Numerical Algorithms for Partially Segregated Elliptic Systems

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Outline

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The Physical and Mathematical Context

Partial Segregation Constraint

$$\prod_{i=1}^{m} u_i(x) = 0 \quad \text{a.e. in } \Omega$$

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- Models competitive interactions among m components ($u_i \geq 0$).
- Arises in multi-state Bose-Einstein condensates and Lotka-Volterra dynamics.

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The Mathematical Challenge

- **Coexistence**: Forces ≥ 1 component to vanish; others may coexist.
- **Nonconvexity**: Produces a **highly nonconvex** admissible set.

Pairwise vs. Partial Segregation

Consider the geometric difference between traditional pairwise segregation and our partial constraint for $m = 3$ case

Pairwise Segregation

- Constraint: $u_i u_j = 0$ for all $i \neq j$.
- **At most one** component is positive at any location.
- Domain is partitioned into mutually exclusive single-component phases.

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Partial Segregation

- Constraint: $u_1 u_2 u_3 = 0$.
- **Up to two** components can coexist at any location.
- Domain is stratified by vanishing and coexistence patterns.

Outline

Assumptions

Boundary Conditions

The domain $\Omega \subset \mathbb{R}^d$, $d \geq 1$, is bounded and has Lipschitz boundary. The boundary data satisfy

$$\phi_i \in H^{1/2}(\partial\Omega) \cap L^\infty(\partial\Omega), \quad \phi_i \geq 0, \quad \prod_{i=1}^{m} \phi_i = 0 \quad \text{a.e. on } \partial\Omega.$$

Moreover, they admit a nonnegative Lipschitz extension $\psi = (\psi_1, \ldots, \psi_m) \in \mathrm{Lip}(\overline{\Omega})^m$ such that $\psi_i|_{\partial\Omega} = \phi_i$ and $\prod_{i=1}^{m} \psi_i = 0$ in Ω.

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The Admissible Set S

$$S := \left\{ U = (u_1, \ldots, u_m) \in (H^1(\Omega))^m : \begin{array}{l} u_i \geq 0 \text{ a.e. in } \Omega, \quad u_i|_{\partial\Omega} = \phi_i, \\ \displaystyle\prod_{i=1}^{m} u_i = 0 \text{ a.e. in } \Omega \end{array} \right\}.$$

The Main Minimization Problem (m=3)

Constrained Dirichlet Energy

The primary goal is to minimize the total Dirichlet energy

$$E(U) = \int_\Omega \sum_{i=1}^{3} |\nabla u_i(x)|^2 \, dx$$

over the boundary-constrained partial-segregation set S.

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Penalized Energy Approximation

To overcome nonconvexity, we relax the constraint by minimizing

$$E^\varepsilon(U) := \frac{1}{2} \sum_{i=1}^{3} \int_\Omega |\nabla u_i|^2 \, dx + \frac{1}{2\varepsilon} \int_\Omega (u_1 u_2 u_3)^2 \, dx$$

over the space

$$\mathcal{A}_\phi := \{U \in (H^1(\Omega))^3 : u_i|_{\partial\Omega} = \phi_i, \;\; i = 1, 2, 3\},$$

analyzing the strong-competition limit $\varepsilon \to 0$.

Strong-Competition Limit ($\varepsilon \to 0^+$)

Before introducing the algorithms, we establish the theoretical limit of the penalized solutions U^ε

Euler-Lagrangian

$$\begin{cases} -\Delta u_i + \dfrac{1}{\varepsilon} u_i \displaystyle\prod_{j \neq i} u_j^2 = 0 & \text{in } \Omega, \\ u_i = \phi_i & \text{on } \partial\Omega. \end{cases} \qquad i = 1, 2, 3.$$

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Theorem (Soave & Terracini, 2024)

As $\varepsilon \to 0$, there exists a subsequence U^{ε_k} converging strongly in $H^1(\Omega; \mathbb{R}^3)$ and in $C^{0,\alpha}(\overline{\Omega}; \mathbb{R}^3)$ to a limit U that is a global minimizer of the constrained problem.

