Phase-Field Approximation of Interface Moving with Local Geometry and Nonlocal Field

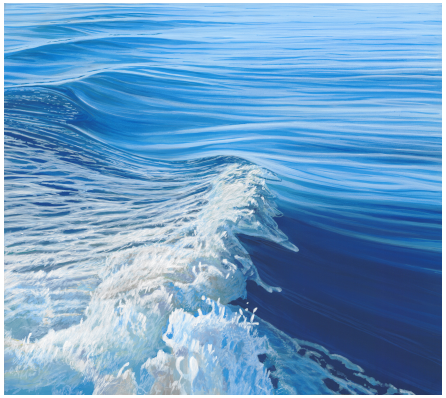
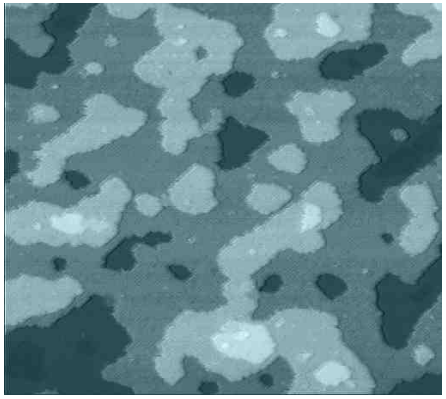
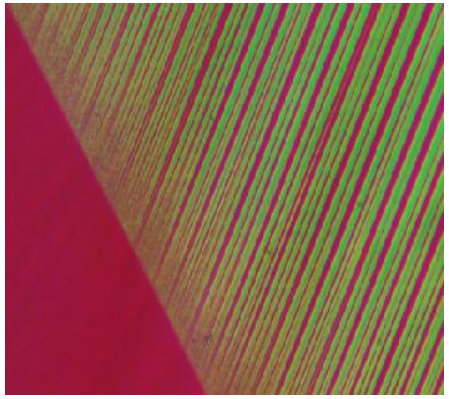
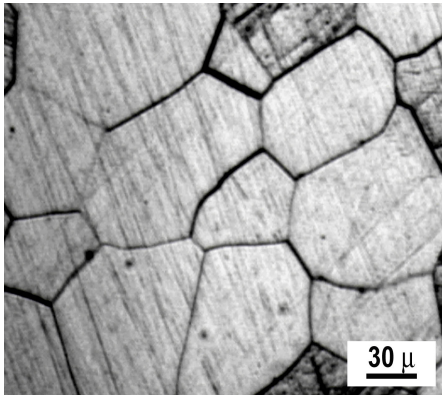
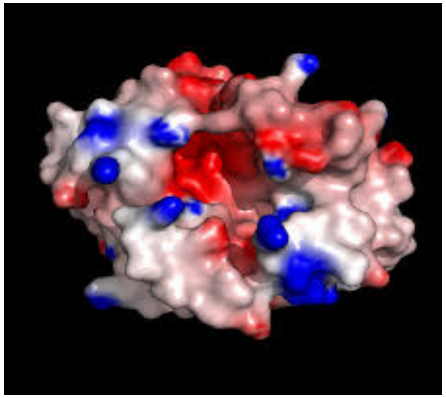
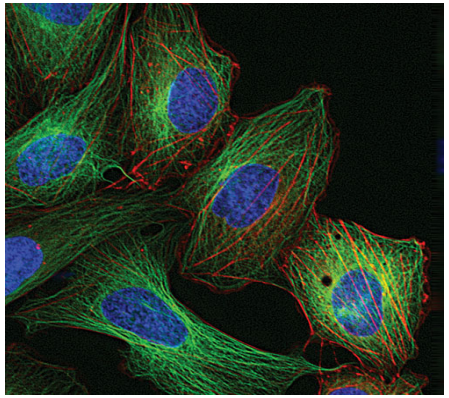
Bo Li

Department of Mathematics
University of California, San Diego

Funding: NIH and NSF

School of Mathematical Sciences, Fudan University
May 25, 2015

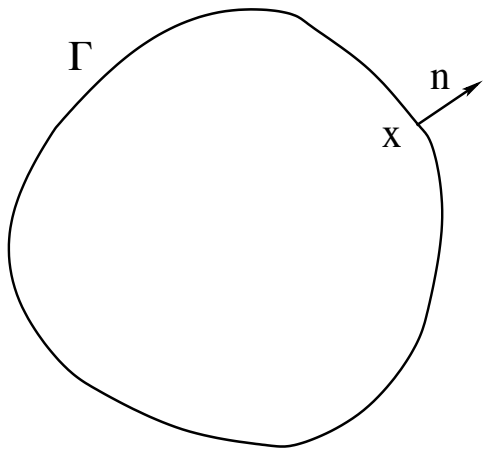
Graphic Pictures





30 μ



Interface motion

Let $x = x(t)$ be a point on a moving interface $\Gamma = \Gamma(t)$.

- Velocity: $\dot{x}(t)$
- Unit normal: $n = n(x)$
- Normal velocity: $v_n = \dot{x} \cdot n(x)$

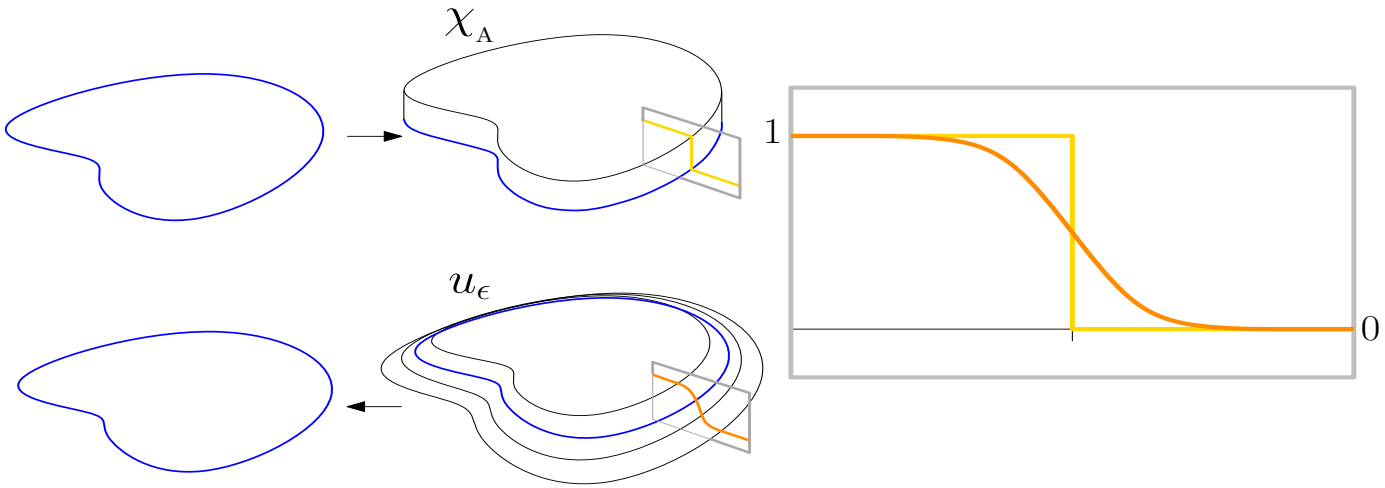


Examples of curvature driven interface motion

- Mean-curvature flow: $v_n = -H$.
  The steepest descent of the energy $E[\Gamma] = \text{area}\,(\Gamma)$.
- Surface diffusion: $v_n = \Delta_\Gamma H$.
- Willmore flow: $v_n = \Delta_\Gamma H + 2H(H^2 - K)$.
  The steepest descent of the energy $E[\Gamma] = \displaystyle\int_\Gamma H^2\, dS$.

Numerical methods for tracking interface motion

- Particle Method
  $x(t+\Delta t) \approx x(t) + \Delta t\, v(x(t))$.
- Level-Set Method (Osher-Sethian 1988)
  - A level-set representation: $\Gamma(t) = \{x \in \mathbb{R}^3 : \phi(x,t) = 0\}$.
  - The level-set equation: $\partial_t \phi + v_n |\nabla \phi| = 0$.
- Phase-Field Method (Langer 1986, Levine 1985, etc.)
  $\Gamma(t) = \{x \in \mathbb{R}^3 : \phi(x,t) = 1/2\}$ with the phase-field function ϕ continuous, $\phi \approx 1$ inside and $\phi \approx 0$ outside the interface.

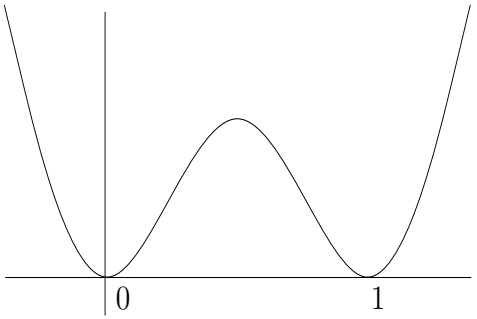


Phase-field model of the mean-curvature flow

Let $\Omega \subset \mathbb{R}^3$ be a smooth and bounded domain. Let $0 < \varepsilon \ll 1$. Consider

$$E_\varepsilon[\phi] = \int_\Omega \left[\frac{\varepsilon}{2} |\nabla \phi|^2 + \frac{1}{\varepsilon} W(\phi) \right] dx,$$

where $W(\phi) = 18\phi^2(\phi - 1)^2$.



Theorem (Modica 1987) Let $\varepsilon_k \downarrow 0$ as $k \uparrow \infty$. Let ϕ_{ε_k} minimize $E_{\varepsilon_k}[\phi]$ among all $\phi \in L^1(\Omega)$, $\phi \geq 0$ in Ω, and the average of ϕ on Ω is a constant $m \in (0,1)$. Let $\phi_{\varepsilon_k} \to \phi_0$ in $L^1(\Omega)$. Then

- $\phi_0 \in \{0, 1\}$ a.e. Ω.
- $P_\Omega(\{\phi_0 = 1\}) = \min\{P_\Omega(A) : A \subset \Omega, |A| = m|\Omega|\}$.
- $\lim_{k\to\infty} E_{\varepsilon_k}(\phi_{\varepsilon_k}) = P_\Omega(\{\phi_0 = 1\})$.

Gradient flow: $\partial_t \phi = -\delta_\phi E_\varepsilon[\phi]$.

$$\partial_t \phi = \varepsilon \Delta \phi - \frac{1}{\varepsilon} W'(\phi) \quad \text{in } \Omega \times (0, \infty).$$

OUTLINE

1. Relaxation of Bending Energy with Fixed Volume and Surface Area
2. Cell Dynamics: Coupling Diffusion Equations with Interface Motion
3. Molecular Solvation: Relxation of Dielectric Boundary
   - Free-Energy Functional and First Variation
   - Matched Asymptotic Analysis
4. Conclusions and Discussions

1. Relaxation of Bending Energy with Fixed Volume and Surface Area

(Banham, Li, & Zhao, PRE 2014)

Sharp-interface formulation:

$$\min_{\Gamma} \frac{\kappa}{2} \int_{\Gamma} H^2 \, dS \quad \text{s.t. vol}\,(\text{interior}\,(\Gamma)) = V \text{ and area}\,(\Gamma) = A.$$

Phase-field formulation: minimize

$$E_\varepsilon[\phi] = \int_\Omega \frac{\kappa}{2\varepsilon} \left[-\varepsilon \Delta \phi + \frac{1}{\varepsilon} W'(\phi) \right]^2 \mathrm{d}x$$
$$+ \frac{1}{2} M_{\mathrm{A}}(\varepsilon) \left[A_\varepsilon(\phi) - A \right]^2 + \frac{1}{2} M_{\mathrm{V}}(\varepsilon) \left[V_\varepsilon(\phi) - V \right]^2,$$
$$A_\varepsilon(\phi) = \int_\Omega \left[\frac{\varepsilon}{2} |\nabla \phi|^2 + \frac{1}{\varepsilon} W(\phi) \right] \mathrm{d}x,$$
$$V_\varepsilon(\phi) = \int_\Omega \phi(x) \, \mathrm{d}x.$$

Du, Liu, & Wang (2005): Convergence of $E_{\varepsilon,\text{bending}}$.

