Flots de courbure moyenne multiphase avec mobilités et applications à la croissance de nanofils

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Motivation

Many physical systems involve several phases and associated interfaces whose shapes minimize a general area energy (under various constraints).

Many restoration problems (in particular, in image processing) require the reconstruction of volumes whose boundaries minimize a general area energy (under various constraints).

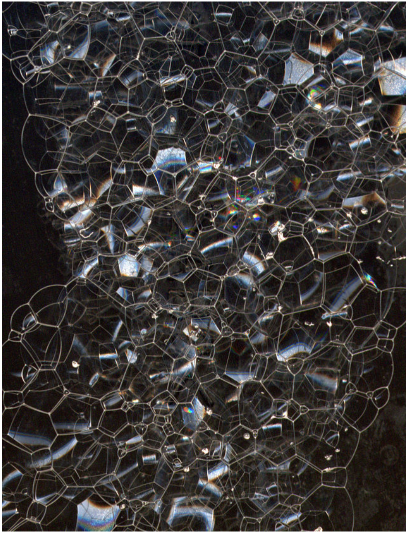
We are interested in simulating such systems, and solving such problems.

Examples: Wetting

Droplet wetting on a lotus leaf
(energy = area)

Bubbles

Bubbles



Soap foam

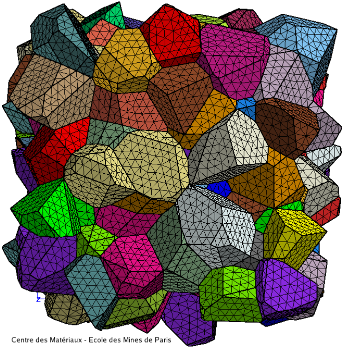
(energy $=$ multiphase area)

Honeycomb

Honeycomb
(energy = 2D multiphase perimeter)

Polycrystalline materials

Silicon



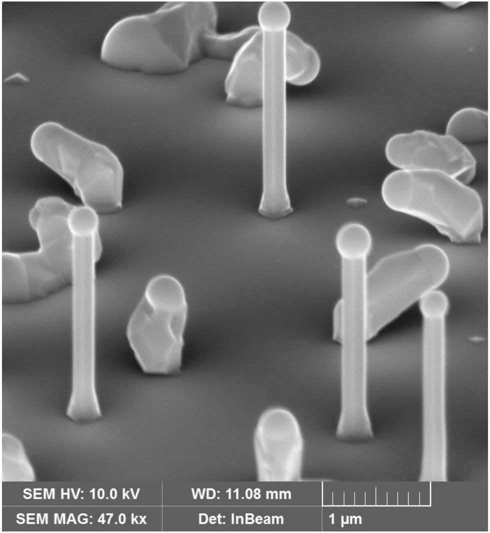
Polycrystalline material

(energy=multiphase inhomogenous area)

$$E(\Sigma_1, \ldots, \Sigma_N) = \frac{1}{2} \sum_{i,j=1}^{N} \sigma_{i,j} \,\mathrm{Area}(\partial\Sigma_i \cap \partial\Sigma_j)$$

($\sigma_{i,j}$ are surface tensions)

Nanowires



Nanowires
(energy = multiphase anisotropic area)

Phases and interfaces

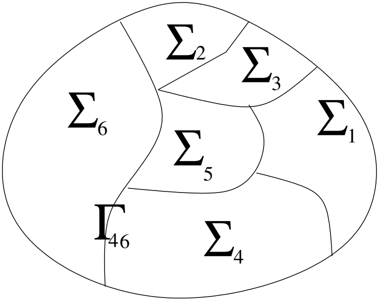
Let $D \subset \mathbb{R}^d$

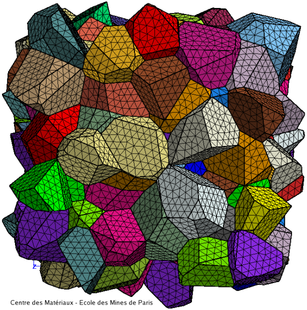
Consider a partition of D in N closed sets $\Sigma_1, \ldots, \Sigma_N$ called phases s.t.

$$D = \bigcup_{i=1}^{N} \Sigma_i$$

$$\Sigma_i \cap \Sigma_j = \partial\Sigma_i \cap \partial\Sigma_j, \quad i \neq j$$

Denote $\Gamma_{ij} = \partial\Sigma_i \cap \partial\Sigma_j$.





Multiphase perimeter

$$E(\Sigma_1, \dots, \Sigma_N) = \frac{1}{2} \sum_{i,j=1}^{N} \sigma_{i,j} \mathcal{H}^{\mathrm{d}-1}(\Gamma_{i,j}) = \frac{1}{2} \sum_{i,j=1}^{N} \sigma_{i,j} \int_{\Gamma_{i,j}} d\Gamma$$

where $\sigma_{i,j} \in \mathbb{R}^{d^2}$ are surface tensions s.t.

$$\begin{array}{l} \sigma_{ii} = 0 \\ \sigma_{ij} = \sigma_{ji} > 0 \quad \forall i \neq j \\ \text{triangle inequality} \qquad \sigma_{ij} + \sigma_{jk} \geq \sigma_{ik} \end{array}$$

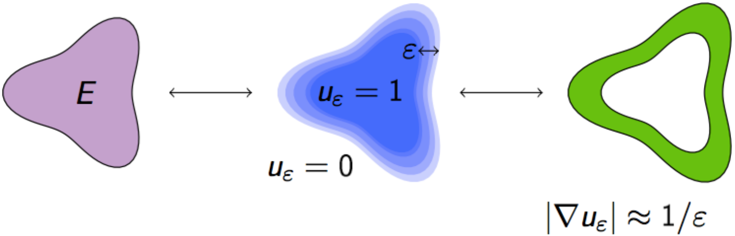
Introduction to Phase Field Approximation

