Bubble Assemblies in Binary/Ternary Systems with Long Range Interaction

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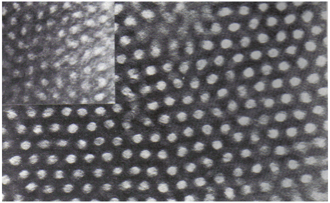
Outline

Diverse Patterns



- Top left: Disc assemblies. Vampire Plecostomus (Image Credit: PlanetCatfish.com);
- Top right: Disc assemblies. cross section of diblock copolymer in cylindrical phase (Image Credit: Peter R. Lewis);
- Bottom left: Lamellar patterns. Marbled Headstander (Image Credit: seriouslyfish.com)
- Bottom right: Core-shell assemblies. Blue Spotted Grouper (Image Credit: flickr.com)

Block copolymers

- When two or more different monomers unite together to polymerize, their result is called a **copolymer**.

- Copolymers can be classified based on how the monomers are arranged along the chain. These include:
    - **Alternating copolymers**
    - **Random copolymers**
    - **Block copolymers**

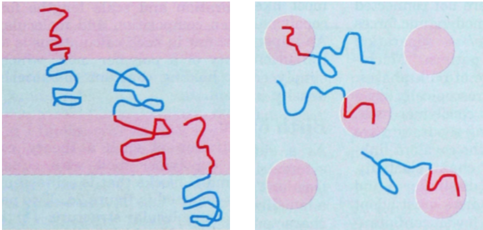
—A—B—A—B—A—B—A—B—A—B—

—A—B—B—B—A—B—A—B—A—A—

—B—B—B—B—B—A—A—A—A—A—

Block copolymers

- Block copolymers comprise two or more homopolymer subunits linked by covalent bonds.
- Block copolymers with two or three distinct blocks are called diblock copolymers and triblock copolymers, resepctively.

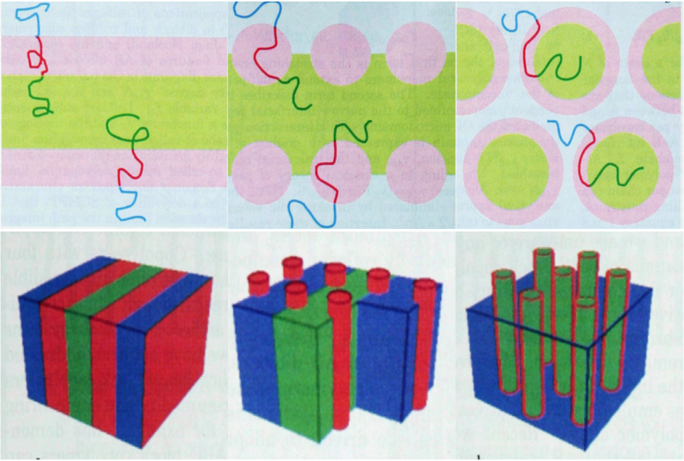


(Image Credit: Frank S. Bates and Glenn H. Fredrickson)

Block copolymers

- Due to incompatibility between blocks, block copolymers undergo a phase separation; but becuase blocks are covalently bonded, they cannot demix macroscopically as water and oil. We call it microphase separation.
- Block copolymers are interesting because they can microphase separate to form periodic nanostructures. For instance, styrene-butadiene-styrene block copolymer is used for shoe soles and adhesives.
- More Commercial use: wine bottle stoppers, jelly candles, outdoor coverings for optical fibre cables, bitumen modifiers, or in artificial organ technology.

Block copolymers



(Image Credit: Frank S. Bates and Glenn H. Fredrickson)

Binary diffuse interface model: Ohta-Kawasaki theory

$$E(\phi) = \int_\Omega \left[\frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{\epsilon}W(\phi)\right] dx + \frac{\gamma}{2}\int_\Omega \left|(-\Delta)^{-\frac{1}{2}}\left(f(\phi)-\omega\right)\right|^2 dx.$$

- Ohta-Kawasaki theory (Ohta-Kawasaki, Macromolecules 1986).
- ϕ: the concentration of one of the two species
  - $\{\phi(x) = 1\}$, A-species rich region;
  - $\{\phi(x) = 0\}$, B-species rich region;
  - $\{0 < \phi(x) < 1\}$, transition layer;
  - $W(\phi) = 18\phi^2(\phi - 1)^2$;
  - γ, strength of long-range repulsion.