Roger & Schätzle (2006): Convergence of $E_{\varepsilon,\text{surface}} + E_{\varepsilon,\text{bending}}$.

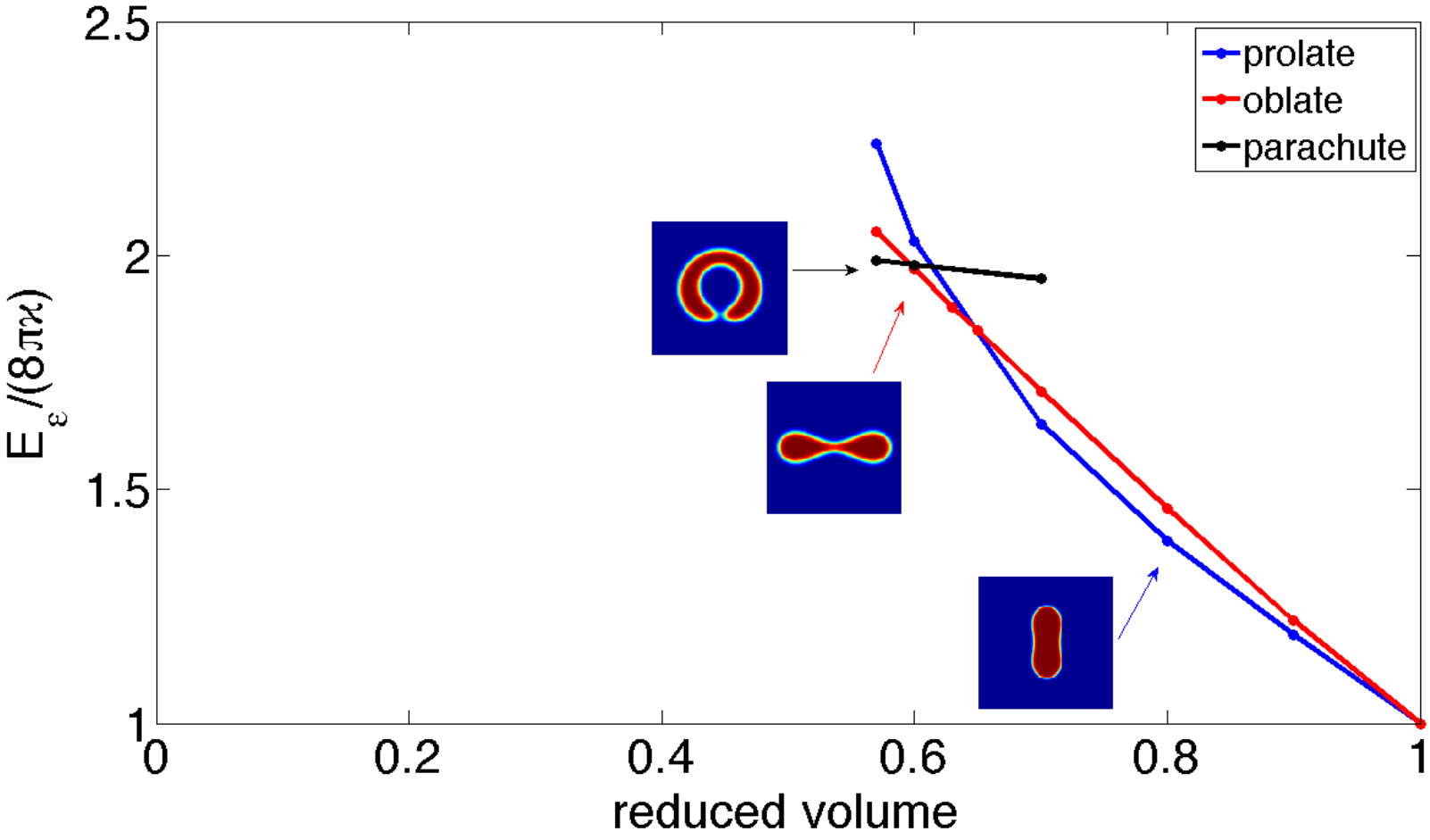
Gradient flow: $\partial_t \phi = -M_\varepsilon \delta E_\varepsilon[\phi]$.

$$\begin{aligned}\frac{\partial \phi}{\partial t} = &-\frac{\kappa M_\varepsilon}{\varepsilon}\left[\varepsilon\Delta - \frac{1}{\varepsilon}W''(\phi)\right]\left[\varepsilon\Delta\phi - \frac{1}{\varepsilon}W'(\phi)\right] \\ &- M_\varepsilon M_{\mathrm{A}}(\varepsilon)\left[A_\varepsilon(\phi) - A\right]\left[-\varepsilon\Delta\phi + \frac{1}{\varepsilon}W'(\phi)\right] \\ &- M_\varepsilon M_{\mathrm{V}}(\varepsilon)\left[V_\varepsilon(\phi) - V\right].\end{aligned}$$

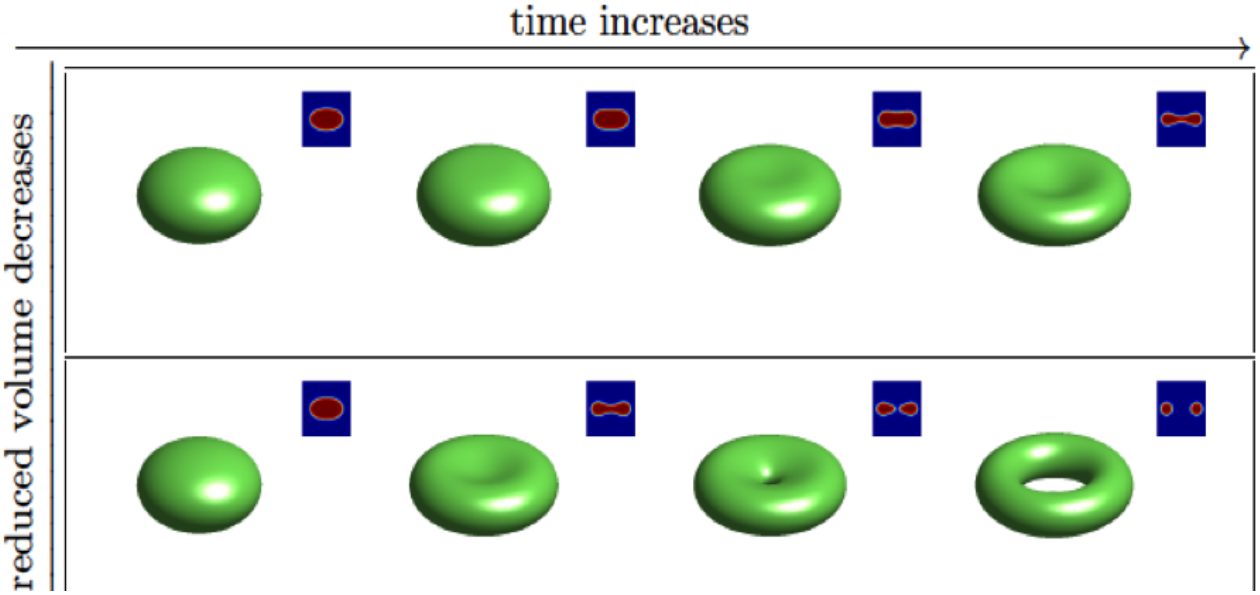
Numerical Methods: Forward Euler, semi-implicit time, and Fourier spectral. $M_\varepsilon = 1/\varepsilon$. Dynamic M_A and M_V values.

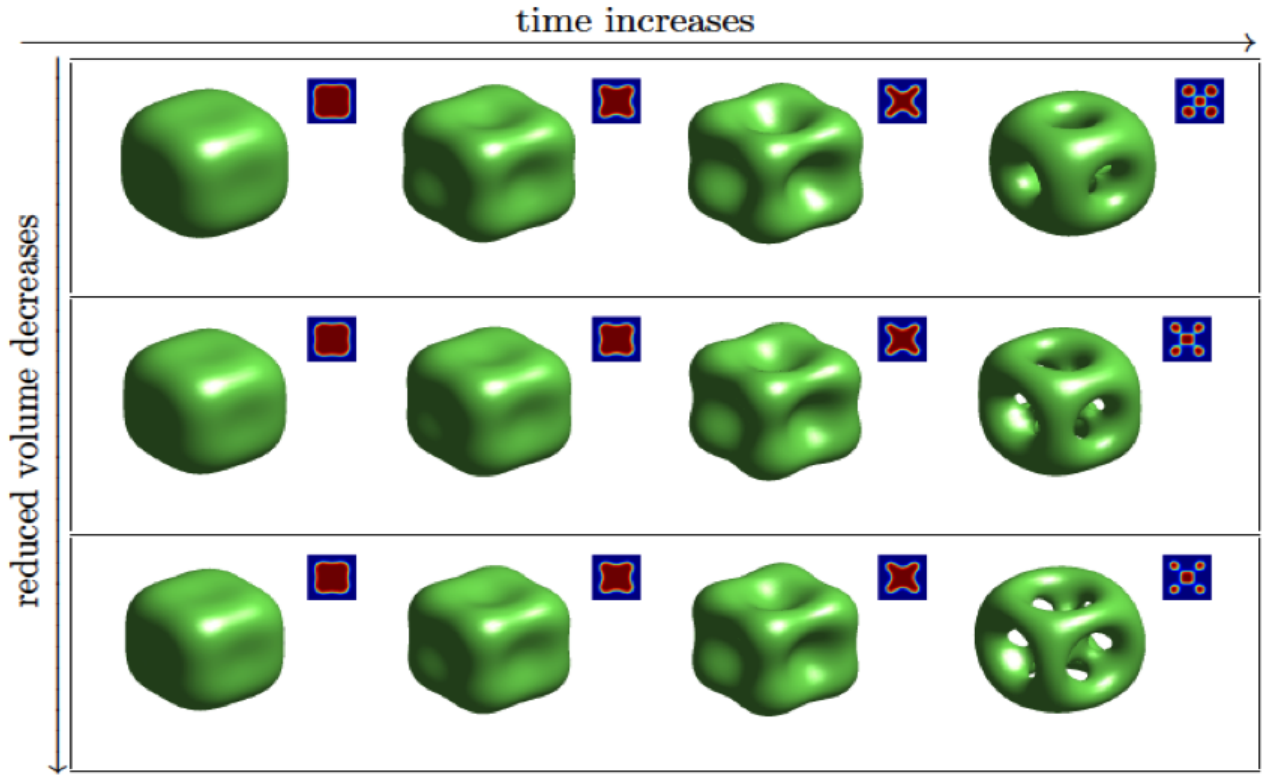
$$\frac{\phi^{(m+1)} - \phi^{(m)}}{\Delta t} = -\varepsilon M(\varepsilon)\kappa\Delta^2\phi^{(m+1)} + B\left[\phi^{(m)}\right], \quad m = 0, 1, \ldots$$