Take a set $E \subset \mathbb{R}^N$ and its characteristic function $\mathbb{1}_E$

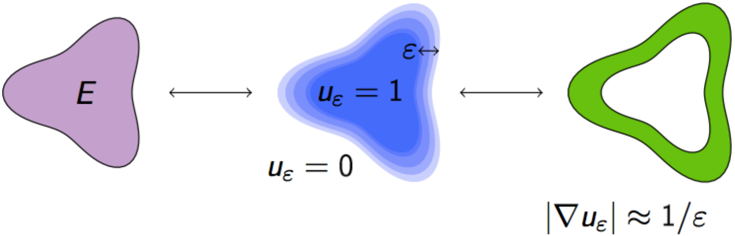
A smooth approximation $u_\varepsilon : \mathbb{R}^N \to [0,1]$ of $\mathbb{1}_E$ is called a phase field.

The set $\{u_\varepsilon = \frac{1}{2}\}$ is an approximation of the boundary ∂E.

The area of ∂E is called the perimeter of E.



Perimeter approximation

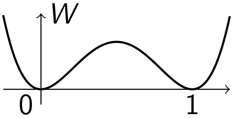


Thus, $\int \varepsilon |\nabla u_\varepsilon|^2 \mathrm{d}x \approx \frac{1}{\varepsilon} \mathit{Area} \approx \frac{1}{\varepsilon} \varepsilon P(E) = P(E) \quad$ as $\varepsilon \to 0$.

However, any constant function has zero energy! How to force u_ε to be close to a characteristic function?

Perimeter approximation

Use a double-well potential, for instance $W(s) = \frac{1}{2}s^2(1-s)^2$.



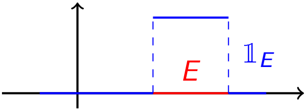
If $\sup_{\varepsilon} \left(\int \frac{1}{\varepsilon} W(u_\varepsilon) \mathrm{d}x \right) < +\infty$ then $u_\varepsilon \to 0$ or 1 a.e. as $\varepsilon \to 0$, i.e. u_ε approximates a characteristic function.

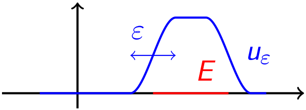
The Van der Waals Cahn-Hilliard functional

Phase field approximation of $P(E)$

If u_ε is a smooth approximation of $\mathbb{1}_E$, the phase-field approximation of $P(E)$ is the Van der Waals-Cahn-Hilliard energy

$$P_\varepsilon(u_\varepsilon) = \int \left(\frac{\varepsilon}{2} |\nabla u_\varepsilon|^2 + \frac{1}{\varepsilon} W(u_\varepsilon) \right) \mathrm{d}x$$





Key idea: replace the highly singular energy P by the smooth energy P_ε.

Phase-field approximation of perimeter

Convergence of P_ε (Modica, Mortola - 1977)

P_ε Γ-converges to

$$P(u) = \begin{cases} \lambda\, P(E) & \text{si } u = \mathbb{1}_E \text{ has bounded variations } (\mathrm{BV}) \\ +\infty & \text{otherwise} \end{cases}$$

(where $\lambda = cst$ depends only on potential W).

Γ-convergence is the right notion of convergence for functionals in a variational context (due to De Giorgi).

Γ-convergence and minimizers

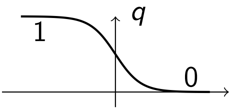
If (F_n) Γ-converges to F and, $\forall n$, u_n is a minimizer of F_n, then every cluster point of (u_n) minimizes F.

In other words: minimizers of P_ε approximate minimizers of P.

Optimal profile

The phase-field optimal profile associated with E is:

$$u_\varepsilon(x) = q\left(\frac{1}{\varepsilon} d_s(x,E)\right) \qquad \text{with} \quad q(s) = \frac{1}{2}(1 - \tanh(\frac{s}{2}))$$



Signed distance

$$d_s(x,E) = d(x,E) - d(x, \mathbb{R}^N \setminus E)$$

Convergences

For a bounded set E

- $u_\varepsilon \to \mathbb{1}_E$
- $P_\varepsilon(u_\varepsilon) \to \lambda P(E)$ if E has finite perimeter

as $\varepsilon \to 0$.

Phase field mean curvature flow

$$u_t = \Delta u - \frac{1}{\varepsilon^2} W'(u)$$

Easy to simulate numerically using a splitting scheme and Fourier series with periodic boundary conditions

Evolution law and equilibrium at interfaces

The Clausius-Duhem inequality in sharp interface theory implies that normal and velocity are proportional:

Interface velocity

$$\frac{1}{m_{ij}} V_{ij} = \sigma_{ij} H_{ij} \quad \text{a.e. } x \in \Gamma_{ij},$$

with m_{ij} the interface mobilities.