Binary diffuse interface model: Ohta-Kawasaki theory

$$E(\phi) = \int_\Omega \left[\frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{\epsilon}W(\phi)\right] dx + \frac{\gamma}{2}\int_\Omega \left|(-\Delta)^{-\frac{1}{2}}(f(\phi)-\omega)\right|^2 dx.$$

- $f(\phi)$: an artificial term for the force localization
  - $f(\phi) = 3\phi^2 - 2\phi^3$;
  - $f(1) = 1, f(0) = 0$, $f(\phi)$ resembles ϕ as an indicator;
  - $f'(1) = f'(0) = 0$, repulsive force is enforced near A-B interface.

Binary diffuse interface model: Ohta-Kawasaki theory

$$E(\phi) = \int_\Omega \left[\frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{\epsilon}W(\phi)\right]dx + \frac{\gamma}{2}\int_\Omega \left|(-\Delta)^{-\frac{1}{2}}(f(\phi)-\omega)\right|^2 dx.$$

- $(-\Delta)^{-1} : \mathring{L}^2_{\text{per}}(\Omega) \to \mathring{H}^1_{\text{per}}(\Omega)$

$$(-\Delta)^{-1}(f(\phi)-\omega) = v \Longleftrightarrow -\Delta v = f(\phi)-\omega.$$

- $(-\Delta)^{-\frac{1}{2}}$ is its positive square root

$$\int_\Omega \left|(-\Delta)^{-\frac{1}{2}}(f(\phi)-\omega)\right|^2 dx = \int_\Omega (-\Delta)^{-1}(f(\phi)-\omega)(f(\phi)-\omega)dx$$
$$= \int_\Omega v(-\Delta v)dx = \int_\Omega |\nabla v|^2 dx.$$

- Volume constraint: $\int_\Omega f(\phi)dx = \omega|\Omega|$

Gradient flow dynamics

- L^2 gradient flow dynamics with volume penalty: penalized Allen-Cahn-Ohta-Kawasaki dynamics (pACOK)

$$\frac{\partial \phi}{\partial t} = \epsilon \Delta \phi - \frac{1}{\epsilon} W'(\phi) - \gamma (-\Delta)^{-1} (f(\phi) - \omega) f'(\phi) \\ - M \left(\int_\Omega f(\phi) dx - \omega |\Omega| \right) f'(\phi).$$

- H^{-1} gradient flow dynamics: Cahn-Hilliard-Ohta-Kawasaki dynamics (CHOK)

$$\frac{\partial \phi}{\partial t} = \quad \Delta \left[\left(-\epsilon \Delta \phi + \frac{1}{\epsilon} W'(\phi) \right) + \gamma (-\Delta)^{-1} (f(\phi) - \omega) f'(\phi) \right].$$

  - $f(\phi) = \phi$, IEQ method (Cheng, Yang and Shen, JCP 2017);
  - $f(\phi) = \phi$, implicit midpoint spectral method (Benesova, Melcher and Suli, SINUM 2014);

Energy stable schemes

- Convex splitting schemes
  - Wang-Wang-Wise, DCDS-A, 2010;
  - Shen-Wang-Wang-Wise, SINUM, 2012;
  - Chen-Conde-Wang-Wang-Wise, JSC, 2012;
  - Chen-Wang-Wang-Wise, JSC, 2014;
- Stabilized semi-implicit schemes
  - Xu-Tang, SINUM, 2006;
  - Li-Qiao-Tang, SINUM, 2016;
  - Ju-Li-Qiao-Zhang, Math. Comput. 2017;
  - Du-Ju-Li-Qiao, JCP, 2018;
- IEQ method
  - Ju-Zhao-Yang-Wang-Shen, 2016-2017;