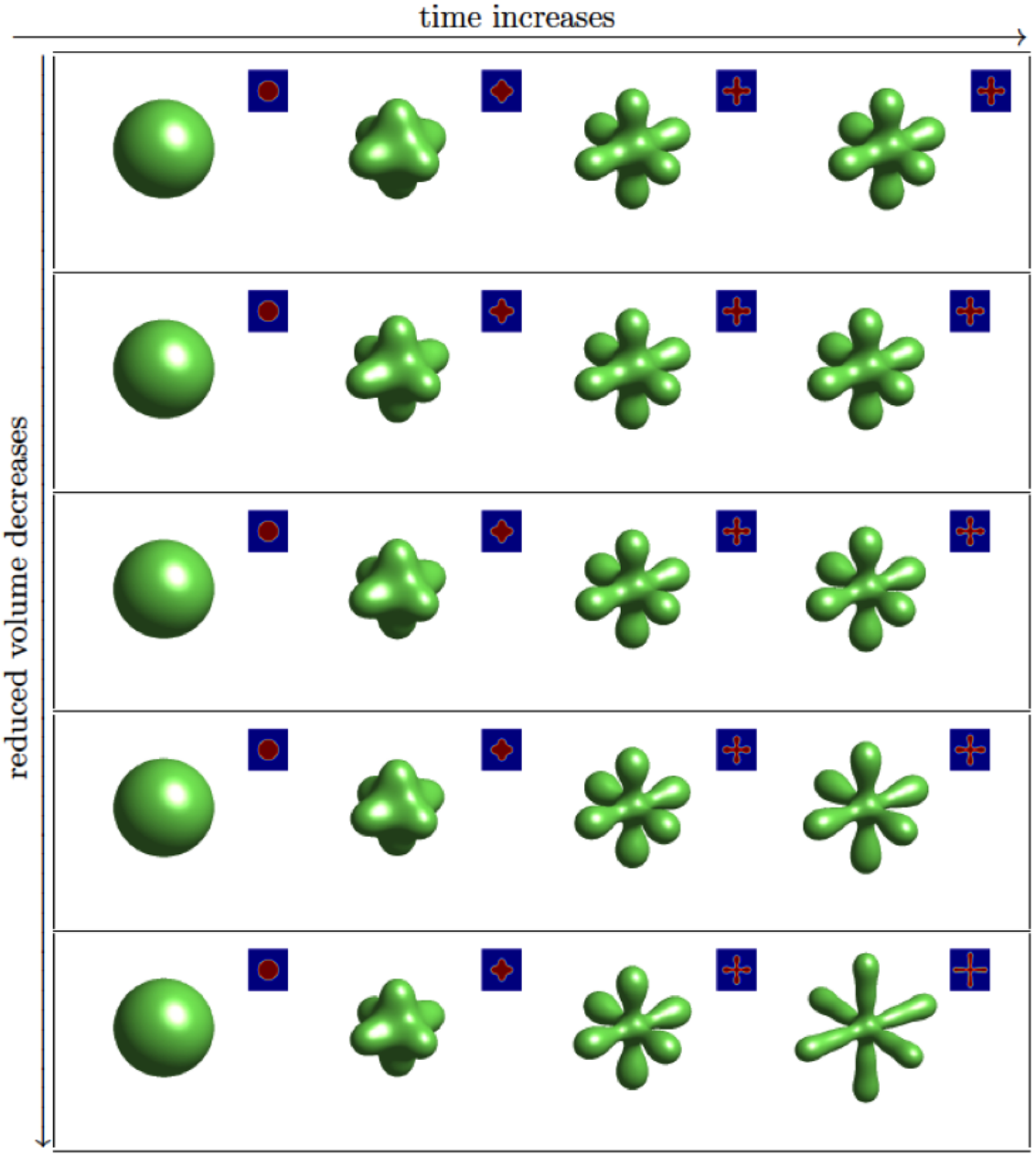
$$\begin{aligned}B[\phi] = &\frac{M(\varepsilon)\kappa}{\varepsilon}\left[\Delta(W'(\phi)) + W''(\phi)\Delta\phi - \frac{1}{\varepsilon^2}W'(\phi)W''(\phi)\right] \\ &- M(\varepsilon)M_{\mathrm{A}}(\varepsilon)\left[A_\varepsilon(\phi) - A\right]\left[-\varepsilon\Delta\phi + \frac{1}{\varepsilon}W'(\phi)\right] \\ &- M(\varepsilon)M_{\mathrm{V}}(\varepsilon)\left[V_\varepsilon(\phi) - V\right]\end{aligned}$$

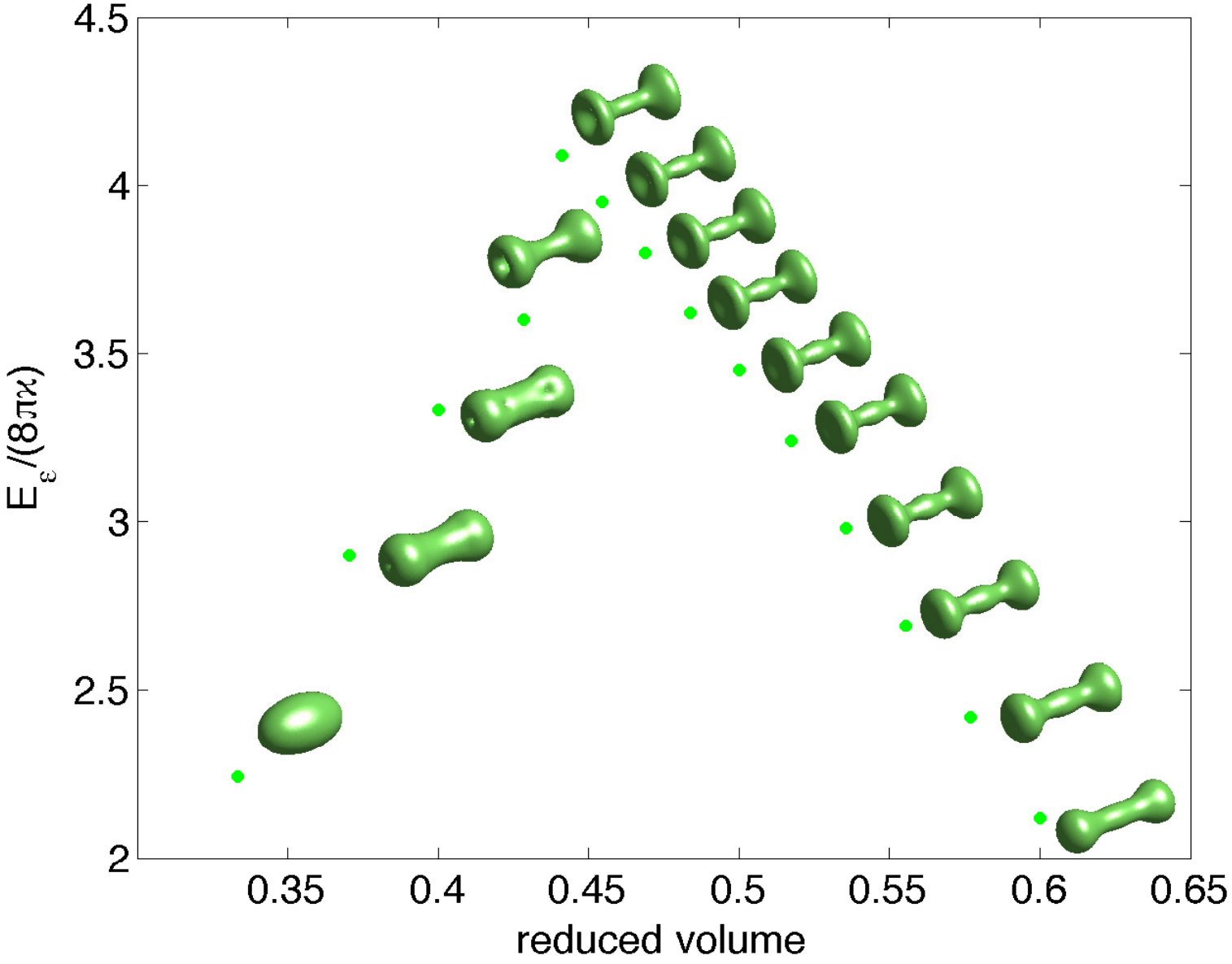


Bending energy vs. reduced volume. Results agree well with the sharp-interface model (Seifert, Berndl, & Lipowsky, 1991).

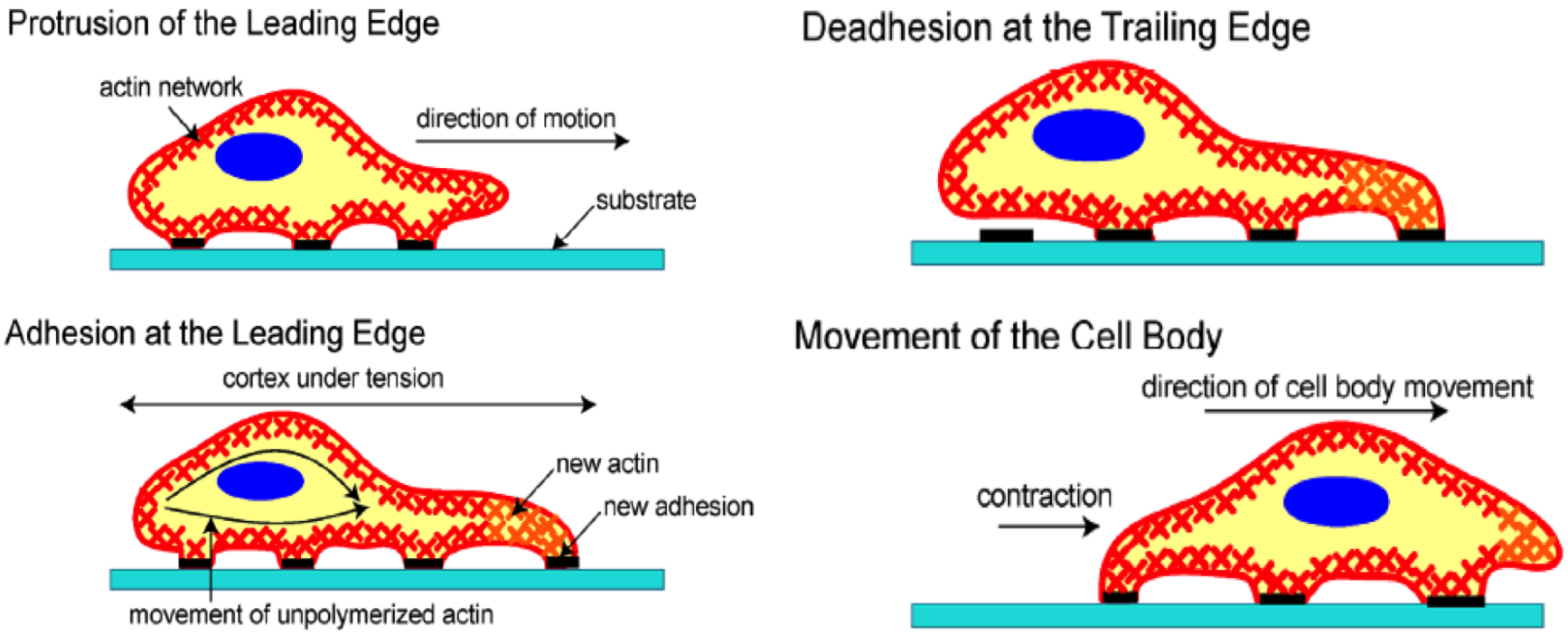

time increases
reduced volume decreases


time increases
reduced volume decreases


reduced volume decreases
time increases


4.5
4
3.5
3
2.5
2
0.35
0.4
0.45
0.5
0.55
0.6
0.65
reduced volume
E_ε/(8πκ)