Furthermore, the limit satisfies

$$u_1 u_2 u_3 \equiv 0 \quad \text{in } \Omega, \qquad \Delta u_i = 0 \quad \text{in } \{u_i > 0\}, \quad i \in \{1, 2, 3\}$$

Non-uniqueness

1D Example

Let $\Omega = (0,1)$ and $m = 3$. We set the boundary data for $U = (u_1, u_2, u_3)$ as follows

$$U(0) = (2,1,0), \qquad U(1) = (0,1,3).$$

Consider the constrained Dirichlet problem

$$\min \left\{ E(U) := \int_0^1 \left(|u_1'(x)|^2 + |u_2'(x)|^2 + |u_3'(x)|^2 \right) dx : U \in S \right\}.$$

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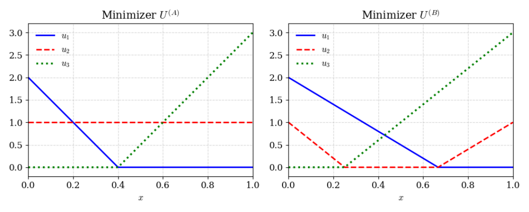
This problem has at least two distinct global minimizers.

$$U^{(A)}(x) = \begin{pmatrix} (2-5x)^+ \\ 1 \\ (5x-2)^+ \end{pmatrix}$$

$$U^{(B)}(x) = \begin{pmatrix} (2-3x)^+ \\ (1-4x)^+ + (3x-2)^+ \\ (4x-1)^+ \end{pmatrix}$$



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Algorithm 1: Iterative Maps T and G

As observed above the penalized energy gives rise to a system of Euler-Lagrange equations. For $U = (u_1, u_2, u_3)$, we define two fixed-point maps:

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1. Jacobi/Picard Map T

$T(U) = V$, where v_i solves the decoupled linear system:

$$-\Delta v_i + \frac{(u_j u_\ell)^2}{\varepsilon} v_i = 0 \quad \text{in } \Omega, \quad v_i|_\Omega = \phi_i \quad (\{i, j, \ell\} = \{1, 2, 3\})$$

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2. Sequential Semi-Implicit Map G

$G(U) = V$, computed sequentially to utilize recent updates immediately:

$$\begin{aligned}
-\Delta v_1 + \varepsilon^{-1}(u_2 u_3)^2 v_1 &= 0 \\
-\Delta v_2 + (2\varepsilon)^{-1} u_3^2 (u_1^2 + v_1^2) v_2 &= 0 \\
-\Delta v_3 + (2\varepsilon)^{-1} \left((u_1 u_2)^2 + (v_1 v_2)^2\right) v_3 &= 0
\end{aligned}$$

Convergence Analysis: Existence and Monotone Sub-sequences

Theorem 1: Existence for every ε

For every $\varepsilon > 0$, the Picard map T has at least one fixed point $U^* \in K$ via Schauder's fixed point theorem. Thus, the penalized system admits a bounded weak solution.

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Theorem 2: Monotone Subsequences

Initializing by harmonic extensions $U^0 = (u_1^0, u_2^0, u_3^0)$, the Picard map $U^{k+1} = T(U^k)$ forms monotonically convergent sub-sequences enclosing every fixed point $U^* = (u_1^*, u_2^*, u_3^*)$

$$U^{2k+1} \uparrow \underline{U}, \quad U^{2k} \downarrow \overline{U} \implies \underline{u_i} \leq u_i^* \leq \overline{u_i}$$

- The full sequence converges iff $\underline{U} = \overline{U}$.
- Gives an *a posteriori* bound $0 \leq \overline{u_i} - \underline{u_i} \leq |u_i^{k+1} - u_i^k|$.

Convergence Analysis: Contraction and Asymptotics

Theorem 3: Explicit Contraction Condition

Let $M = \max \|\phi_i\|_{L^\infty}$ and λ_Ω be the first Dirichlet eigenvalue. If

$$L_T := \frac{4M^4}{\varepsilon \lambda_\Omega} < 1$$

- T has a unique fixed point.
- The Picard iteration converges in L^2 space.