Stabilized semi-implicit schemes for pACOK

Penalized Ohta-Kawasaki energy:

$$E[\phi] = \int_\Omega \left[\frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{\epsilon}W(\phi)\right] dx + \frac{\gamma}{2}\int_\Omega \left|(-\Delta)^{-\frac{1}{2}}\left(f(\phi)-\omega\right)\right|^2 dx + \frac{M}{2}\left(\int_\Omega f(\phi)dx - \omega|\Omega|\right)^2,$$

- $E_l[\phi] = \int_\Omega \frac{\epsilon}{2}|\nabla\phi|^2 + \frac{\kappa}{2\epsilon}\phi^2 + \frac{\gamma}{2}\beta\left|(-\Delta)^{-\frac{1}{2}}(\phi-\omega)\right|^2 dx;$
- $E_n[\phi] = E_l[\phi] - E[\phi];$
- Semi-discrete scheme:

$$\frac{\phi^{n+1}-\phi^n}{\tau} = -\frac{\delta E_l}{\delta\phi}(\phi^{n+1}) + \frac{\delta E_n}{\delta\phi}(\phi^n).$$

Stabilized semi-implicit schemes for pACOK

Semi-discrete scheme:

$$\frac{\phi^{n+1} - \phi^n}{\tau} = -\frac{\delta E_l}{\delta \phi}(\phi^{n+1}) + \frac{\delta E_n}{\delta \phi}(\phi^n).$$

- Unconditional unique solvability: all eigenvalues of the following operator are positive

$$\left(\left(\frac{1}{\tau} + \frac{\kappa}{\epsilon} \right) I - \epsilon\Delta + \gamma\beta(-\Delta)^{-1} \right) \phi^{n+1} = F^n$$

Stabilized semi-implicit schemes for pACOK

Semi-discrete scheme:

$$\frac{\phi^{n+1}-\phi^n}{\tau} = -\frac{\delta E_c}{\delta \phi}(\phi^{n+1}) + \frac{\delta E_e}{\delta \phi}(\phi^n).$$

- Unconditional energy stability:

$$E[\phi^{n+1}] \leq E[\phi^n],$$

provided that

$$\kappa \geq \frac{L_W}{2} + \epsilon\Big(\frac{\gamma L_f}{2}\|(-\Delta)^{-1}\|_\infty \max\{\omega, 1-\omega\} + \frac{M}{2}|\Omega|\left(L_p^2 + L_f \max\{\omega, 1-\omega\}\right)\Big);$$

$$\beta \geq \frac{L_p^2}{2}.$$

  - Quadratic and linear extensions of W and f, respectively;
  - L_W, L_f are upper bounds of $|W''|, |f''|$;
  - L_p is Lipschitz constant of f.

Spectral collocation approximation for space

- $\Omega = [-X, X) \times [-Y, Y) \subset \mathbb{R}^2$;
- N_x and N_y are two positive even integers, $h_x = \frac{2X}{N_x}$ and $h_y = \frac{2Y}{N_y}$;
- $\Omega_h = \Omega \cap (h_x\mathbb{Z} \otimes h_y\mathbb{Z})$;
- Index sets:

$$S_h = \left\{(i,j) \in \mathbb{Z}^2 | 1 \le i \le N_x, 1 \le j \le N_y\right\},$$
$$\hat{S}_h = \left\{(k,l) \in \mathbb{Z}^2 | -\frac{N_x}{2} + 1 \le k \le \frac{N_x}{2}, -\frac{N_y}{2} + 1 \le j \le \frac{N_y}{2}\right\}.$$

- periodic grid functions on Ω_h:

$$\mathcal{M}_h = \left\{f : \Omega_h \to \Omega | f_{i+mN_x, j+nN_y} = f_{ij}, \forall (i,j) \in S_h, \forall (m,n) \in \mathbb{Z}^2\right\}.$$

- Discrete inner products and norms:

$$\langle f, g\rangle_h = h_x h_y \sum_{(i,j)\in S_h} f_{ij} g_{ij}, \|f\|_{h,L^2} = \sqrt{\langle f, f\rangle_h}, \|f\|_{h,L^\infty} = \max_{(i,j)\in S_h} |f_{ij}|;$$
$$\langle \mathbf{f}, \mathbf{g}\rangle_h = h_x h_y \sum_{(i,j)\in S_h} \left(f_{ij}^1 g_{ij}^1 + f_{ij}^2 g_{ij}^2\right), \|\mathbf{f}\|_{h,L^2} = \sqrt{\langle \mathbf{f}, \mathbf{f}\rangle_h}.$$