2. Cell Dynamics



Ananthakrishnan & Ehrlicher (2007)

Phase-field model (Levine, Rapple, Camley, *et al.* PRL, PNAS, 2010–2014)

$$\partial_t \phi + u \cdot \nabla \phi = \hat{\gamma} \left[\varepsilon \Delta \phi - W'(\phi)/\varepsilon - \varepsilon |\nabla \phi| \nabla \cdot (\nabla \phi / |\nabla \phi|) \right]$$

$$\nu_0 \nabla \cdot \left[\phi \left(\nabla u + (\nabla u)^T \right) \right] + \nabla \cdot \sigma_{\mathrm{poly}} + \nabla \cdot \sigma_{\mathrm{myo}} + F_{\mathrm{mem}} + F_{\mathrm{adh}} = \xi u$$

$$\partial_t (\phi \rho_{\mathrm{a}}) + \nabla \cdot (\phi \rho_{\mathrm{a}} u) = \nabla \cdot (\phi D_{\mathrm{a}} \nabla \rho_{\mathrm{a}}) + \phi f \left(\rho_{\mathrm{a}}, \rho_{\mathrm{a}}^{\mathrm{cyt}} \right)$$

$$\partial_t (\phi \rho_{\mathrm{m}}) + \nabla \cdot (\phi \rho_{\mathrm{m}} u) = \nabla \cdot (\phi D_{\mathrm{m}}(\rho_{\mathrm{a}}) \nabla \rho_{\mathrm{m}})$$

$$\sigma_{\mathrm{poly}} = -\eta_{\mathrm{a}}^0 \rho_{\mathrm{a}} \varepsilon \nabla \phi \otimes \nabla \phi$$

$$\sigma_{\mathrm{myo}} = \eta_{\mathrm{m}}^0 \rho_{\mathrm{m}} I$$

$$F_{\mathrm{mem}} = -\gamma \left[\varepsilon \Delta \phi - W'(\phi)/\varepsilon \right] \nabla \phi + \kappa \varepsilon \left[\Delta - W''(\phi)/\varepsilon \right] \left[\Delta \phi - W''(\phi)/\varepsilon^2 \right] \nabla \phi$$

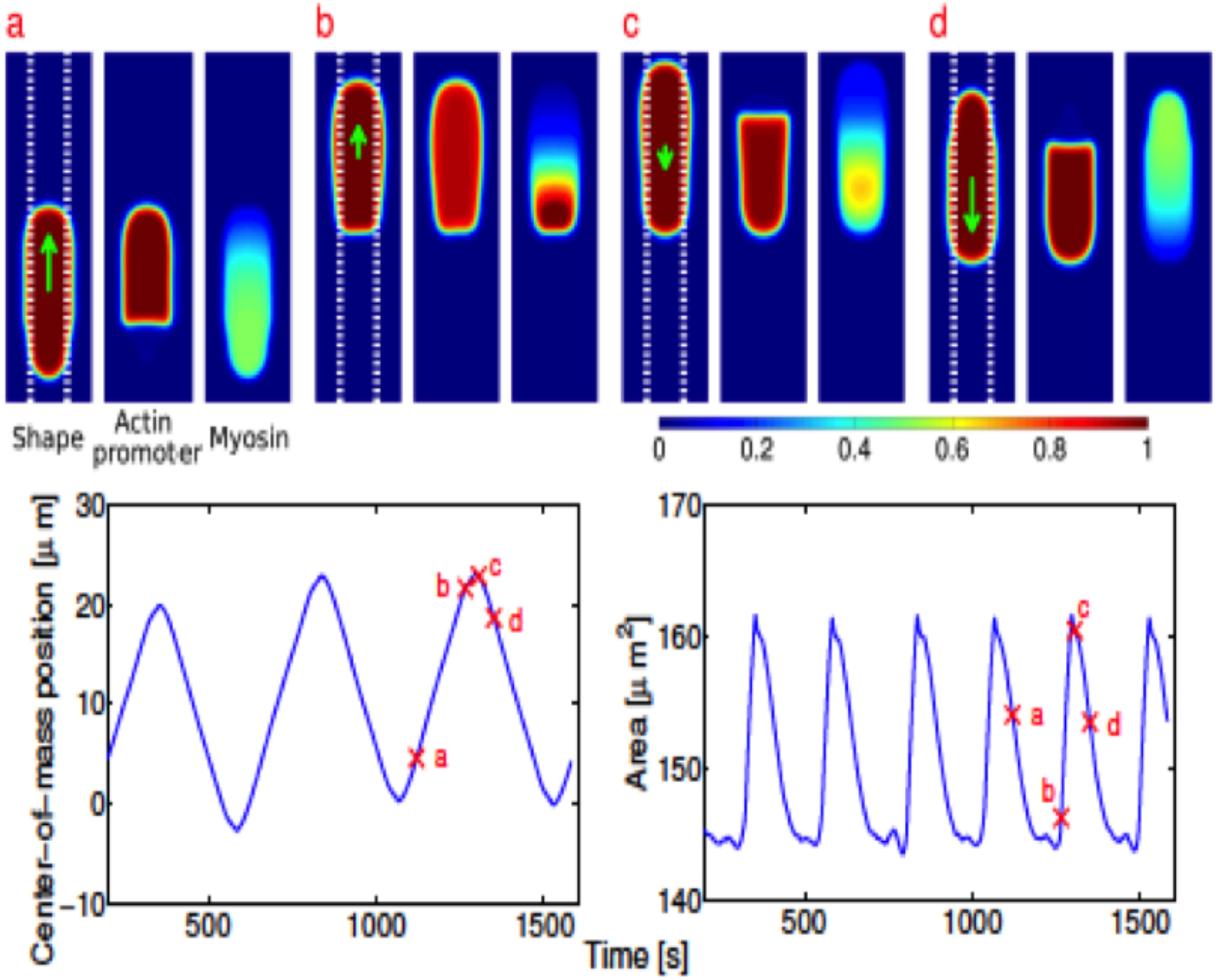
$$F_{\mathrm{adh}} = F_{\mathrm{grip}} + F_{\mathrm{slip}} = -k_{\mathrm{grip}}(x - x_0) - k_{\mathrm{slip}} u$$

$$f \left(\rho_{\mathrm{a}}, \rho_{\mathrm{a}}^{\mathrm{cyt}} \right) = k_{\mathrm{b}} \left[\rho_{\mathrm{a}}^2 / (K_{\mathrm{a}}^2 + \rho_{\mathrm{a}}^2) + \kappa_{\mathrm{a}} \right] \rho_{\mathrm{a}}^{\mathrm{cyt}} - k_{\mathrm{c}} \rho_{\mathrm{a}}$$

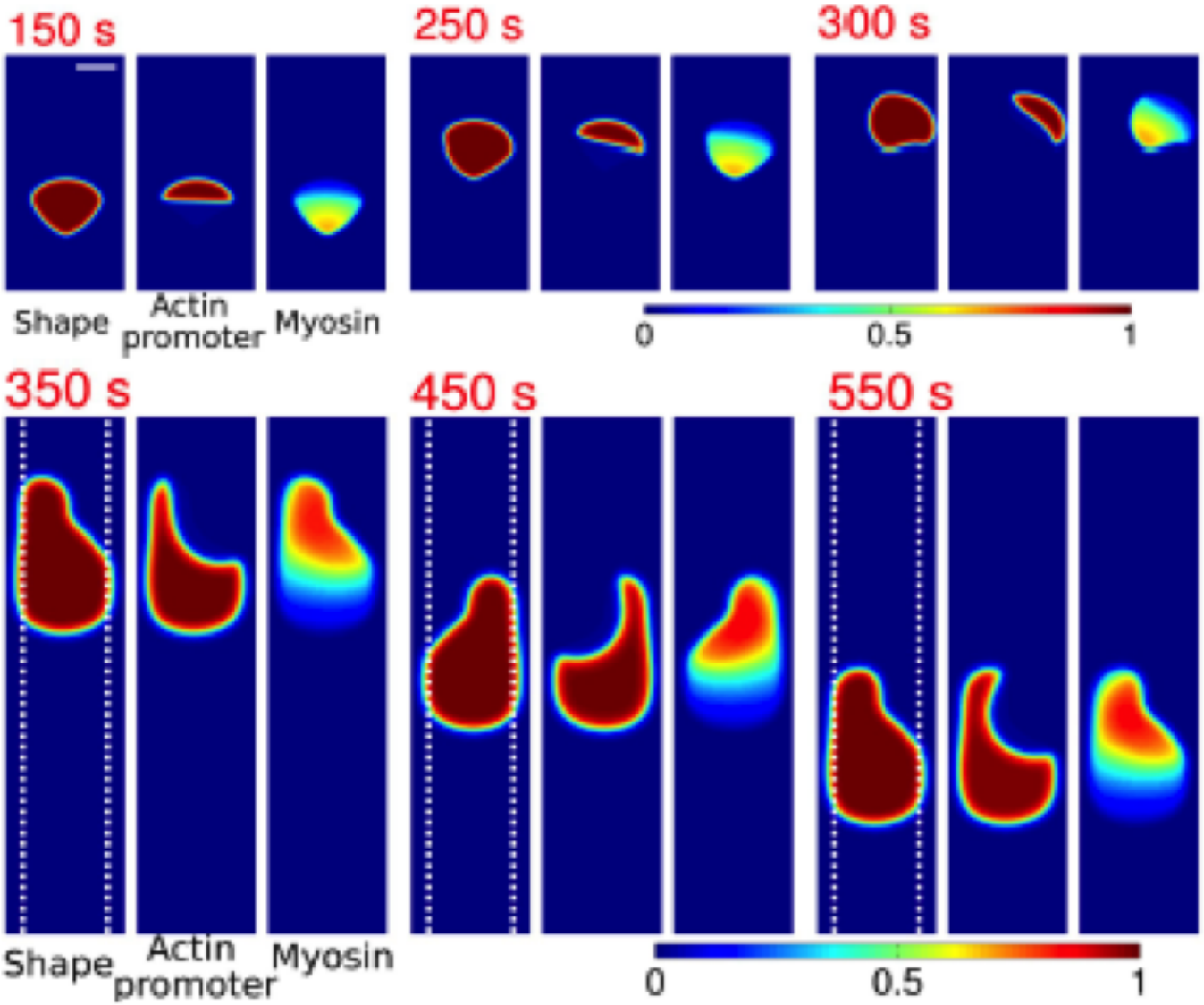
$$\int_\Omega \phi \left(\rho_{\mathrm{a}} + \rho_{\mathrm{a}}^{\mathrm{cyt}} \right) dx = \text{ constant}$$

$$D_{\mathrm{m}}(\rho_{\mathrm{a}}) = \rho_{\mathrm{a}}^0 / (1 + \rho_{\mathrm{a}} / K_{\mathrm{D}})$$

Cell moves on a patterned substrate.