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Theorem 4: Interior Exponential Smallness

In subdomains $V \Subset \Omega$ with uniformly positive competition $\left(\prod_{j\neq i} u_j^k\right)^2 \geq \delta$, the components u_i^k decay **exponentially** away from the boundary as $\varepsilon \to 0^+$, i.e. for every compact $K_0 \subset V$ holds

$$\|u_i^{k+1}\|_{L^\infty(K_0)} \leq C \exp\left(-c\sqrt{\frac{\delta}{\varepsilon}}\right)$$

Outline

Pointwise Projection Operator

We define the partial segregation set in $\mathbb{R}^3$ as follows

$$\Sigma := \{a = (a_1, a_2, a_3) \in \mathbb{R}^3 : a_i \geq 0, a_1 a_2 a_3 = 0\}.$$

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Projection $\mathcal{P}$: For $v \in L^2(\Omega)^3$, we define $\mathcal{P}v$ pointwise. To handle ties deterministically, lets fix $x_0 \in \Omega$, then

$$k^*(x_0) := \min \operatorname*{argmin}_{r \in \{1,2,3\}} (v_r(x_0))^+$$

where $s^+ = \max\{s, 0\}$. The projected components are then

$$(\mathcal{P}v)_i(x_0) = \begin{cases} (v_i(x_0))^+, & i \neq k^*(x_0) \\ 0, & i = k^*(x_0) \end{cases}$$

Pointwise Projection Operator

Lemma

Let

$$W := \{w \in L^2(\Omega)^3 : w(x) \in \Sigma \text{ for a.e. } x \in \Omega\}.$$

Then for every $v \in L^2(\Omega)^3$ *we have* $\mathcal{P}v \in W$ *and*

$$\|v - \mathcal{P}v\|^2_{L^2(\Omega)^3} = \min_{w \in W} \|v - w\|^2_{L^2(\Omega)^3}.$$

Thus $\mathcal{P}$ *is a projection onto* W.

Discrete Projected-Gradient Method

Discrete Formulation: Let $z_i \in \mathbb{R}^{N_I}$ be the interior nodal values of component i, and let A be the Dirichlet matrix for $-\Delta_h$. Here b_i are the boundary data contributions.

Discrete Dirichlet Energy

$$F_h(z) := \frac{1}{2}\sum_{i=1}^{3} z_i^\top A z_i + \sum_{i=1}^{3} b_i^\top z_i, \qquad \nabla_i F_h(z) = A z_i + b_i$$

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Discrete Feasible Set

$$W_h := \{z \in (\mathbb{R}^{N_I})^3 : (z_1(r), z_2(r), z_3(r)) \in \Sigma \text{ for every interior node } r\}.$$

Discrete Projected-Gradient Method

Exact Projected-Gradient Method

Let $z^0 \in W_h$, tolerance $\mathrm{tol} > 0$, and $0 < \tau < 1/\lambda_{\mathsf{max}}(A)$

- $\tilde{z}^{k+1} = z^k - \tau(Az^k + b)$
- $z_{k+1} = \mathcal{P}_h \tilde{z}^{k+1}$.
- **If** $\|z^{k+1} - z^k\|_2 \leq \mathrm{tol}$, **break**!

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Proposition: Exact Descent

Let $L_h := \lambda_{\max}(A)$ and $0 < \tau < \frac{1}{L_h}$. Suppose

$$z^{k+1} \in \operatorname*{argmin}_{z \in W_h} \left\| z - \left(z^k - \tau \nabla F_h(z^k)\right) \right\|_2^2 .$$

Then

$$F_h(z^{k+1}) \leq F_h(z^k) - \left(\frac{1}{2\tau} - \frac{L_h}{2} \right) \|z^{k+1} - z^k\|_2^2 .$$

Consequently, the energy is non-increasing and

$$\|z^{k+1} - z^k\|_2 \to 0.$$

Algorithm 2: Discrete Projected-Gradient Method

Projected-Gradient Method via Nesterov Acceleration

Let $z^0 \in W_h$, $z^{-1} \equiv z^0$, $t_0 = 1$, initial step $\tau > 0$, shrink factor $\rho \in (0,1)$, optional bias $\eta \geq 0$, tolerance $\mathrm{tol} > 0$.

