogMod2 = 8.676 + 2.007 LogEps
S 0.0379180
R-Sq 99.9%
R-Sq(adj) 99.9%
LogMod2
-1
-2
-3
-4
-5
-6.8
-6.6
-6.4
-6.2
-6.0
-5.8
-5.6
-5.4
-5.2
-5.0
LogEps

Anisotropy

Two basic approaches we have used.
1. The usual phase field equations arise from truncating Fourier expansion after q^2 (so we have second order). The molecular anisotropy is largely "averaged out" when we do this. By retaining higher order Fourier modes, and using higher order differential equations, we can obtain the classical Gibbs-Thomson-Herring relation (in $2d$) at the interface:

$$u[s]_E = -(\sigma + \sigma'')\kappa$$

and its dynamical generalization.
In $3d$ things are more complicated.

A new approach to anisotropy (with or w/o non-local interactions) in arbitrary spatial dimension

Idea of working directly on the integral form (avoiding higher order DEs).
Include non-local interactions.
The entropic part of the free energy involves

$$\{\phi_k \ln \phi_k + (1 - \phi_k) \ln(1 - \phi_k)\}$$

is often approximated in applications by a smooth double well potential, denoted $W(\phi_k)$, which takes its minimum values on the bulk (i.e., single phase) material.

1. These ideas lead to a free energy:

$$F[\phi] = \sum_{k,l} \frac{1}{4} J_{kl} \left(\phi_k - \phi_l\right)^2 + \sum_k W(\phi_k) + \sum_k uG(\phi_k).$$

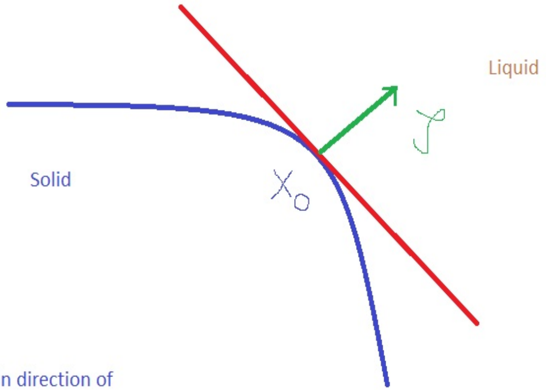
The free energy in the continuum limit:

$$\mathcal{F}[\phi] = \frac{1}{4} \int J_\varepsilon(x-y)(\phi(x) - \phi(y))^2 dxdy + \int W(\phi(x))dx + \int uG(\phi(x))\, dx$$

where $J_\varepsilon(z) = \varepsilon^{-N} J(\varepsilon^{-1} z)$, ε is an atomic length scale; $G(\phi)$ represent the entropy difference per unit volume. For simplicity we assume $\Omega = \mathbb{R}^d$ with $d \geq 2$.

2. The phase field equation can be obtained by the assumption that the variational derivative of the free energy should be proportional to the time derivative of the phase field, i.e.,

$$\alpha\varepsilon^2 \phi_t = J_\varepsilon * \phi - \phi - W'(\phi) + \varepsilon u G'(\phi)$$



Traveling wave in direction of zeta at point x_0.

The surface tension is the difference per unit area between the free energy with the interface and without, i.e.,

$$\sigma = \frac{\mathcal{F}[\phi] - (\mathcal{F}[-1] + \mathcal{F}[1])/2}{Area}..$$

$$\begin{aligned}\sigma(\zeta) &:= \int_{\mathbb{R}} \left\{ W(Q(\zeta, z)) + \frac{1}{2} Q(\zeta, z)(Q(\zeta, z) - (j * Q)(\zeta, z) \right\} dz \\ &= \int_{\mathbb{R}} \left(W(Q(\zeta, z)) - \tfrac{1}{2} Q(\zeta, z) W'(Q(\zeta, z)) \right) dz,\end{aligned}$$

where the second line is obtained by making use of equation

$$\begin{aligned} 0 &= [(j * Q)(\zeta, z) - Q(\zeta, z)] - W'(Q(\zeta, z)) \\ \pm 1 &= \lim_{z \to \pm\infty} Q(\zeta, z), \quad Q(\zeta, 0) = 0 \end{aligned}$$

When $\zeta = \hat{n}$, i.e., the points located on the interface, $\sigma(\zeta) = \sigma(\hat{n})$ corresponds to the surface tension of the interface.

Notation

Let $h(x, t)$ be the signed distance (positive in the liquid) from the point x to Γ_t, the limit interface between liquid and solid at time t. Then, in the local coordinate system $(s', h) := \left(s^1, ..., s^{N-1}, h\right) \in \mathbb{R}^N$, one has

$$x = x_0(s') + h\hat{n}(s'),$$

where $\hat{n}$ is the unit normal. Thus, with these definitions, $D^2 h$ and $\overrightarrow{\nabla}\hat{n}$ are $N \times N$ matrices with components $\left(D^2 h\right)_{ij} = \partial h_i / \partial x_j$ and $\left(\overrightarrow{\nabla}\hat{n}\right)_{ij} = \partial \hat{n}_i / \partial x_j$ and are related to each other in the following way

$$\overrightarrow{\nabla} h = \hat{n}^T \quad \textit{and} \quad D^2 h = \overrightarrow{\nabla}\hat{n}.$$