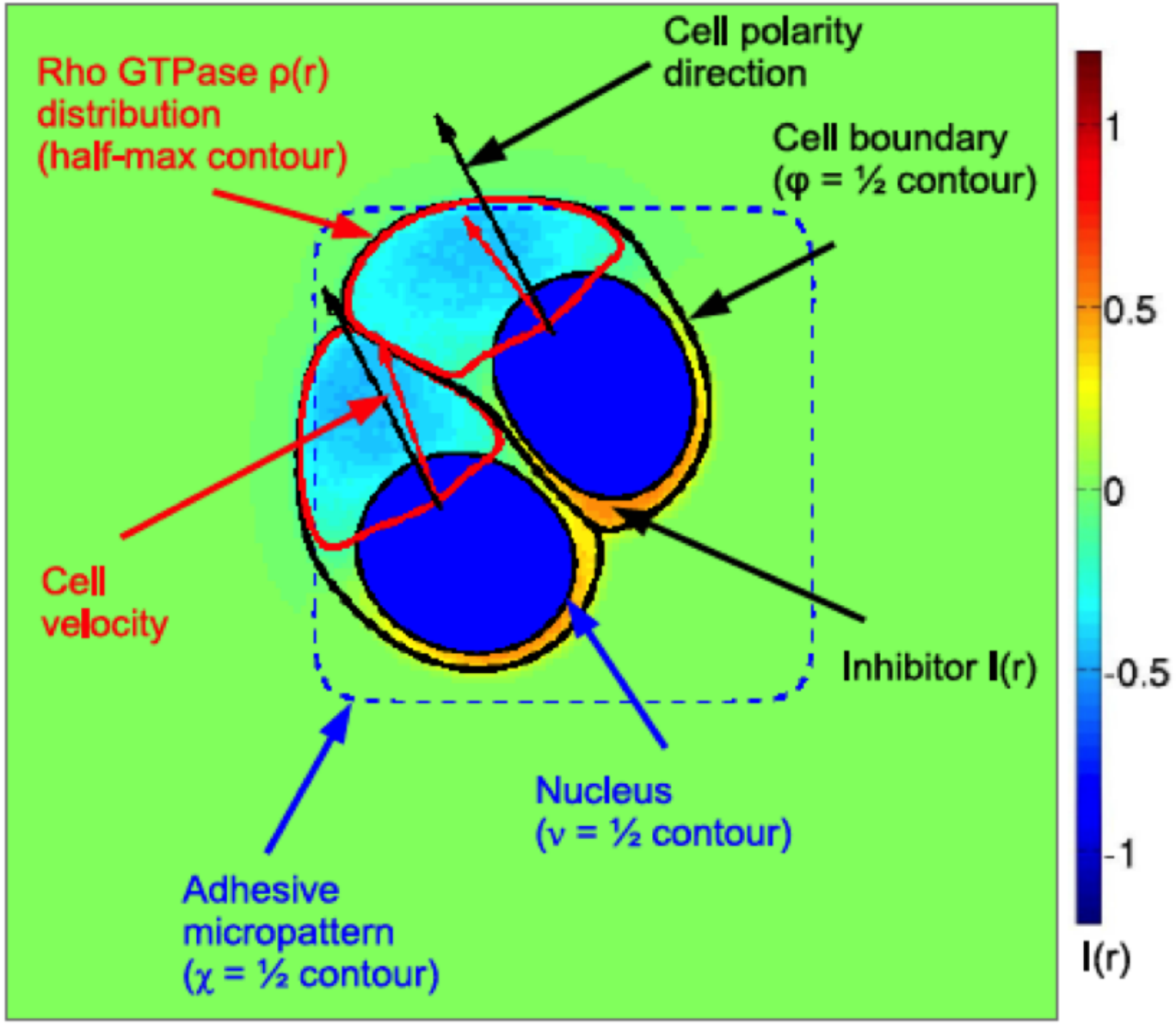


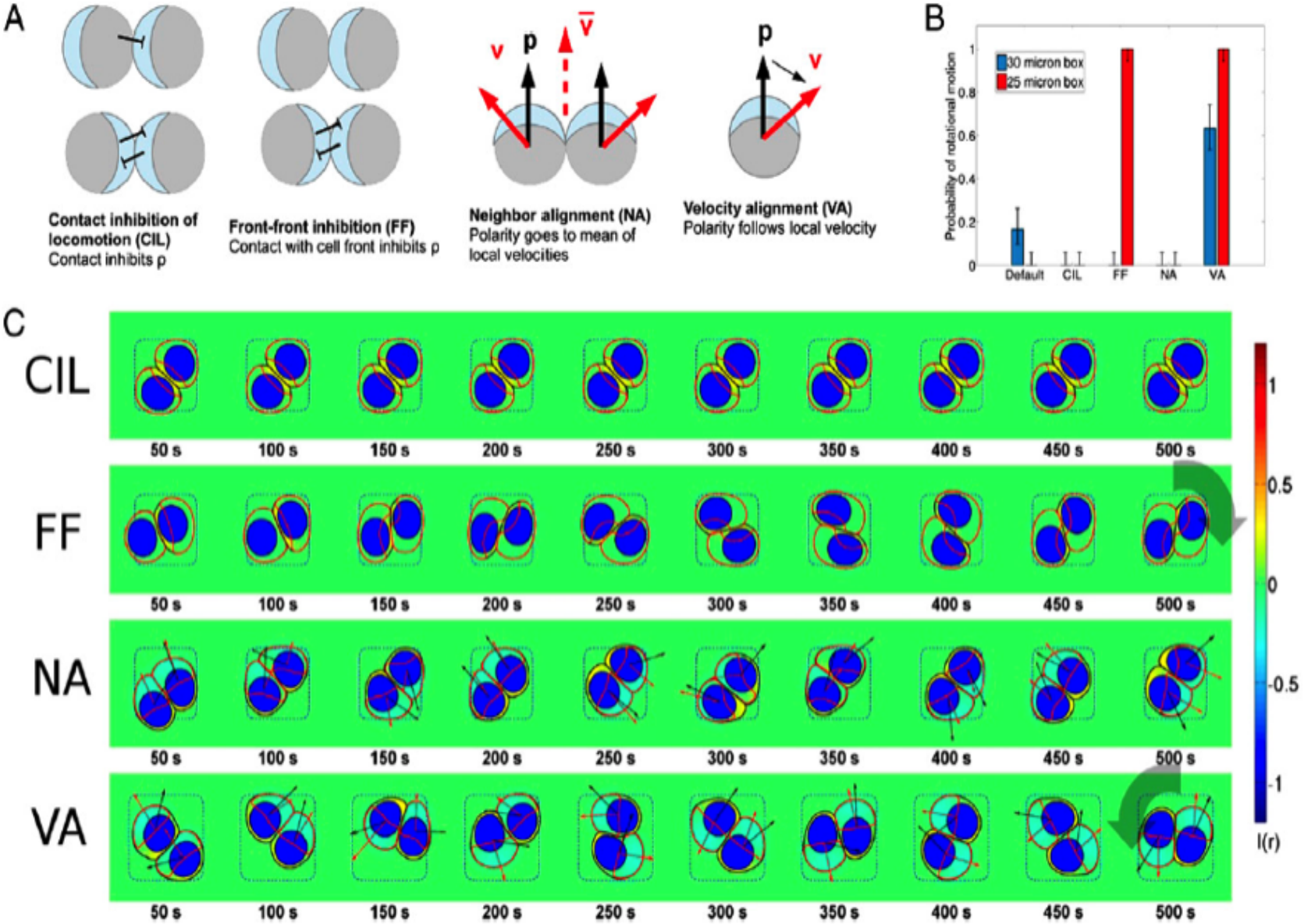
Periodic migraion of a cell on a patterned substrate.



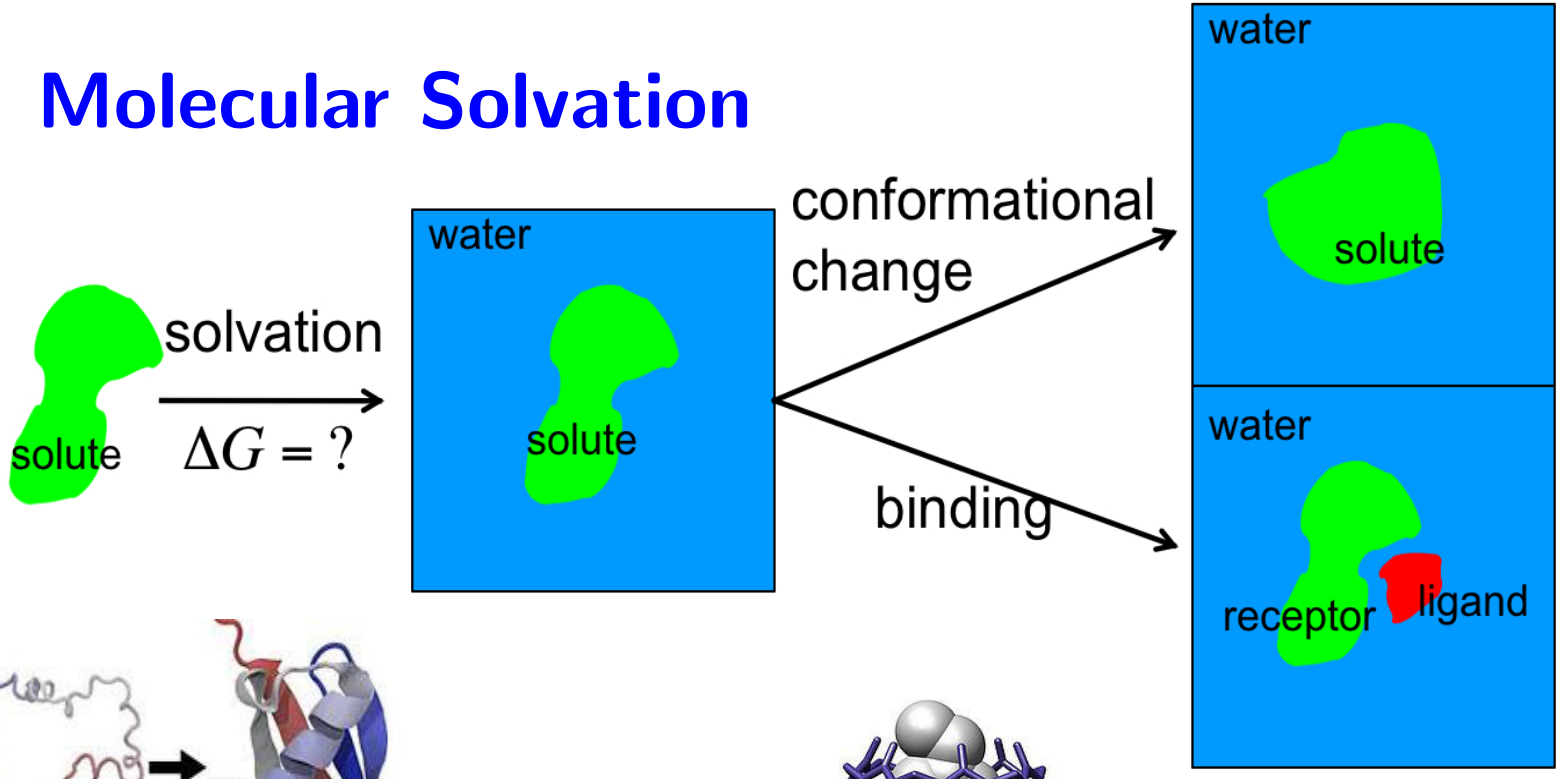
Cell craws on a patterned substrate: bipedaling and turning.