- $\widehat{t}_{k+1} = \frac{1+\sqrt{1+4t_k^2}}{2}, \quad \beta_k = \frac{t_k - 1}{\widehat{t}_{k+1}}$
- $y^k = z^k + \beta_k(z^k - z^{k-1})$
- **Repeat** (Backtracking):
  - $r^k = y^k - \tau \nabla F_h(y^k)$
  - $\tilde{z}^{k+1} = \frac{r^k + \eta z^k}{1+\eta}$
  - $z^{\mathrm{trial}} = \mathcal{P}_h(\tilde{z}^{k+1})$
  - **If** $F_h(z^{\mathrm{trial}}) > F_h(z^k)$, then reject step. Set $y^k = z^k$ (reset momentum), shrink $\tau \leftarrow \tau \cdot \rho$, and flag $t_{k+1} = 1$.
- **Until** $F_h(z^{\mathrm{trial}}) \leq F_h(z^k)$
- Accept step: $z^{k+1} = z^{\mathrm{trial}}$. If not flagged, $t_{k+1} = \widehat{t}_{k+1}$.
- **If** $\|z^{k+1} - z^k\|_2 \leq \mathrm{tol}$, **break**!

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Initialization

Because the partial-segregation problem is highly non-convex, algorithms are sensitive to initialization. We employ robust start-up heuristics

Initialization via Harmonic Extensions

- Initial interior values are generated by solving the discrete harmonic equation:

$$-\Delta u_i^0 = 0 \quad \text{in } \Omega, \quad u_i^0|_{\partial\Omega} = \phi_i$$

- For the Projected-Gradient method, this u^0 is immediately pointwise projected via $\mathcal{P}_h$ to ensure feasibility.

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ε-Continuation (Penalty Method)

- The system is exceedingly stiff for $\varepsilon \to 0$.
- We utilize a continuation schedule: solve for a larger ε, and use the converged state as a **warm-start** for the next, smaller ε.
- The final strong-competition limit is captured at $\varepsilon = 10^{-9}$.

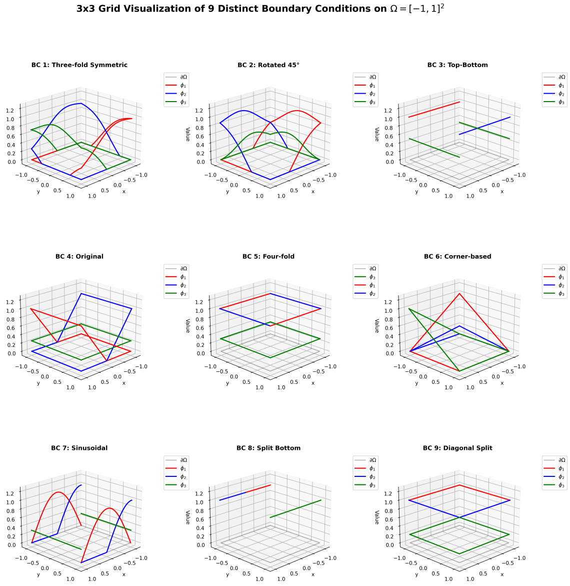
Outline

Boundary Conditions

We test both algorithms on $\Omega = [-1, 1]^2$ using 9 discrete boundary configurations ($\theta = \arctan(y, x)$).