Herring's condition (equilibrium at triple points)

If x is a triple-junction between phases i, j, k, then

$$\sigma_{ij} n_{ij} + \sigma_{jk} n_{jk} + \sigma_{ki} n_{ki} = 0,$$

Multiphase mean curvature flow: the additive case I

Assumption: $\exists\ \sigma_i \geq 0$ such as $\sigma_{ij} = \sigma_i + \sigma_j$.
Always true for three phases

Then

$$\boldsymbol{P}(\Omega_1, \Omega_2, \cdots, \Omega_N) = \frac{1}{2} \sum_{1 \leq i < j \leq N} \sigma_{ij} \int_{\Gamma_{ij}} 1 d\sigma = \sum_{i}^{N} \sigma_i \int_{\partial \Omega_i} 1 d\sigma.$$

can be approximated by

$$\boldsymbol{P}_\varepsilon(\boldsymbol{u}) = \begin{cases} \frac{1}{2} \sum_{i=1}^{N} \int_Q \sigma_i \left(\varepsilon \frac{|\nabla u_i|^2}{2} + \frac{1}{\varepsilon} W(u_i) \right) dx, & \text{if } \sum_{i=1}^{N} u_i = 1, \\ +\infty & \text{otherwise.} \end{cases}$$

Multiphase mean curvature flow: the additive case II

The L^2 gradient flow is

$$\partial_t u_k^\varepsilon = \sigma_k \left[\Delta u_k^\varepsilon - \frac{1}{\varepsilon^2} W'(u_k^\varepsilon)\right] + \lambda^\varepsilon, \quad \forall k = 1, \ldots, N,$$

where the Lagrange multiplier field λ^ε comes from $\sum_{k=1}^N u_k^\varepsilon = 1$.

Method of matched asymptotic expansions:
If $\Omega_i^\varepsilon = \left\{x \in D; u_i(x,t) \geq \frac{1}{2}\right\}$, then around the interface Γ_{ij}^ε the solution $\boldsymbol{u}^\varepsilon$ satisfies

$$\begin{cases} u_i^\varepsilon & = q\left(\frac{dist(x,\Omega_i^\varepsilon)}{\varepsilon}\right) + O(\varepsilon), \\ u_j^\varepsilon & = 1 - q\left(\frac{dist(x,\Omega_i^\varepsilon)}{\varepsilon}\right) + O(\varepsilon), \\ u_k^\varepsilon & = O(\varepsilon), \text{ for k } \in \{1,2,\ldots,N\} \setminus \{i,j\} \end{cases}$$

Moreover, for the associated normal velocity: $V_{ij}^\varepsilon = \frac{1}{2}\sigma_{ij} H_{ij} + O(\varepsilon)$.

The convergence is only linear.

Multiphase mean curvature flow: the additive case III

Localize now the Lagrange multiplier (see [Bretin-Denis, 2017]) to improve the accuracy:

$$\partial_t u_k^\varepsilon = \sigma_k \left[\Delta u_k^\varepsilon - \frac{1}{\varepsilon^2} W'(u_k^\varepsilon) \right] + \lambda^\varepsilon \sqrt{2W(u_k)} \quad \forall k = 1, \dots, N,$$

Then, near Γ_{ij}^ε:

$$\begin{cases} u_i^\varepsilon & = q\left(\frac{dist(x, \Omega_i^\varepsilon)}{\varepsilon} \right) + O(\varepsilon^2), \\ u_j^\varepsilon & = 1 - q\left(\frac{dist(x, \Omega_i^\varepsilon)}{\varepsilon} \right) + O(\varepsilon^2), \\ u_k^\varepsilon & = O(\varepsilon^2), \text{ for k } \in \{1, 2, \dots, N\} \setminus \{i, j\}, \end{cases}$$

with $V_{ij}^\varepsilon = \frac{1}{2}\sigma_{ij} H_{ij} + O(\varepsilon)$.

The convergence is quadratic

Incorporating the mobilities: the energy viewpoint

[Garcke-Nestler-Stoth'99] propose to plug the mobilities m_{ij} directly in the Cahn-Hilliard energy:

$$\boldsymbol{P}_\varepsilon(\boldsymbol{u}) = \int_Q \varepsilon f(\boldsymbol{u}, \nabla \boldsymbol{u}) + \frac{1}{\varepsilon} W(\boldsymbol{u}) dx,$$

where $f(\boldsymbol{u}, \nabla \boldsymbol{u}) = \sum_{i<j} m_{ij}\sigma_{ij} \left| u_i \nabla u_j - u_j \nabla u_i \right|^2$ and

$$W(\boldsymbol{u}) = 9 \sum_{i,j=1, i<j}^{N} \frac{\sigma_{ij}}{m_{ij}} u_i^2 u_j^2 + \sum_{i<j<k} \sigma_{ijk} u_i^2 u_j^2 u_k^2.$$

The term $\sum_{i<j<k} \sigma_{ijk} u_i^2 u_j^2 u_k^2$ is a penalization term, with σ_{ijk} ufficiently large as to ensure the Γ-convergence of $\boldsymbol{P}_\varepsilon$ to $\boldsymbol{P}$.

As the mobilities appear in the energy form (and not only in the flow of $\boldsymbol{P}_\varepsilon$), the size of the diffuse interface Γ_{ij} depends on m_{ij}.

This is a limitation for high contrast mobilities, and degenerate mobilities cannot be handled.

Incorporating the mobilities: the metric viewpoint

Define the gradient flow of $\boldsymbol{P}_\varepsilon$ with respect to a weighted scalar product:

$$\langle \boldsymbol{u}, \boldsymbol{v} \rangle_{L^2_A(Q,\mathbb{R}^d)} = \int_Q (\boldsymbol{A}\boldsymbol{u}) \cdot \boldsymbol{v}\, dx$$

where the matrix $\boldsymbol{A}$ depends on mobilities m_{ij}.

Additive mobilities

Assumption: there exist $m_i \geq 0$ such as

$$\frac{1}{m_{ij}} = \frac{1}{m_i} + \frac{1}{m_j}.$$

Then, choosing $\boldsymbol{A} = \boldsymbol{M}^{-1}$ with

$$M_{ij} = \begin{cases} m_i & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

leads to the Allen-Cahn system:

$$\partial_t u_k^\varepsilon = m_k \left[\sigma_k \left(\Delta u_k^\varepsilon - \frac{1}{\varepsilon^2} W'(u_k^\varepsilon) \right) + \lambda^\varepsilon \sqrt{2W(u_k)} \right], \quad \forall k \in \{1, 2, \cdots, N\}$$

where the Lagrange multiplier field λ^ε is, as usual, associated with the constraint $\sum u_i^\varepsilon = 1$.