Spectral collocation approximation for space

- 2D discrete Fourier transform (DFT):

$$\hat{f}_{kl} = \frac{1}{N_x N_y} \sum_{(i,j)\in S_h} f_{ij} \exp\left(-\mathrm{i}\frac{k\pi}{X}x_i\right) \exp\left(-\mathrm{i}\frac{l\pi}{Y}y_j\right), \quad (k,l)\in \hat{S}_h,$$

- 2D inverse DTF (iDFT) :

$$f_{ij} = \sum_{(k,l)\in \hat{S}_h} \hat{f}_{kl} \exp\left(\mathrm{i}\frac{k\pi}{X}x_i\right) \exp\left(\mathrm{i}\frac{l\pi}{Y}y_j\right), \quad (i,j)\in S_h.$$

- Let $\widehat{\mathcal{M}}_h = \{Pf \,|\, f \in \mathcal{M}_h\}$ and define the operators $\hat{D}_x, \hat{D}_y$ on $\widehat{\mathcal{M}}_h$ as

$$(\hat{D}_x \hat{f})_{kl} = \left(\frac{\mathrm{i}k\pi}{X}\right)\hat{f}_{kl}, \quad (\hat{D}_y \hat{f})_{kl} = \left(\frac{\mathrm{i}l\pi}{X}\right)\hat{f}_{kl}, \quad (k,l)\in \hat{S}_h,$$

- Fourier spectral approximations to the the spatial operators $\partial_x, \partial_{xx}$:

$$D_x = P^{-1}\hat{D}_x P, \quad D_y = P^{-1}\hat{D}_y P, \quad D_x^2 = P^{-1}\hat{D}_x^2 P, \quad D_y^2 = P^{-1}\hat{D}_y^2 P.$$

Spectral collocation approximation for space

- Discrete gradient, divergence and Laplace operators are given respectively by

$$\nabla_h f = (D_x f, D_y f)^T, \nabla_h \cdot \mathrm{f} = D_x f^1 + D_y f^2,$$
$$\Delta_h f = D_x^2 f + D_y^2 f = P^{-1}(\hat{D}_x^2 + \hat{D}_y^2) P f.$$

- Let $\mathring{\mathcal{M}}_h = \{f \in \mathcal{M}_h | \langle f, 1 \rangle_h = 0\}$ be the collections of all periodic grid functions with zero mean. Define $(-\Delta_h)^{-1} : \mathring{\mathcal{M}}_h \to \mathring{\mathcal{M}}_h$ as

$$(-\Delta_h)^{-1} f = u \Longleftrightarrow -\Delta_h u = f.$$

- In terms of DFT and iDFT, we define it as

$$\begin{aligned} (-\Delta_h)^{-1} f &= -P^{-1}(\hat{D}_x^2 + \hat{D}_y^2)^{-1} P f \\ &= -P^{-1} \begin{cases} \left[\left(\frac{k\pi}{X}\right)^2 + \left(\frac{l\pi}{Y}\right)^2 \right]^{-1} \hat{f}_{kl}, & (k, l) \neq (0, 0) \\ 0, & (k, l) = (0, 0) \end{cases} \end{aligned}$$

Uniform L^∞ bound of $(-\Delta_h)^{-1}$

Lemma

For any functions $f \in \mathcal{M}_h$, we have

$$\|f\|_{h,L^\infty} \leq C_s \|f\|_{h,H^s}$$

provided $s > d/2, d = 2, 3$, where C_s is a constant only depending on s and independent of h.