Also, the velocity of the interface at an arbitrary point $x_0 \in \Gamma_t$ be expressed as

$$v\left(x_0, t\right) = \frac{\partial h\left(x_0, t\right)}{\partial t}.$$

Main Theorem

The solution ϕ of

$$\begin{aligned}\alpha\varepsilon^2\phi_t &= J_\varepsilon * \phi - \phi - W'(\phi) + \varepsilon u G'(\phi)\\ (u + \frac{1}{2}\phi)_t &= \Delta u\end{aligned}$$

admits a formal asymptotic expansion only if the Gibbs-Thomson-Herring condition (with linear kinetics) is satisfied, i.e.,

$$u + \alpha(\hat{n})v + \mathrm{Trace}\left\{\overrightarrow{\nabla}\hat{n}\ D^2\sigma(\hat{n})\right\} = 0.$$

Using tensor notation this can also be expressed as

$$u + \alpha(\hat{n})v + \overrightarrow{\nabla}\hat{n}\ : D^2\sigma(\mathbf{n}) = 0.$$

The Wulff shape is the shape of a solid under the undercooling temperature $u := 1$.

- $2d$ example with anisotropy, $J(x,y) =: \bar{J}(r,\theta)$.
- We will compute the Wulff shape by (i) utilizing the planar solutions, (ii) calculating the corresponding surface free energy $\bar{\sigma}(\theta) =: \sigma(\hat{n})$, and (iii) solving the differential equation

$$\bar{\sigma}(\theta) + \bar{\sigma}''(\theta) = -u\,[s]_E\,/\kappa(\theta)$$

Let $\bar{J}(r, \theta)$ be given by

$$\bar{J}(r, \theta) = f_0(r) + \delta \cos(n\theta) f_1(r), \qquad r = \sqrt{x^2 + y^2}, \quad \tan\theta = \frac{y}{x},$$

As an illustration, we choose the following:

$$n = 6, \qquad f_0(r) = \frac{e^{-r^2}}{\pi}, \qquad f_1(r) = -\frac{r^6 e^{3-2r^2}}{27\pi} .$$

For $\hat{n} = (\cos\theta, \sin\theta)$ we have

We integrate $\bar{J}$ in the direction orthogonal to the normal to obtain $\bar{j}$

$$\begin{aligned} \bar{j}(\theta, z) \quad &: \quad = \int_{-\infty}^{\infty} \bar{J}\left(\sqrt{z^2 + l^2},\ \theta + \arctan \frac{l}{z}\right) dl \\ &= \quad \hat{j}(\delta \cos n\theta, z) \end{aligned}$$

where

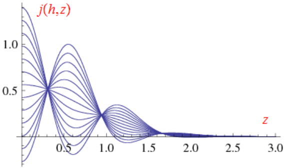
$$\begin{aligned} \hat{j}(h, z) \quad &= \quad j_0(z) + hj_n(z) \\ j_0(z) \quad &: \quad = 2\int_0^{\infty} f_0(\sqrt{z^2 + l^2}) dl \\ j_n(z) \quad &: \quad = 2\int_0^{\infty} f_1(\sqrt{z^2 + l^2}) \cos(n \arctan \frac{l}{z}) dl \end{aligned}$$

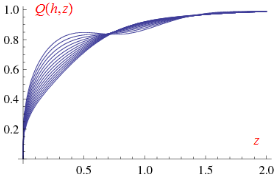
In our example, we have (recall $\delta \cos(n\theta)$ is form of anisotropy with $n = 6$)

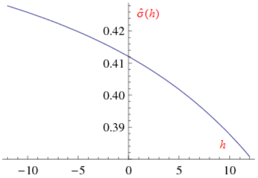
$$j_0(z) = \frac{e^{-z^2}}{\sqrt{\pi}}, \qquad j_6(z) = \frac{e^{3-2z^2}(15 - 180z^2 + 240z^4 - 64z^6)}{1728\sqrt{2\ \pi}}.$$

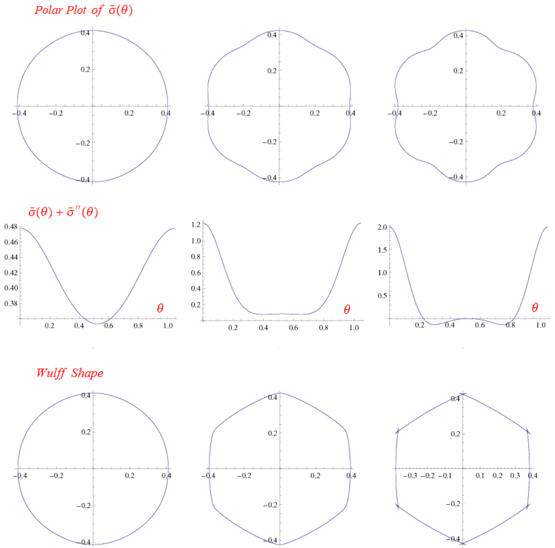
Increasing δ (amplitude of anisotropy) means equil shape is more like a hexagon. At at critical value of δ, one obtains sharp vertices of a hexagon.

Plots of $\hat{j}(h,z)$, $Q(h,z)$ and $\hat{\sigma}(h)$. Horizontal axis is z in first two graphs.









Polar Plot of $\bar{\sigma}(\theta)$
$\bar{\sigma}(\theta) + \bar{\sigma}''(\theta)$
θ
θ
θ
Wulff Shape

Thank you!