Additive mobilities

Then, around the interface Γ_{ij}, the solution $\boldsymbol{u}^\varepsilon$ satisfies (formally):

$$\begin{cases} u_i^\varepsilon & = q\left(\frac{dist(x,\Omega_i^\varepsilon)}{\varepsilon}\right) + O(\varepsilon^2), \\ u_j^\varepsilon & = 1 - q\left(\frac{dist(x,\Omega_i^\varepsilon)}{\varepsilon}\right) + O(\varepsilon^2), \\ u_k^\varepsilon & = O(\varepsilon^2), \text{ for k } \in \{1,2,\dots,N\} \setminus \{i,j\}, \end{cases}$$

with

$$\frac{1}{m_{ij}} V_{ij}^\varepsilon = \sigma_{ij} H_{ij} + O(\varepsilon).$$

The convergence is quadratic.

General mobilities

Define

$$A_{ij} = \begin{cases} -\frac{1}{m_{ij}} & \text{if} i \neq j \\ 0 & \text{if } i = j. \end{cases}$$

which leads to

$$\boldsymbol{A}\partial_t \boldsymbol{u}^\varepsilon = \sigma \Delta \boldsymbol{u}^\varepsilon - \frac{1}{\varepsilon^2} W'(\boldsymbol{u}^\varepsilon) + \lambda^\varepsilon \sqrt{2W(\boldsymbol{u}^\varepsilon)},$$

where, for all $k \in \{1, 2, \cdots, N\}$,

$$(\sigma \Delta \boldsymbol{u})_k = \sigma_k \Delta u_k, \quad W'(\boldsymbol{u})_k = W'(u_k) \text{ and } \quad (\sqrt{2W(\boldsymbol{u})})_k = \sqrt{2W(u_k)}.$$

This system is well-posed as soon as $\boldsymbol{A}$ is semi-definite positive on $(1, 1, \cdots, 1)^\perp$, which in turn imposes some restriction on the choice of the mobilities m_{ij}.

General mobilities

Around the interface $\Gamma_{ij}^{\varepsilon}$, the solution $\boldsymbol{u}^{\varepsilon}$ satifies (formally)

$$\begin{cases} u_i^{\varepsilon} & = q\left(\frac{dist(x,\Omega_i^{\varepsilon})}{\varepsilon}\right) + O(\varepsilon), \\ u_j^{\varepsilon} & = 1 - q\left(\frac{dist(x,\Omega_i^{\varepsilon})}{\varepsilon}\right) + O(\varepsilon), \\ u_k^{\varepsilon} & = O(\varepsilon), \text{ for k } \in \{1,2,\dots,N\} \setminus \{i,j\}, \end{cases}$$

with

$$\frac{1}{m_{ij}} V_{ij}^{\varepsilon} = \sigma_{ij} H_{ij} + O(\varepsilon).$$

The model is of order 1 only.

Numerical approximation

A robust, accurate, fast, and convergent scheme can be designed thanks to the previous considerations.

It is heavily based on Fourier representation.

Numerical iterative scheme

1. L^2-gradient flow of the Cahn-Hilliard energy without constraint: let $\boldsymbol{u}^{n+1/2}$ be an approximation of $\boldsymbol{v}(\delta_t)$ where $\boldsymbol{v} = (v_1, v_2, \ldots, v_N)$ is the solution of

$$\begin{cases} \partial_t v_k(x,t) & = m_k \sigma_k \left[\Delta v_k(x,t) - \frac{1}{\varepsilon^2} W'(v_k(x,t))\right] \quad \forall (x,t) \in Q \times [0, \\ \boldsymbol{v}(x,0) & = \boldsymbol{u}^n(x), \quad \forall x \in Q \text{ with periodic boundary conditions.} \end{cases}$$

2. Projection onto the partition and volume constraints: for all $k \in \{1, 2, \ldots, N\}$ define u_k^{n+1} by

$$u_k^{n+1} = u_k^{n+1/2} + m_k \lambda^{n+1} \sqrt{2W(u_k^{n+1/2})} + m_k \mu_k^{n+1} G_k(\boldsymbol{u}^{n+1/2}),$$

where λ^{n+1} and μ_i^{n+1} are defined to satisfy the discrete constraints $\sum_{k=1}^N u_k^{n+1} = 1$ and $\int_Q u_k^{n+1} = V_k^{n+1} = \mathrm{V}ol_k((n+1)\delta_t)$.

In the special case of nanowires VLS growth, $\boldsymbol{u} = (u_S, u_L, u_V)$ and the potentials G_k are:

$$G_L(\boldsymbol{u}) = \sqrt{2W(u_L)}, \quad G_S(\boldsymbol{u}) = u_S u_L, \text{ and } \quad G_V(\boldsymbol{u}) = u_V u_L.$$

Numerical scheme

1. Use a semi-implicit Fourier spectral scheme;
2. All projections can be computed explicitly.

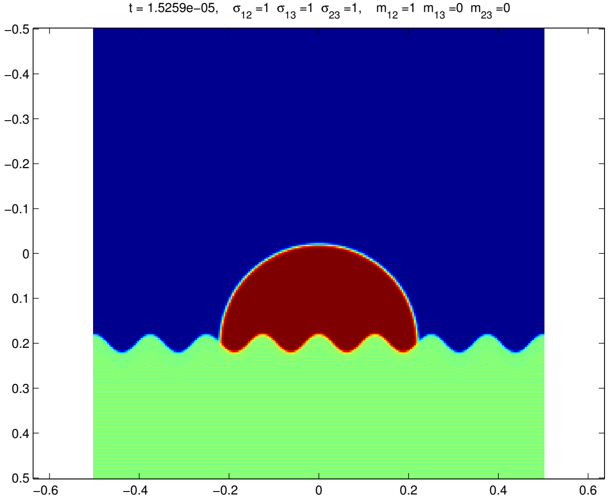
Highly contrasted and even degenerate mobilities can be handled!