- Discrete H^s norms for $f \in \mathcal{M}_h$:

$$\|f\|_{h,H^s}^2 = \sum_{(k,l)\in\hat{S}_h} \Big(1 + (k^2 + l^2)^s\Big) |\hat{f}_{kl}|^2.$$

- Taking $s = 2$, we can have an estimate on C_2:

$$C_2^2 = \sum_{(k,l)\in\mathbb{Z}^2} \frac{1}{1 + (k^2 + l^2)^2} \leq 1 + 4 \cdot \frac{\pi^2}{6} + \frac{\pi^2}{2}.$$

Uniform L^∞ bound of $(-\Delta_h)^{-1}$

Lemma

Let any $u, f \in \mathcal{M}_h$ be such that $-\Delta_h u = f$, then we have

$$\|u\|_{h,L^\infty} \leq C_\infty \|f\|_{h,L^\infty}, \tag{1}$$

where C_∞ is independent of h. In other words, $\|(-\Delta_h)^{-1}\|_{h,L^\infty} \leq C_\infty$ is uniformly bounded.

- $\|u\|_{h,L^\infty} \leq C_2 \|u\|_{h,H^2} \leq C_\infty \|f\|_{h,L^\infty}$;
- $C_\infty = C_2 \sqrt{(1 + C_p^4)|\Omega|}$;
- $C_p \leq \frac{\max\{X,Y\}}{\pi}$.

Energy stability for full discrete schemes of pACOK

Find $\phi_h^{n+1} = (\phi_{ij}^{n+1}) \in \mathcal{M}_h$ such that

$$\begin{aligned}
\frac{\phi_h^{n+1} - \phi_h^n}{\tau} &= \epsilon \Delta_h \phi_h^{n+1} - \frac{\kappa_h}{\epsilon}\phi_h^{n+1} - \gamma\beta_h(-\Delta_h)^{-1}(\phi_h^{n+1} - \omega) \\
&+ \frac{1}{\epsilon}\left[\kappa_h \phi_h^n - W'(\phi_h^n)\right] \\
&+ \gamma\left[\beta_h(-\Delta_h)^{-1}(\phi_h^n - \omega) - (-\Delta_h)^{-1}(f(\phi_h^n) - \omega)f'(\phi_h^n)\right] \\
&- M\left[\langle f(\phi_h^n), 1\rangle_h - \omega|\Omega|\right] f'(\phi_h^n).
\end{aligned}$$

- Unconditional unique solvability.

Energy stability for full discrete schemes of pACOK

Define a discrete analogy of the energy $E[\phi]$:

$$E_h[\phi_h] = \frac{\epsilon}{2}\|\nabla_h \phi_h\|_{h,L^2}^2 + \frac{1}{\epsilon}\langle W(\phi_h), 1\rangle_h + \frac{\gamma}{2}\|(-\Delta_h)^{-\frac{1}{2}}(f(\phi_h - \omega))\|_{h,L^2}^2 + \frac{M}{2}\left(\langle f(\phi_h), 1\rangle_h - \omega|\Omega|\right)^2.$$

Theorem

For any $\tau > 0$, the ϕ_h^{n+1} determined by the full discrete scheme satisfies:

$$E_h[\phi_h^{n+1}] \leq E_h[\phi_h^n],$$

provided that the constants κ_h and β_h satisfy

$$\kappa_h \geq \frac{L_W}{2} + \epsilon\Big(\frac{\gamma L_f}{2}\|(-\Delta_h)^{-1}\|_{h,\infty} \max\{\omega, 1-\omega\} + \frac{M}{2}|\Omega|\left(L_p^2 + L_f \max\{\omega, 1-\omega\}\right)\Big); \quad \beta_h \geq \frac{L_p^2}{2}.$$

Numerical experiments: binary system

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Ternary diffuse interface model: Ohta-Nakazawa theory

$$E(\phi_1,\phi_2) = \int_\Omega \left[\frac{\epsilon}{2}\left(|\nabla\phi_1|^2 + |\nabla\phi_2|^2 + \nabla\phi_1\cdot\nabla\phi_2\right) + \frac{1}{2\epsilon}W_T(\phi_1,\phi_2)\right]dx$$
$$+ \sum_{i,j=1}^{2}\frac{\gamma_{ij}}{2}\int_\Omega \left[(-\Delta)^{-\frac{1}{2}}\left(f(\phi_i)-\omega_i\right)(-\Delta)^{-\frac{1}{2}}\left(f(\phi_j)-\omega_j\right)\right]dx.$$