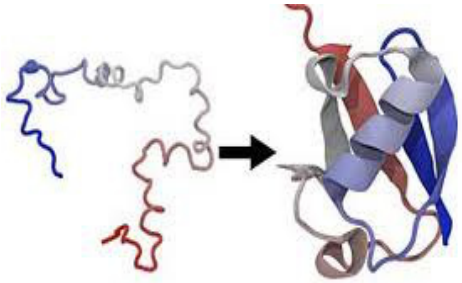
Persistent rotational motion of cells on micropatterns



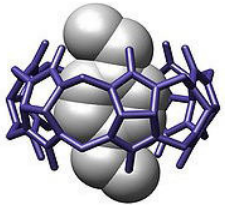

A
Contact inhibition of locomotion (CIL)
Contact inhibits p
Front-front inhibition (FF)
Contact with cell front inhibits p
Neighbor alignment (NA)
Polarity goes to mean of local velocities
Velocity alignment (VA)
Polarity follows local velocity
B
30 micron box
25 micron box
Probability of rotational motion
Default
CIL
FF
NA
VA
C
CIL
FF
NA
VA
50 s
100 s
150 s
200 s
250 s
300 s
350 s
400 s
450 s
500 s
I(r)

3. Molecular Solvation

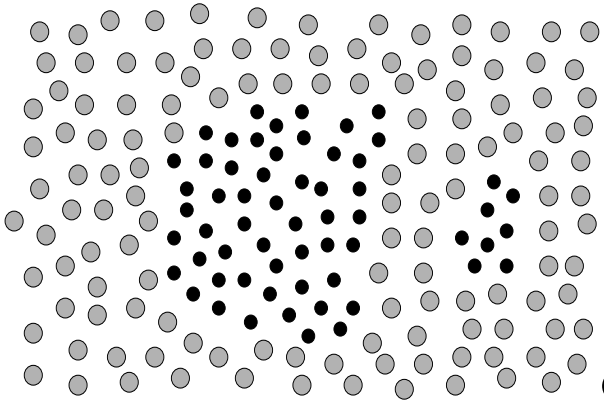




protein folding

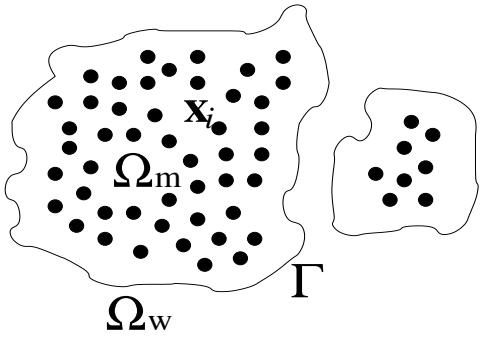


molecular recognition

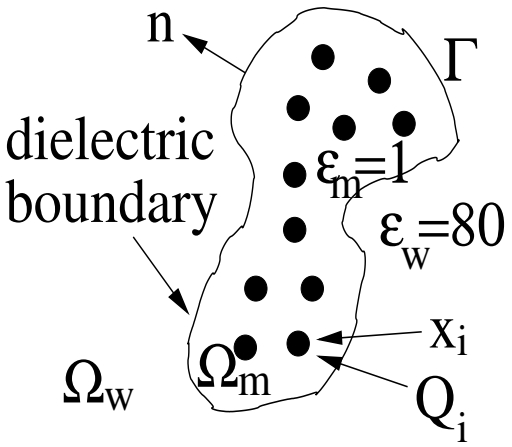


explicit solvent

implicit solvent



Variational implicit-solvent model (VISM) (Dzubiella, Swanson, & McCammon, PRL & JCP 2006; Cheng, Zhou, Wang, Guo, Che, Dzubiella, Li, McCammon, *et al.*, JCP, PRL, JCP, JCTC, JCC, SIAP, 2007–2015)



Free-energy functional

$$G_{\text{total}}[\Gamma] = P\,\text{vol}\,(\Omega_{\text{m}}) + \gamma_0\,\text{area}\,(\Gamma) + \rho_{\text{w}} \int_{\Omega_{\text{w}}} U_{\text{vdW}}\, dV + G_{\text{ele}}[\Gamma]$$

$$U(x) = U_{\text{vdW}}(x) = \sum_{i=1}^{N} U_{\text{LJ}}^{(i)}(|x - x_i|)$$

The Poisson–Boltzmann (PB) theory

$$G_{\text{ele}}[\Gamma] = \int_{\Omega} \left[-\frac{\varepsilon_\Gamma}{2} |\nabla \psi|^2 + f\psi - \chi_{\text{w}} B(\psi) \right] dx$$

$$\nabla \cdot \varepsilon_\Gamma \nabla \psi - \chi_{\text{w}} B'(\psi) = -f$$

$$B(\psi) = \beta^{-1} \sum_{i=1}^{M} c_i^{\infty} \left(e^{-\beta q_i \psi} - 1 \right)$$

Phase-field VISM (P-VISM) model (Li & Zhao, SIAP 2013, Zhao *el al.* JCP 2013, Li & Liu SIAP 2015 (submitted))

Let $\Omega \subset \mathbb{R}^3$ be a smooth and bounded domin that contains all x_i ($i \leq i \leq N$). Let $0 < \xi \ll 1$. Define the free-energy functional

$$
\begin{aligned}
F_\xi[\phi] = P \int_\Omega \phi^2 \, \mathrm{d}x + \gamma_0 \int_\Omega \left[\frac{\xi}{2} |\nabla \phi|^2 + \frac{1}{\xi} W(\phi) \right] \mathrm{d}x \\
+ \rho_{\mathrm{w}} \int_\Omega (\phi - 1)^2 U \, \mathrm{d}x \\
+ \int_\Omega \left[-\frac{\varepsilon(\phi)}{2} |\nabla \psi_\phi|^2 + f \psi_\phi - (\phi - 1)^2 B(\psi_\phi) \right] \mathrm{d}x,
\end{aligned}
$$

where ψ_ϕ is determined by the phase-field PB equation together with boundary conditions

$$
\nabla \cdot \varepsilon(\phi) \nabla \psi_\phi - (\phi - 1)^2 B'(\psi_\phi) = -f \quad \text{in } \Omega, \tag{1}
$$

$$
\psi_\phi = \psi_\infty \qquad \text{on } \partial\Omega. \tag{2}
$$

Assumptions

- The functions f and ψ_∞ are smooth and bounded.
- $\varepsilon = \varepsilon(\phi) \in C^1(\mathbb{R})$, $\varepsilon(\phi) = \varepsilon_{\mathrm{w}}\varepsilon_0$ if $\phi \le 0$, $\varepsilon(1) = \varepsilon_{\mathrm{m}}\varepsilon_0$ if $\phi \ge 1$, and $\varepsilon(\phi)$ is strictly monotonic in $[0, 1]$.
- The function $U : \mathbb{R}^3 \setminus \{x_1, \ldots, x_N\} \to \mathbb{R}$ is smooth and bounded below, $U(x_i) = \infty$ $(1 \le i \le N)$, and $U(\infty) = 0$.
- $B \in C^2(R)$ is strictly convex, minimized at 0, $B(\pm\infty) = \infty$, and $B'(\pm\infty) = \infty$.

Two examples of $\varepsilon = \varepsilon(\phi)$.

$$\varepsilon(\phi) = \begin{cases} \varepsilon_{\mathrm{w}}\varepsilon_0 & \text{if } \phi \le 0, \\ \dfrac{\varepsilon_{\mathrm{p}}\varepsilon_0 e^{\tan(\pi(\phi-1/2))} + \varepsilon_{\mathrm{w}}\varepsilon_0 e^{-\tan(\pi(\phi-1/2))}}{e^{\tan(\pi(\phi-1/2))} + e^{-\tan(\pi(\phi-1/2))}} & \text{if } 0 < \phi < 1, \\ \varepsilon_{\mathrm{p}}\varepsilon_0 & \text{if } \phi \ge 1. \end{cases}$$

$$\varepsilon(\phi) = \begin{cases} \varepsilon_{\mathrm{w}}\varepsilon_0 & \text{if } \phi \le 0, \\ \dfrac{1}{2}(\varepsilon_{\mathrm{w}}\varepsilon_0 - \varepsilon_{\mathrm{p}}\varepsilon_0)\cos\pi\phi + \dfrac{1}{2}(\varepsilon_{\mathrm{w}}\varepsilon_0 + \varepsilon_{\mathrm{p}}\varepsilon_0) & \text{if } 0 < \phi < 1, \\ \varepsilon_{\mathrm{p}}\varepsilon_0 & \text{if } \phi \ge 1. \end{cases}$$

Free-Energy Functional and First Variation

Theorem 1. (Li & Liu, 2015 (submitted)) For any $\phi \in H_0^1(\Omega)$, there exists a unique weak solution $\psi_\phi \in H^1(\Omega)$ to the boundary-value problem (**??**) and (**??**). Moreover, $\psi_\phi \in L^\infty(\Omega)$ and

$$\begin{aligned}
&\|\psi_\phi\|_{H^1(\Omega)} \leq C\left(1 + \|\phi\|_{L^2(\Omega)}\right), \\
&\|\chi_{\{\phi\neq 1\}}\psi_\phi\|_{L^\infty(\Omega)} \leq C, \\
&\|\psi_\phi\|_{L^\infty(\Omega)} \leq C\left(1 + \|\phi\|^2_{H^1(\Omega)}\right).
\end{aligned}$$

Proof. Step 1. Let $\hat{\psi}_\phi \in H^1(\Omega)$ be the unique weak solution to

$$\begin{aligned}
&\nabla \cdot \varepsilon(\phi)\nabla\hat{\psi}_\phi = -f \quad \text{in } \Omega, \\
&\hat{\psi}_\phi = \psi_\infty \quad \text{on } \partial\Omega.
\end{aligned}$$

Standard elliptic theory implies that $\hat{\psi}_\phi \in H^1(\Omega) \cap L^\infty(\Omega)$, and

$$\|\hat{\psi}_\phi\|_{H^1(\Omega)} + \|\hat{\psi}_\phi\|_{L^\infty(\Omega)} \leq C.$$

Step 2. By direct methods in the calculus of variations, there exists a unique minimizer, $u = u_\phi \in H_0^1(\Omega)$, of the functional $I : H_0^1(\Omega) \to \mathbb{R} \cup \{+\infty\}$ defined by

$$I[v] = \int_\Omega \left[\frac{\varepsilon(\phi)}{2} |\nabla v|^2 + (\phi - 1)^2 B(v + \hat{\psi}_\phi) \right] \mathrm{d}x \quad \forall v \in H_0^1(\Omega).$$

Let $\lambda > 0$ be such that $B'(\lambda + \hat{\psi}_\phi) > 1$ and $B'(-\lambda + \hat{\psi}_\phi) < -1$ a.e. on Ω. We prove that $|u| \leq \lambda$ a.e. on $\{\phi \neq 1\}$. Define

$$u_\lambda(x) = \begin{cases} -\lambda & \text{if } u(x) < -\lambda, \\ u(x) & \text{if } -\lambda \leq u(x) \leq \lambda, \\ \lambda & \text{if } u(x) > \lambda. \end{cases}$$

Then $I[u_\lambda] \geq I[u]$ and $|\nabla u_\lambda| \leq |\nabla u|$ a.e. Ω. These together with the convexity of B imply that

$$
\begin{aligned}
0 &\geq \int_\Omega \chi_{\{u>\lambda\}}(\phi-1)^2 \left[B(u+\hat{\psi}_\phi) - B(\lambda+\hat{\psi}_\phi)\right] \mathrm{d}x \\
&\qquad + \int_\Omega \chi_{\{u<-\lambda\}}(\phi-1)^2 \left[B(u+\hat{\psi}_\phi) - B(-\lambda+\hat{\psi}_\phi)\right] \mathrm{d}x \\
&\geq \int_\Omega \chi_{\{u>\lambda\}}(\phi-1)^2 B'(\lambda+\hat{\psi}_\phi)(u-\lambda)\mathrm{d}x \\
&\qquad + \int_\Omega \chi_{\{u<-\lambda\}}(\phi-1)^2 B'(-\lambda+\hat{\psi}_\phi)(u+\lambda)\mathrm{d}x \\
&= \int_\Omega \chi_{\{|u|>\lambda\}}(\phi-1)^2 |\,|u|-\lambda\,|\,\mathrm{d}x \geq 0.
\end{aligned}
$$

This implies that $|u| \leq \lambda$ a.e. Ω.