Simulations for various mobilities/surface tensions I

Blue=1, Red=2, Green=3

$m = (m_{12}, m_{13}, m_{23}) = (1, 0, 0)$,

$\sigma = (1, 1, 1)$



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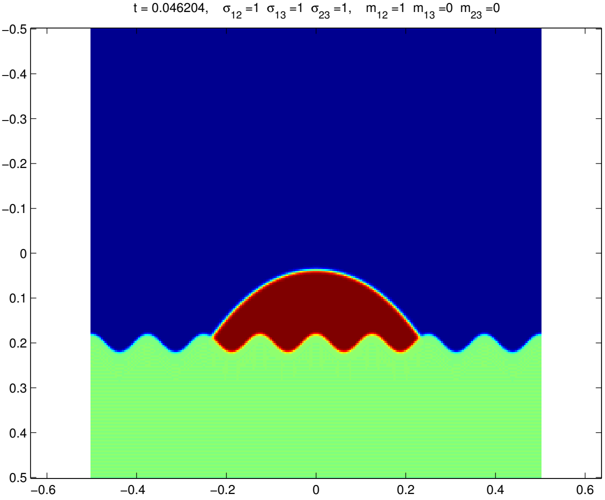

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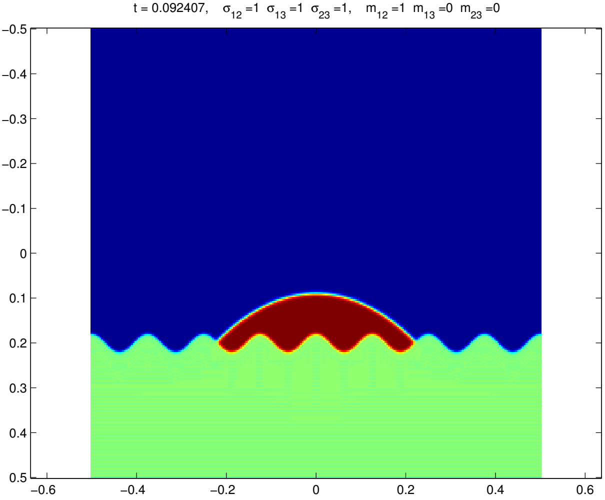

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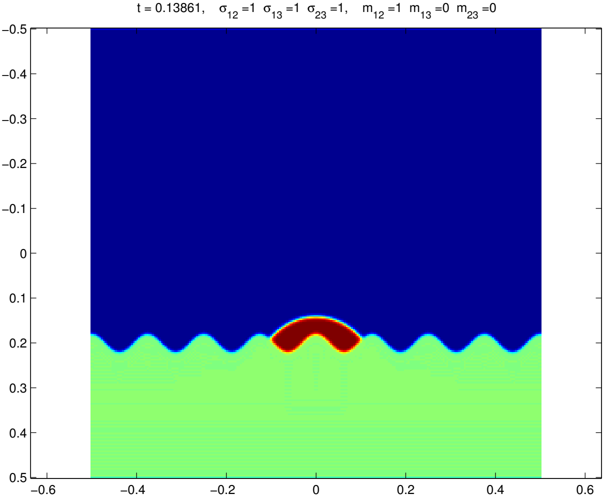
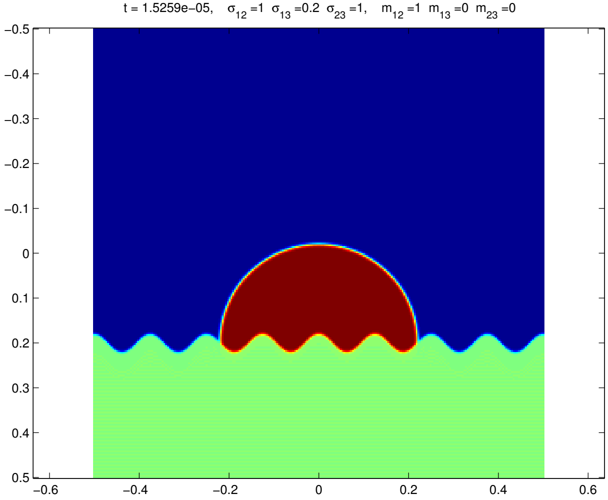


Simulations for various mobilities/surface tensions II

Blue=1, Red=2, Green=3

$m = (m_{12}, m_{13}, m_{23}) = (1, 0, 0)$,

$\sigma = (1, 0, 2.1)$



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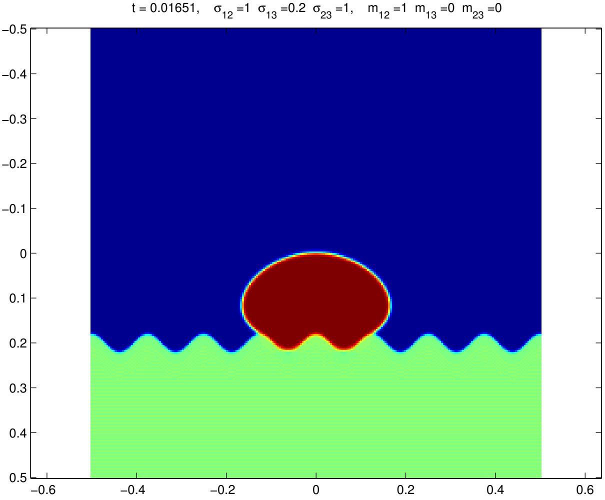