- Ohta-Nakazawa theory for ABC-type copolymers (Nakazawa-Ohta, Macromolecules 1993).
- $\phi_1, \phi_2, 1-\phi_1-\phi_2$ label A, B, C rich regions, respectively.
- $W_T(\phi_1,\phi_2) := W(\phi_1) + W(\phi_2) + W(1-\phi_1-\phi_2)$.
- Volume constraints:

$$\int_\Omega f(\phi_i)dx = \omega_i|\Omega|, \quad i = 1, 2.$$

- Symmetric $[\gamma_{ij}]_{2\times 2}$: long-range interaction strengths.

penalized Allen-Cahn-Ohta-Nakazawa dynamics (pACON)

$$\begin{aligned}\frac{\partial \phi_i}{\partial t} = &\ \epsilon \Delta \phi_i + \frac{\epsilon}{2}\Delta \phi_j - \frac{1}{2\epsilon}\frac{\partial W_T}{\partial \phi_i} \\ &- \gamma_{ii}(-\Delta)^{-1}(f(\phi_i) - \omega_i)f'(\phi_i) \\ &- \gamma_{ij}(-\Delta)^{-1}(f(\phi_j) - \omega_j)f'(\phi_i) \\ &- M_i\left[\int_\Omega f(\phi_i)dx - \omega|\Omega|\right] f'(\phi_i), \quad i = 1, 2,\ j \neq i.\end{aligned}$$

Stabilized semi-implicit scheme for pACON

$$
\begin{aligned}
\frac{\phi_1^{n+1}-\phi_1^n}{\tau} &= \epsilon\Delta\phi_1^{n+1} + \frac{\epsilon}{2}\Delta\phi_2^n - \frac{\kappa_1}{2\epsilon}\phi_1^{n+1} - \frac{1}{2\epsilon}\left(\frac{\partial W_T}{\partial\phi_1}(\phi_1^n) - \kappa_1\phi_1^n\right) \\
&\quad - \gamma_{11}\beta_{11}(-\Delta)^{-1}(\phi_1^{n+1}-\omega_1) - \gamma_{12}(-\Delta)^{-1}(f(\phi_2^n)-\omega_2)f'(\phi_2^n) \\
&\quad - \gamma_{11}\left[(-\Delta)^{-1}(f(\phi_1^n)-\omega_1)f'(\phi_1^n) - \beta_{11}(-\Delta)^{-1}(\phi_1^n-\omega_1)\right] \\
&\quad - M_1\left[\int_\Omega f(\phi_1^n)dx - \omega_1|\Omega|\right] f'(\phi_1^n), \\
\frac{\phi_2^{n+1}-\phi_2^n}{\tau} &= \epsilon\Delta\phi_2^{n+1} + \frac{\epsilon}{2}\Delta\phi_1^{n+1} - \frac{\kappa_2}{2\epsilon}\phi_2^{n+1} - \frac{1}{2\epsilon}\left(\frac{\partial W_T}{\partial\phi_2}(\phi_2^n) - \kappa_2\phi_2^n\right) \\
&\quad - \gamma_{22}\beta_{22}(-\Delta)^{-1}(\phi_2^{n+1}-\omega_2) - \gamma_{21}(-\Delta)^{-1}(f(\phi_1^{n+1})-\omega_1)f'(\phi_1^{n+1}) \\
&\quad - \gamma_{22}\left[(-\Delta)^{-1}(f(\phi_2^n)-\omega_2) - \beta_{22}(-\Delta)^{-1}(\phi_2^n-\omega_2)\right] \\
&\quad - M_2\left[\int_\Omega f(\phi_2^n)dx - \omega_2|\Omega|\right] f'(\phi_2^n),
\end{aligned}
$$

- $(\phi_1^n,\phi_2^n) \to (\phi_1^{n+1},\phi_2^n) \to (\phi_1^{n+1},\phi_2^{n+1})$;
- $E[\phi_1^{n+1},\phi_2^{n+1}] \le E[\phi_1^{n+1},\phi_2^n] \le E[\phi_1^n,\phi_2^n]$ for properly chosen $\kappa_1,\kappa_2,\beta_{11},\beta_{22}$.