The minimizer is the unique solution to the corresponding Euler–Lagrange equation. Standard arguments lead to

$$
\begin{aligned}
\|u\|_{H^1(\Omega)} &\leq C\left(1+\|\phi\|_{L^2(\Omega)}\right), \\
\|u\|_{L^\infty(\Omega)} &\leq C\left(1+\|\phi\|^2_{H^1(\Omega)}\right).
\end{aligned}
$$

Step 3. Let $\psi_\phi = u + \hat{\psi}_\phi$. **Q.E.D.**

Theorem 2 (Li & Liu 2015 (submitted)) Let $\phi \in H_0^1(\Omega)$ and $\eta \in L^\infty(\Omega) \cap H_0^1(\Omega)$ be such that $(\phi - 1)^2 U \in L^1(\Omega)$ and $\eta^2 U \in L^1(\Omega)$. Then

$$\delta_\phi F_\xi[\phi][\eta] = \int_\Omega \left\{ \gamma_0 \xi \nabla\phi \cdot \nabla\eta + \left[2P\phi + \frac{\gamma_0}{\xi} W'(\phi) + 2\rho_{\mathrm{w}}(\phi - 1)U \right.\right.$$
$$\left.\left. - \frac{\varepsilon'(\phi)}{2} |\nabla\psi_\phi|^2 - 2(\phi - 1)B(\psi_\phi) \right] \eta \right\} dx.$$

Remark. Formally, we have

$$\delta_\phi F_\xi[\phi] = 2P\phi - \gamma_0 \left[\xi\Delta\phi - \frac{1}{\xi} W'(\phi) \right] + 2\rho_{\mathrm{w}}(\phi - 1)U$$
$$- \frac{\varepsilon'(\phi)}{2} |\nabla\psi_\phi|^2 - 2(\phi - 1)B(\psi_\phi).$$

Only consider

$$F_{\mathrm{ele},\xi}[\phi] := \int_\Omega \left[-\frac{\varepsilon(\phi)}{2}|\nabla\psi_\phi|^2 + f\psi_\phi - (\phi-1)^2 B(\psi_\phi) \right] \mathrm{d}x,$$

$$\begin{aligned} &\nabla\cdot\varepsilon(\phi)\nabla\psi_\phi - (\phi-1)^2 B'(\psi_\phi) = -f \quad \text{in } \Omega, \\ &\psi_\phi = \psi_\infty \qquad \text{on } \partial\Omega. \end{aligned}$$

Heuristics: use $\delta\phi$ as the test function in the weak form of PBE.

$$\begin{aligned} \delta_\phi F_{\mathrm{ele},\xi}[\phi]\delta\phi = \int_\Omega \Big[&-\frac{\varepsilon'(\phi)}{2}\delta\phi|\nabla\psi_\phi|^2 - \varepsilon(\phi)\nabla\psi_\phi\cdot\nabla\delta_\phi\psi_\phi + \rho_{\mathrm{f}}\delta_\phi\psi_\phi \\ &- 2(\phi-1)\delta\phi V(\psi_\phi) - (\phi-1)^2 V'(\psi_\phi)\delta_\phi\psi_\phi \Big] \mathrm{d}x \\ = \int_\Omega &\left[-\frac{\varepsilon'(\phi)}{2}|\nabla\psi_\phi|^2 - 2(\phi-1)V(\psi_\phi) \right] \delta\phi\,\mathrm{d}x, \end{aligned}$$

We now prove that

$$\delta_\phi F_{\mathrm{ele},\xi}[\phi][\eta] = \int_\Omega \left[-\frac{1}{2}\varepsilon'(\phi)|\nabla\psi_\phi|^2 - 2(\phi-1)B(\psi_\phi) \right] \eta\, dx.$$

Step 1. By the week formulations, Poincaré's inequality, Hölder's inequality, and Theorem 1 to obtain

$$\|\psi_{\phi+t\eta} - \psi_\phi\|_{H^1(\Omega)} \leq C(\phi,\eta)|t| \qquad \text{if } |t| \leq 1.$$

Step 2. Use the weak formulations to get

$$\begin{aligned}
&F_{\mathrm{ele},\xi}[\phi + t\eta] - F_{\mathrm{ele},\xi}[\phi] \\
&\quad = \int_\Omega \frac{1}{2}\varepsilon(\phi + t\eta)|\nabla\psi_{\phi+t\eta} - \nabla\psi_\phi|^2 dx \\
&\qquad - \int_\Omega \frac{1}{2}\left[\varepsilon(\phi + t\eta) - \varepsilon(\phi)\right]|\nabla\psi_\phi|^2 dx \\
&\qquad - \int_\Omega \left[(\phi + t\eta - 1)^2 - (\phi - 1)^2\right] B(\psi_\phi)\, dx \\
&\qquad - \int_\Omega (\phi + t\eta - 1)^2 \left[B(\psi_{\phi+t\eta}) - B(\psi_\phi)\right. \\
&\qquad\qquad \left. - B'(\psi_{\phi+t\eta})(\psi_{\phi+t\eta} - \psi_\phi)\right] dx \\
&\quad =: \Lambda_1(t) - \Lambda_2(t) - \Lambda_3(t) - \Lambda_4(t).
\end{aligned}$$

Step 3. Step 1 and the Lebesgue Dominated Convergence Theorem imply that $\Lambda_1(t)/t \to 0$ as $t \to 0$, and

$$\lim_{t\to 0} \frac{\Lambda_2(t)}{t} = \int_\Omega \frac{1}{2}\varepsilon'(\phi)|\nabla\psi_\phi|^2\eta\,dx,$$

$$\lim_{t\to 0} \frac{\Lambda_3(t)}{t} = \int_\Omega 2(\phi-1)B(\psi_\phi)\eta\,dx.$$

Taylor expand $g(b) := B(b) - B(a) - B'(b)(b-a)$ to get

$$g(b) = g(a) + g'(a+\mu(b-a))(b-a) = -\mu B''(a+\mu(b-a))(b-a)^2.$$

With $a = \psi_\phi$ and $b = \psi_{\phi+t\eta}$, we obtain by the fact that $\psi_\phi \in L^\infty(\Omega)$, the Cauchy–Schwarz inequality, the imbedding $H^1(\Omega) \hookrightarrow L^4(\Omega)$, and Step 1 that

$$\begin{aligned}\left|\frac{\Lambda_4(t)}{t}\right| &\le \frac{C(\phi,\eta)}{t}\int_\Omega (\phi+t\eta-1)^2|\psi_{\phi+t\eta}-\psi_\phi|^2 dx \\ &\le \frac{C(\phi,\eta)}{t}\|(\phi+t\eta-1)^2\|_{L^2(\Omega)}\|\psi_{\phi+t\eta}-\psi_\phi\|^2_{H^1(\Omega)} \\ &\to 0 \quad \text{as } t\to 0.\end{aligned}$$

Matched Asymptotic Analysis

Consider the relaxation dynamics

$$\partial_t \phi = -2P\,\phi + \gamma_0 \left[\xi \Delta \phi - \frac{1}{\xi} W'(\phi)\right] - 2\rho_{\mathrm{w}}(\phi - 1)U$$
$$+ \frac{1}{2}\varepsilon'(\phi)|\nabla \psi|^2 + 2(\phi - 1)B(\psi),$$
$$\nabla \cdot \varepsilon(\phi)\nabla \psi - (\phi - 1)^2 B'(\psi) = -\rho_{\mathrm{f}},$$
$$\phi = 0 \qquad \text{on } \partial\Omega,$$
$$\psi = \psi_\infty \qquad \text{on } \partial\Omega,$$

Determine a fast time scale. Electrostatic relaxation is instaneous. So, consider

$$\partial_t \phi = \xi \Delta \phi - \frac{1}{\xi} W'(\phi).$$

Perturb the unstable equilibrium $\phi_0(x) = 1/2$ to get the most unstable mode $k_{\mathrm{c}} = 0$ and the fastest growth rate $\omega(k_{\mathrm{c}}) = O(1/\xi)$. Therefore, the fast time scale is $T = t/\xi$.

Fast time scale. Assume $T = t/\xi$ and

$$\phi(x,t) = \phi_0(x,T) + \xi\phi_1(x,T) + \xi^2\phi_2(x,T) + \cdots,$$
$$\psi(x,t) = \psi_0(x,T) + \xi\psi_1(x,T) + \xi^2\psi_2(x,T) + \cdots,$$

where all ϕ_i and ψ_i are smooth and bounded functions that satisfy

$$\phi_i = 0 \quad (i \geq 0), \quad \psi_0 = \psi_\infty, \quad \text{and} \quad \psi_i = 0 \ (i \geq 1) \quad \text{on } \partial\Omega.$$

Plug these into the governing equations and group terms with the same order of ξ to get

$$\partial_T \phi_0 = -\gamma_0 W'(\phi_0):$$
$$\forall x \in \Omega,\ \phi_0(x,T) \to 0 \text{ or } 1 \text{ exponentially as } T \to \infty,$$
$$\nabla \cdot \varepsilon(\phi_0)\nabla\psi_0 - (\phi_0 - 1)^2 B'(\psi_0) = -f.$$

Regular time scale. Assume

$$\phi(x,t) = \phi_0(x,t) + \xi\phi_1(x,t) + \xi^2\phi_2(x,t) + \cdots ,$$
$$\psi(x,t) = \psi_0(x,t) + \xi\psi_1(x,t) + \xi^2\psi_2(x,t) + \cdots ,$$

where all ϕ_i and ψ_i are smooth and bounded functions that satisfy

$$\phi_i = 0 \quad (i \geq 0), \quad \psi_0 = \psi_\infty, \quad \text{and} \quad \psi_i = 0 \ (i \geq 1) \quad \text{on } \partial\Omega.$$

Leading order equations

$$\begin{aligned} &W'(\phi_0) = 0, \\ &\partial_t\phi_0 = -2P\phi_0 - \gamma_0 W''(\phi_0)\phi_1 - 2\rho_{\mathrm{w}}(\phi_0 - 1)U \\ &\qquad\qquad + \frac{1}{2}\varepsilon'(\phi_0)|\nabla\psi_0|^2 + 2(\phi_0 - 1)B(\psi_0), \\ &\nabla\cdot\varepsilon(\phi_0)\nabla\psi_0 - (\phi_0 - 1)^2 B'(\psi_0) = -f. \end{aligned}$$

Consequences: (1) $\phi_0 = 0$ or 1; (2) $\{\phi_0 = 0\} \neq \emptyset$ by the BC; and (3) $\{\phi_0 = 1\} \neq \emptyset$ by the property of U and the second equation.

Conclusion: These expansions do not hold in the entire region.

Assumptions

- The entire region is the union of an outer and inner region.
- The outer region is the union of $\Omega_\xi^+(t) := \{x \in \Omega : \phi(x,t) \approx 1\}$ (the solute region) and $\Omega_\xi^-(t) := \{x \in \Omega : \phi(x,t) \approx 0\}$ (the solvent region).
- The inner region is a thin layer of width $O(\xi)$ that centers around the closed and smooth interface $\Gamma_\xi(t) = \{x \in \Omega : \phi(x,t) = 1/2\}$ enclosing $\Omega_\xi^+(t)$.
- This interface is $O(\xi)$-close to a smooth interface $\Gamma(t)$ that is independent of ξ.
- The solutions in the inner region and outer region match asymptotically.