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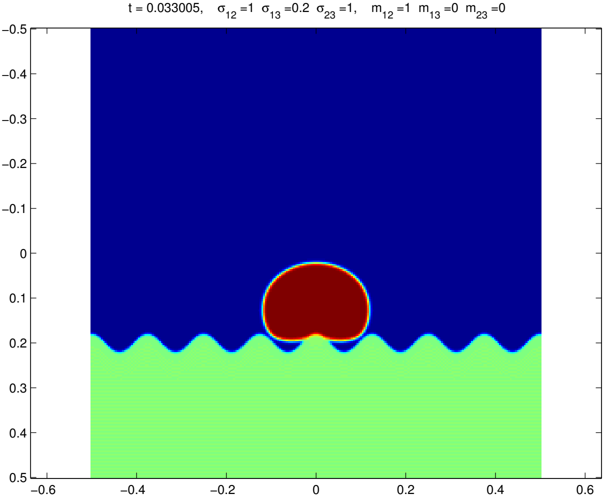

Simulations for various mobilities/surface tensions II

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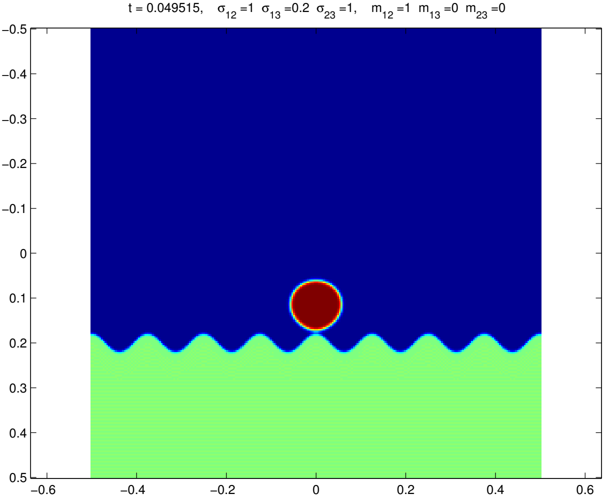
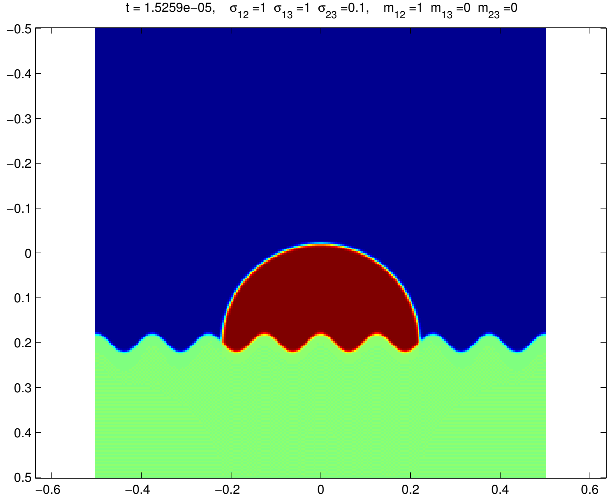


Simulations for various mobilities/surface tensions III

Blue=1, Red=2, Green=3

$m = (m_{12}, m_{13}, m_{23}) = (1, 0, 0)$,

$\sigma = (1, 1, 0.2)$



Simulations for various mobilities/surface tensions III

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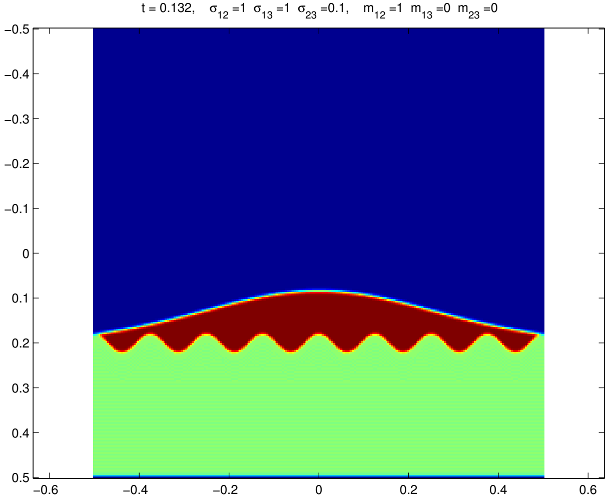

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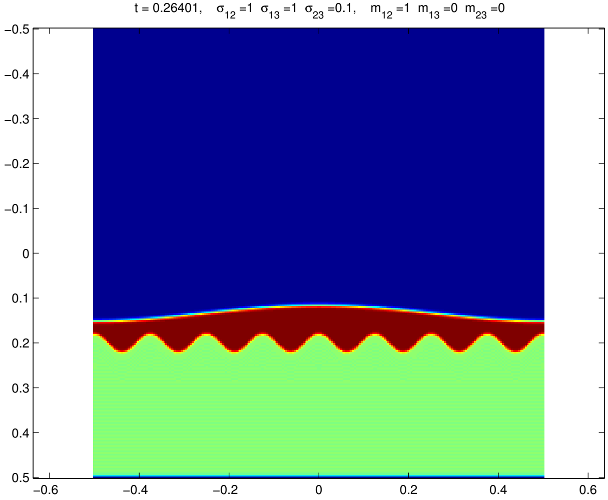