Numerical experiments: ternary systems

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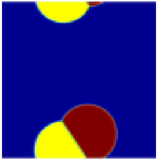
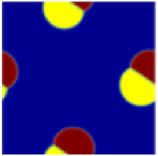
Numerical experiments: ternary systems

Double bubble assemblies (small γ_{12})

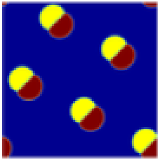
The effect of $\gamma_{11} = \gamma_{22}$



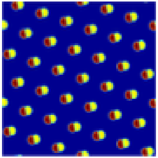
$\gamma_{11} = 0$



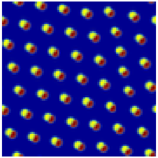
$\gamma_{11} = 200$



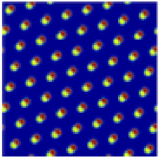
$\gamma_{11} = 1000$



$\gamma_{11} = 20000$

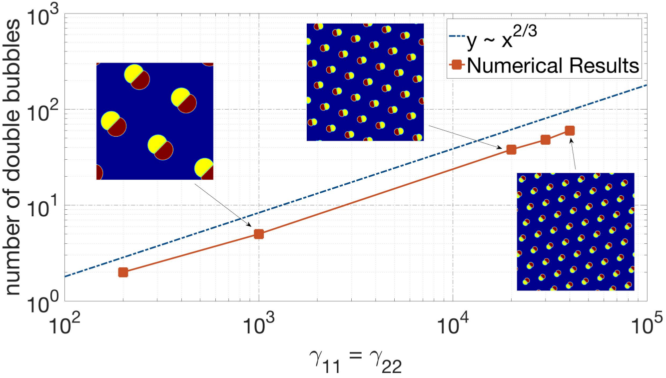


$\gamma_{11} = 30000$



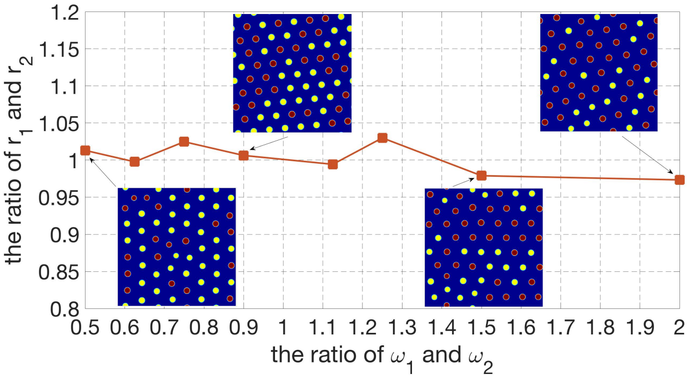
$\gamma_{11} = 40000$

Number of double bubbles obeys $\frac{2}{3}$-law



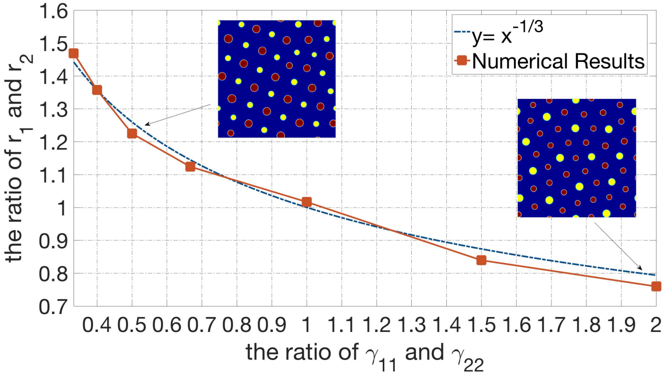
Single bubble assemblies (large γ_{12})

Size of red/yellow bubbles is independent of their volume fraction. In this case, we take $\gamma_{11} = \gamma_{22}$.