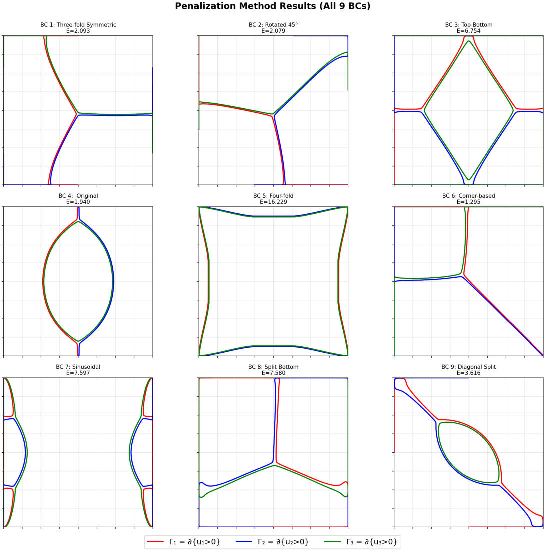
BC	**Definition on the open edges of $\partial\Omega$**
1	$\phi_i = \max\{0, \cos(\theta - 2\pi i/3)\}$, $i = 1, 2, 3$
2	$\phi_i = \max\{0, \cos(\theta - 2\pi i/3 - \pi/4)\}$, $i = 1, 2, 3$
3	$\phi_1 = 1$ on $y = -1$; $\phi_2 = 1$ on $y = 1$; $\phi_3 = 0.5$ on $x = \pm 1$
4	$\phi_1 = x^+$; $\phi_2 = (-x)^+$; $\phi_3 = 0.25$ on $\partial\Omega$
5	$\phi_1 = 1$ on $y = \pm 1$; $\phi_2 = 1$ on $x = \pm 1$; $\phi_3 = 0.3$ on $\partial\Omega$
6	$\phi_i = \max\{0, 1 - \lvert z - c_i \rvert/2\}$; $c_1 = (-1, -1)$, $c_2 = (1, 1)$, $c_3 = (1, -1)$
7	$\phi_1 = \sin(\pi(x + 1)/2)$ on $y = \pm 1$; $\phi_2 = (\cos(\pi(x + 1)/2))^+$ on $y = \pm 1$; $\phi_3 = 0.3$ on $x = \pm 1$
8	$\phi_1 = 1$ on $y = -1, x < 0$; $\phi_2 = 1$ on $y = -1, x > 0$; $\phi_3 = 1$ on $y = 1$
9	$\phi_1 = 1$ on $y = -1$ or $x = -1$; $\phi_2 = 1$ on $y = 1$ or $x = 1$; $\phi_3 = 0.2$ on $\partial\Omega$

Boundary Conditions



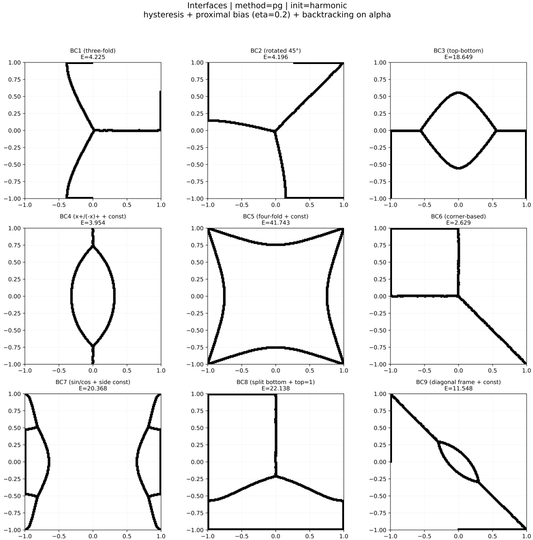
Penalization Method Across 9 Configurations

- At fixed ε, solutions are strictly positive in the interior (weak max principle).
- Free boundaries are approximated via threshold interfaces: $\Gamma_{i,h}^{\varepsilon,\delta} := \partial\{x \in \Omega_h : u_{i,h}^{\varepsilon}(x) > \delta\}$.
- Computed with $\delta = 10^{-5}$ and ε-continuation down to 10^{-9}.



Projected-Gradient Method Across 9 Configurations

- Evaluated on a 201×201 grid ($h = 0.01$).
- Parameters: $\tau_0 = 3 \times 10^{-6}$, $\rho = 0.5$, $\eta = 0.2$.
- Exhibits similar qualitative interface geometries to the penalized method.



Thank You!