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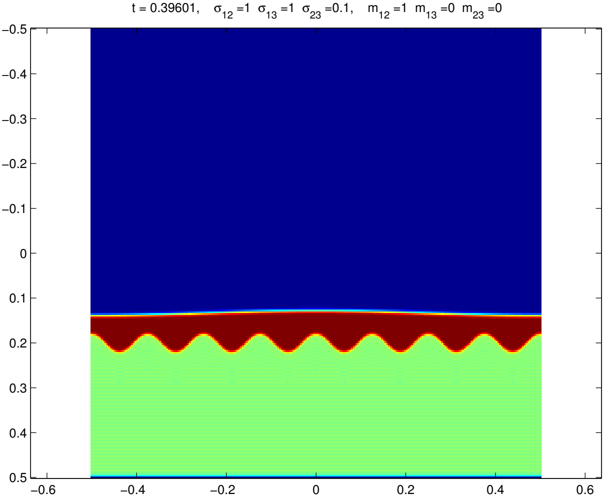
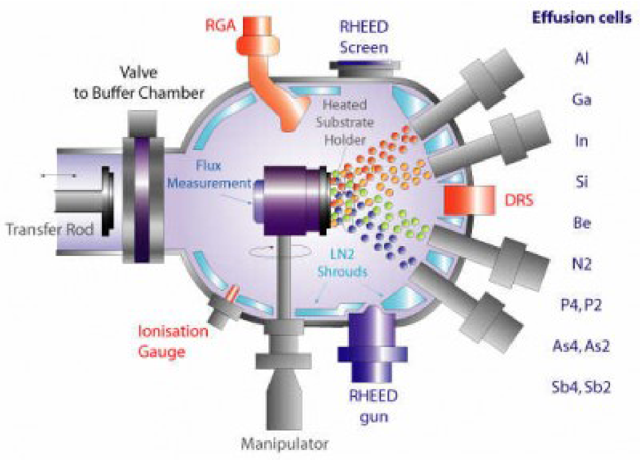
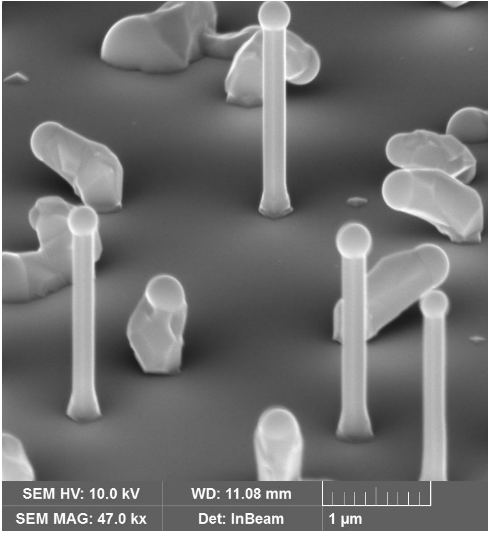


Molecular Beam Epitaxy

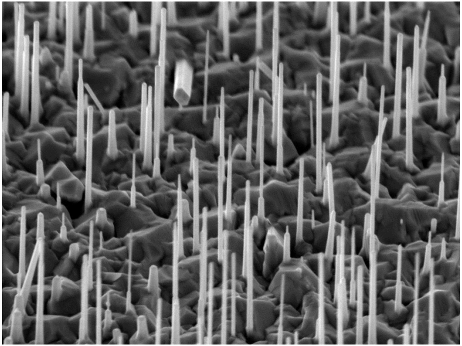
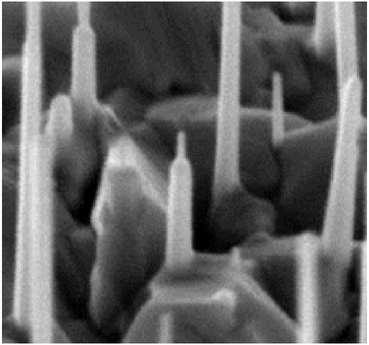