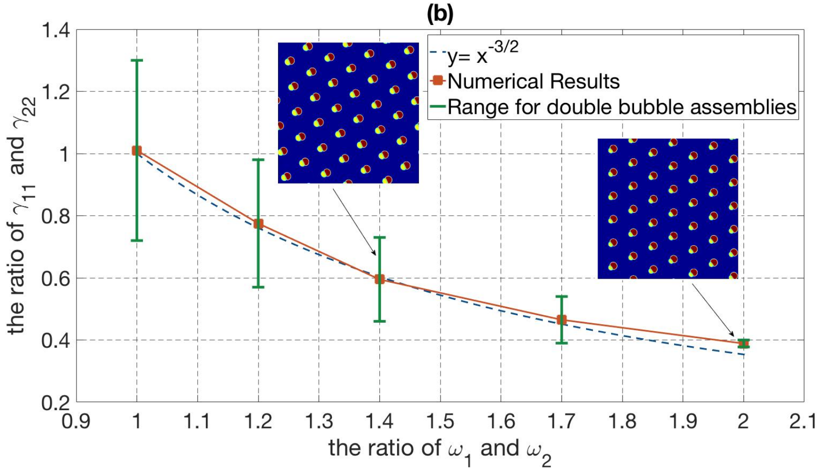


Single bubble assemblies (large γ_{12})

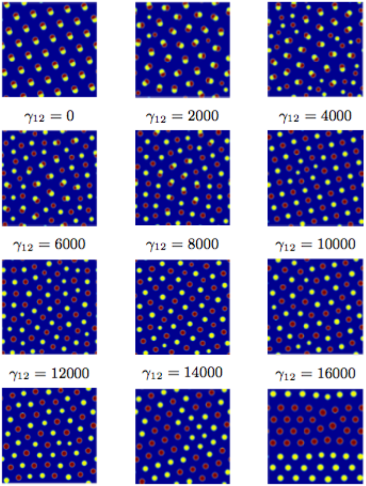
Size of red/yellow bubbles depends on $\frac{\gamma_{11}}{\gamma_{22}}$ via $\frac{1}{3}$-law.



When will double bubble assemblies appear?



Double bubble to single bubble assemblies: effect of γ_{12}



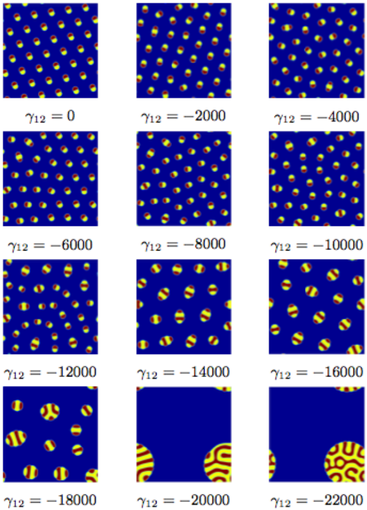
$\gamma_{12} = 0$ $\gamma_{12} = 2000$ $\gamma_{12} = 4000$

$\gamma_{12} = 6000$ $\gamma_{12} = 8000$ $\gamma_{12} = 10000$

$\gamma_{12} = 12000$ $\gamma_{12} = 14000$ $\gamma_{12} = 16000$

$\gamma_{12} = 18000$ $\gamma_{12} = 20000$ $\gamma_{12} = 22000$

Double bubble to single bubble assemblies: effect of γ_{12}



Ongoing works

A more general system of $N+1$ constituents

$$
\begin{aligned}
&E^N[\phi_1,\cdots,\phi_N] \\
&= \int_\Omega \frac{\epsilon}{2} \sum_{\substack{i,j=0 \\ i\le j}}^N \nabla\phi_i\cdot\nabla\phi_j + \frac{1}{2\epsilon}\left[\sum_{i=1}^N W(\phi_i) + W\Big(1-\sum_{i=1}^N \phi_i\Big)\right] dx \\
&\quad + \sum_{i,j=1}^N \frac{\gamma_{ij}}{2}\int_\Omega \Big[(-\Delta)^{-\frac{1}{2}}\left(f(\phi_i)-\omega_i\right)(-\Delta)^{-\frac{1}{2}}\left(f(\phi_j)-\omega_j\right)\Big] dx,
\end{aligned}
$$

- Ternary system ($N=2$): 3d simulations, new patterns;
- Quaternary system ($N=3$): 2d and 3d simulations, new patterns.

Ongoing works

- L^∞ bound of ϕ^n for pACOK;
- Error estimates for the fully discrete schemes of pACOK;
- Higher order schemes and energy stabilities;
- etc.

Thank you!