Local coordinates for a point x in the inter region:

$$x = \Phi(y,t) + \xi z(t) n(y,t).$$

- $\Phi(\cdot,t) : Q(t) \to \Gamma_\xi(t)$ a smooth, principal-curvature parameterization, and $Q(t) \subset \mathbb{R}^3$ is an $O(\xi)$-neighborhood of $\Gamma_\xi(t)$ and $\Gamma(t)$.
- $z(t) = s(x,t)/\xi$ with $s(x,t) = \pm \mathrm{dist}\,(x, \Gamma_\xi(t))$.
- $n(y,t) = \nabla_x s(x,t)$ is the unit normal to $\Gamma_\xi(t)$ at $\Phi(y,t)$.
- The normal velocity is $v(y,t) = \partial_t \Phi(y,t) \cdot n(y,t)$.
- The mean curvature is $H(y,t) = \nabla_y \cdot n(y,t)/2$.

Assume the inner expansions

$$\phi(x,t) = \tilde{\phi}_0(z,y,t) + \xi\tilde{\phi}_1(z,y,t) + \xi^2\tilde{\phi}_2(z,y,t) + \cdots ,$$
$$\psi(x,t) = \tilde{\psi}_0(z,y,t) + \xi\tilde{\psi}_1(z,y,t) + \xi^2\tilde{\psi}_2(z,y,t) + \cdots ,$$

where all $\tilde{\phi}_i$ and $\tilde{\psi}_i$ are smooth and bounded functions that satisfy

$$\tilde{\phi}_i = 0 \quad (i \geq 0), \quad \tilde{\psi}_0 = \psi_\infty, \quad \text{and} \quad \tilde{\psi}_i = 0 \ (i \geq 1) \quad \text{on } \partial\Omega.$$

Leading order equations: $\partial_z\tilde{\psi}_0 = 0$ and

$$-v\,\partial_z\tilde{\phi}_0 = \gamma_0\left[\partial_{zz}^2\tilde{\phi}_0 - W'(\tilde{\phi}_0)\right].$$

Matching conditions: $\tilde{\phi}_0(\infty) = 1$, $\tilde{\phi}_0(-\infty) = 0$, and $\partial_z\tilde{\phi}_0(\pm\infty) = 0$. Hence

$$-v\int_{-\infty}^{\infty}\left(\partial_z\tilde{\phi}_0\right)^2 dz = \gamma_0\left[\frac{1}{2}(\partial_z\tilde{\phi}_0)^2 - W(\tilde{\phi}_0)\right]\Bigg|_{z=-\infty}^{z=\infty} = 0.$$

Therefore $v = 0$. To the leading order, the interface does not move at this time scale.

Slow time scale: $\tau = \xi t$.

Outer expansions

$$W'(\phi_0) = 0,$$
$$\nabla \cdot \varepsilon(\phi_0)\nabla\psi_0 - (\phi_0 - 1)^2 B'(\psi_0) = -f.$$

Use the local coordinate

$$x = \Phi(y, \tau) + \xi z(\tau) n(y, \tau)$$

to assume the local inner expansions

$$\phi(x, t) = \tilde{\phi}_0(z, y, \tau) + \xi\tilde{\phi}_1(z, y, \tau) + \xi^2\tilde{\phi}_2(z, y, \tau) + \cdots,$$
$$\psi(x, t) = \tilde{\psi}_0(z, y, \tau) + \xi\tilde{\psi}_1(z, y, \tau) + \xi^2\tilde{\psi}_2(z, y, \tau) + \cdots,$$

where all $\tilde{\phi}_i$ and $\tilde{\psi}_i$ are smooth and bounded functions that satisfy

$$\tilde{\phi}_i = 0 \quad (i \geq 0), \quad \tilde{\psi}_0 = \psi_\infty, \quad \text{and} \quad \tilde{\psi}_i = 0 \ (i \geq 1) \quad \text{on } \partial\Omega.$$

Also, expand

$$U(x) = U(\Phi(y), \tau) + O(\xi) = \tilde{U}_0(y, \tau) + O(\xi).$$

Leading order equations

$$0 = \partial_z \tilde{\psi}_0,$$

$$0 = \partial_{zz}^2 \tilde{\phi}_0 - W'(\tilde{\phi}_0),$$

$$-v\,\partial_z \tilde{\phi}_0 = -2P\tilde{\phi}_0 + \gamma_0 \left[2H\tilde{\phi}_0 + \partial_{zz}^2 \tilde{\phi}_1 - W''(\tilde{\phi}_0)\tilde{\phi}_1\right]$$

$$-2\rho_{\mathrm{w}}(\tilde{\phi}_0 - 1)\tilde{U}_0 + \frac{1}{2}\varepsilon'(\tilde{\phi}_0)\left[|\nabla_{\Gamma(\tau)}\tilde{\psi}_0|^2 + (\partial_z \tilde{\psi}_1)^2\right] + 2(\tilde{\phi}_0 - 1)B(\tilde{\psi}_0),$$

$$\partial_z \left[\varepsilon(\tilde{\phi}_0)\partial_z \tilde{\psi}_1\right] = 0.$$

Matching conditions

$$\lim_{z\to\pm\infty} \tilde{\phi}_0(z, y, \tau) = \phi_0^{\pm}(x, \tau),$$

$$\lim_{z\to\pm\infty} \tilde{\psi}_0(z, y, \tau) = \psi_0^{\pm}(x, \tau),$$

$$\tilde{\psi}_1(z, y, \tau) = \left(\psi_1^{\pm} + z\nabla\psi_0^{\pm} \cdot \nabla s\right)(x, \tau) + o(1) \qquad \text{as } z \to \pm\infty.$$

We have then

$$\tilde{\phi}_0(z, y, \tau) = \tilde{\phi}_0(z) = 0.5\left[1 + \tanh(3z)\right],$$

$$\partial_z \tilde{\psi}_1(z, y, \tau) = \nabla\psi_0^{\pm}(x, \tau) \cdot \nabla s(x, \tau) + o(1) \quad \text{as } z \to \pm\infty.$$

First and fourth equations imply

$$\psi_0^- = \psi_0^+ \quad \text{and} \quad \varepsilon_{\mathrm{w}}\varepsilon_0 \nabla \psi_0^- \cdot n = \varepsilon_{\mathrm{p}}\varepsilon_0 \nabla \psi_0^+ \cdot n \quad \text{on } \Gamma(\tau).$$

Thus, ψ_0 is a solution to the boundary-value problem of the PB equation.

Multiply the v equation by $\partial_z \tilde{\psi}_0$ and integrate against z from $-\infty$ to ∞ to get

$$-vS = \int_{-\infty}^{\infty} R_1(z)\tilde{\phi}_0'(z)\mathrm{d}z + \int_{-\infty}^{\infty} R_2(z)\tilde{\phi}_0'(z)\mathrm{d}z + \int_{-\infty}^{\infty} R_3(z)\tilde{\phi}_0'(z)\mathrm{d}z,$$

$$S := \int_{-\infty}^{\infty} \left[\tilde{\phi}_0'(z)\right]^2 \mathrm{d}z = 1,$$

$$R_1(z) := -2P\tilde{\phi}_0 - 2\rho_{\mathrm{w}}(\tilde{\phi}_0 - 1)\tilde{U}_0 + 2(\tilde{\phi}_0 - 1)B(\tilde{\psi}_0),$$

$$R_2(z) := \gamma_0 \left[2H\partial_z\tilde{\phi}_0 + \partial_{zz}^2\tilde{\phi}_1 - W''(\tilde{\phi}_0)\tilde{\phi}_1\right],$$

$$R_3(z) := \frac{1}{2}\varepsilon'(\tilde{\phi}_0)\left[|\nabla_{\Gamma(\tau)}\tilde{\psi}_0|^2 + (\partial_z\tilde{\psi}_1)^2\right].$$

Integration by parts and matching conditions imply

$$\int_{-\infty}^{\infty} R_1(z)\tilde{\phi}_0'(z)\,\mathrm{d}z = -P + \rho_{\mathrm{w}} U - B(\psi_0),$$
$$\int_{-\infty}^{\infty} R_2(z)\tilde{\phi}_0'(z)\mathrm{d}z = 2\gamma_0 H.$$

Using in addition the interface conditions for ψ_0 on $\Gamma(\tau)$ to obtain

$$\int_{-\infty}^{\infty} R_3(z)\tilde{\phi}_0'(z)\,\mathrm{d}z = \frac{1}{2}(\varepsilon_{\mathrm{p}}\varepsilon_0 - \varepsilon_{\mathrm{w}}\varepsilon_0)|\nabla_{\Gamma(\tau)}\psi_0|^2 + \frac{1}{2}\left(\frac{1}{\varepsilon_{\mathrm{w}}\varepsilon_0} - \frac{1}{\varepsilon_{\mathrm{p}}\varepsilon_0}\right)\left|\varepsilon_{\Gamma(\tau)}\nabla\psi_0 \cdot n\right|^2.$$

Finally, the normal velocity is

$$v = P - 2\gamma_0 H - \rho_{\mathrm{w}} U + \frac{1}{2}\left(\frac{1}{\varepsilon_{\mathrm{p}}\varepsilon_0} - \frac{1}{\varepsilon_{\mathrm{w}}\varepsilon_0}\right)\left|\varepsilon_{\Gamma(\tau)}\nabla\psi_0 \cdot n\right|^2 + \frac{1}{2}(\varepsilon_{\mathrm{w}}\varepsilon_0 - \varepsilon_{\mathrm{p}}\varepsilon_0)|\nabla_{\Gamma(\tau)}\psi_0|^2 + B(\psi_0).$$

Exactly the same as in the sharp-interface model!

4. Conclusions and Discussions

Summary of Work and Issues

- Phase-field models for complex interface motion:
  - relaxation of bending energy;
  - coupling the diffusion of actin promoters and myosin in cell motion;
  - relaxation of dielectric boundaries with Poisson–Boltzmann electrostatics.
- Matched asymptotic analysis to validate phase-field models.
- Relatively easy numerical implementation. Challenging in high resolution and efficient computations.
- Rate of conference of a phase-field model to the sharp-interface model?

Current and Future Work

- Gamma-convergence of phase-field model to the sharp-interface model for molecular solvation: energies and forces.
- Incorporate fluctuations in the phase-field formulation for moving interfaces.
- Couple particle dynamics with phase-field description of interfaces.
- More applications: biofilms, protein folding, etc.?

References

- B. Li & Y. Zhao, SIAM J. Applied Math., 73, 1–23, 2013.
- Y. Zhao, Y.-Y. Kwan, J. Che, B. Li, & J. A. McCammon, J. Chem. Phys., 139, 024111, 2013.
- B. A. Camley, Y. Zhao, B. Li, H. Levine, & W.-J. Rappel, Phys. Rev. Lett., 111, 158102, 2013.
- B. A. Camley, Y. Zhang, Y. Zhao, B. Li, E. Ben-Jacob, H. Levine, & W.-J. Rappel, Proc. Natl Acad. Sci. USA, 111, 14770–14775, 2014.
- T. Banham, B. Li, & Y. Zhao, Phys. Rev. E, 90, 033308, 2014.
- B. Li & Y. Liu, SIAM J. Applied Math, 2015 (submitted).
- Y. Liu, B. A. Camley, W.-J. Rappel, & B. Li (in preparation).
- S. Dai & B. Li (in preparation).
- J. Wen, Y. Zhao, H. Sun, & B. Li (in preparation).

Thank you!