Nanowires

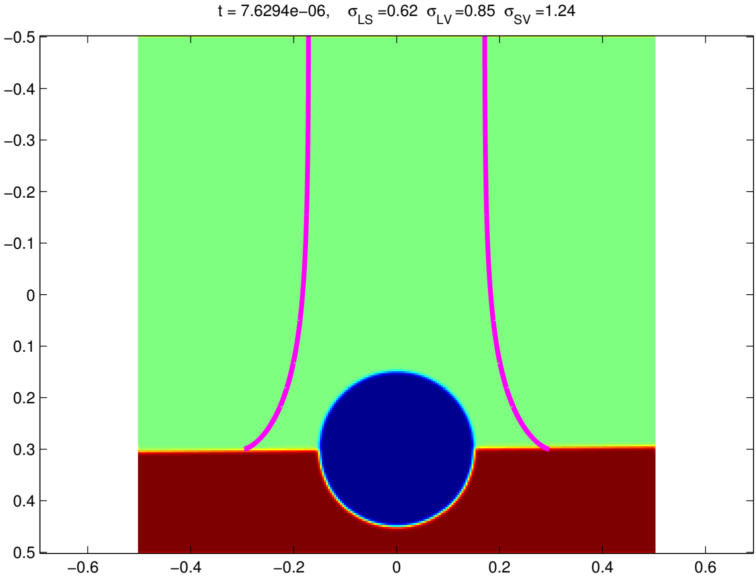


Nanowires

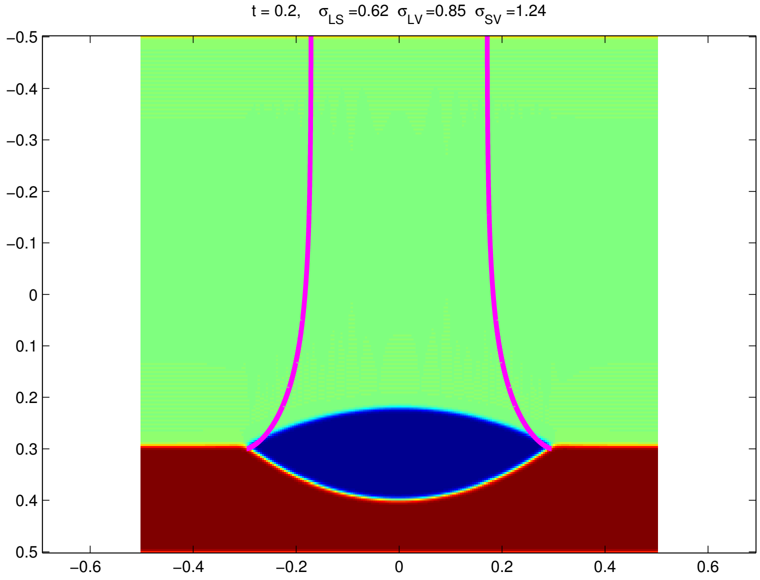
Nanowires with thinning

Nanowire growth with $\sigma_{Ge} = (0.62, 0.85, 1.24)$



Nanowire growth with $\sigma_{Ge} = (0.62, 0.85, 1.24)$



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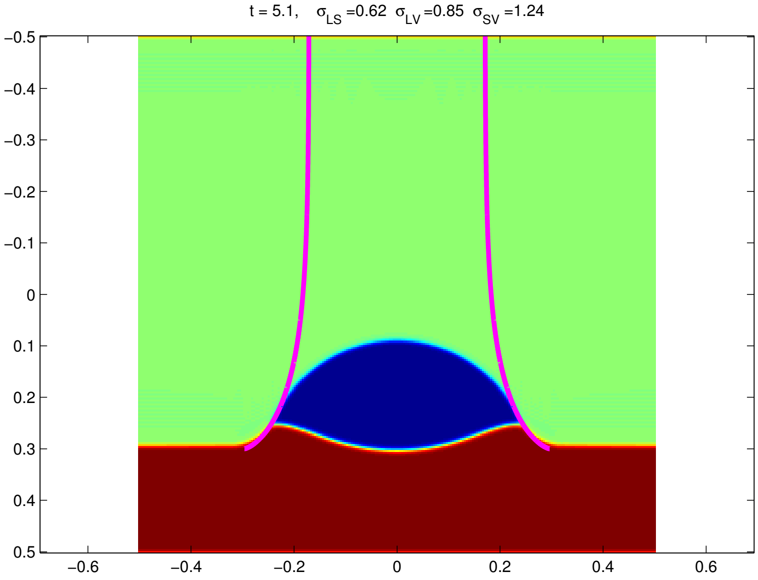
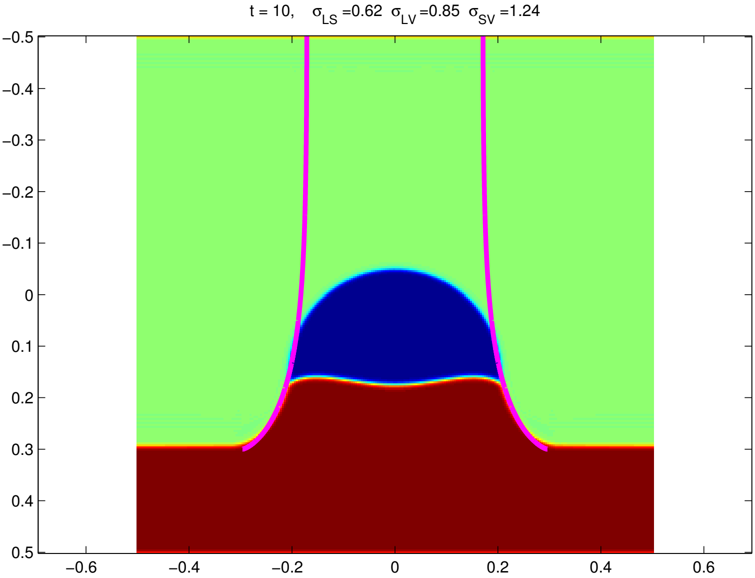


Nanowire growth with $\sigma_{Ge} = (0.62, 0.85, 1.24)$



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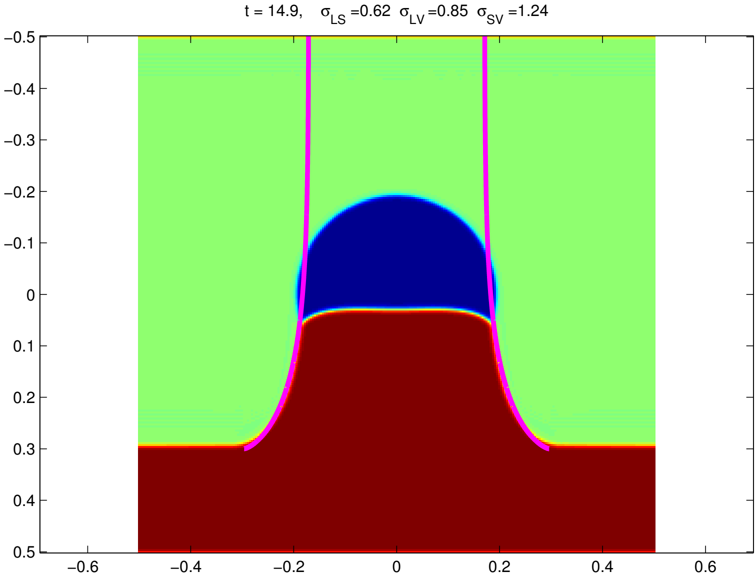

Nanowire growth with $\sigma_{Ge} = (0.62, 0.85, 1.24)$