Cellular flow control design for mixing based on the least action principle

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Optimal mixing via fluid flow?

- Advective mechanisms for fluid transport and mixing

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- Advective mechanisms for fluid transport and mixing
  - Advection-dominant mixing, where molecular diffusion is negligible
  - Pure advective mechanisms for designing velocity fields that induce complex and chaotic mixing (even with perfectly regular velocity fields*)
  - How time-variation in the velocity can generate chaotic transport, achievable through either *active* or *passive* approaches

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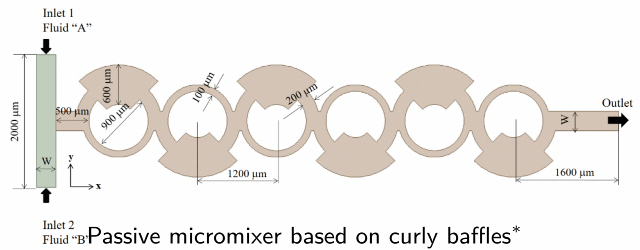
Advective mechanisms: active approaches

- Active approaches: supply an energy to the system.
- For example, stirring a fluid back and forth can generate fluctuating velocities with respect to the flow barriers, therefore engenders transport across them to achieve better mixing.

Advective mechanisms: passive approaches

- Passive approaches do not supply energy, but use passive mechanisms to aid velocity agitations.
- For example, one can have bends or curves in microchannels to passively generate anomalous velocities. Even if the flow in the curved channel remains steady, it can cause unsteady flows across flow barriers and generating transport.

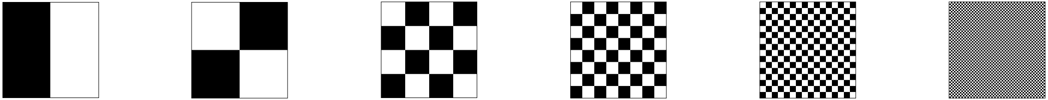


Passive micromixer based on curly baffles*

*M. Juraeva, D.-J. Kang, Design and mixing analysis of a passive micromixer based on curly baffles, Micromachines, 14(9), 1795, 2023.

Mixing modeled by transport equation

- Knowing the velocity field itself, however, does not provide us information of mixing;
- One way of quantifying mixing is to assign each particle a value, say, $\theta(t, x)$, which is conserved as it moves around in the flow.



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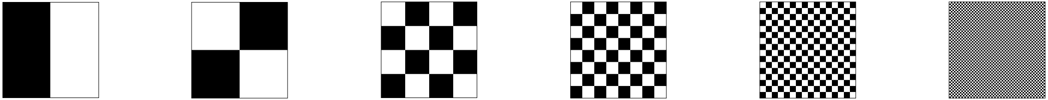

- The total rate of change of $\theta(t,x(t))$ as the fluid parcels moving through a flow field can be described by the *Eulerian specification* of $v(t,x(t))$, which is governed by the transport equation

$$\frac{\partial\theta}{\partial t} + v\cdot\nabla\theta = 0, \quad \theta(0) = \theta_0, \quad x \in \Omega,$$

where $\Omega \subset \mathbb{R}^d, d = 2,3$, is an open, bounded and connected domain, with a regular boundary Γ.
  - θ: mass concentration or density distribution
  - v: incompressible velocity field with no-penetration BC, that is, $\nabla\cdot v = 0, \quad v\cdot n|_\Gamma = 0$.

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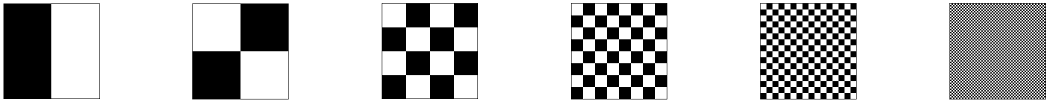

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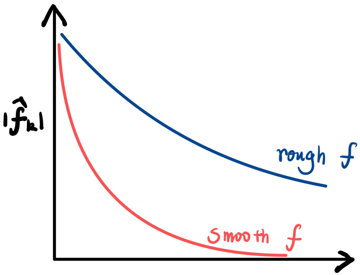
  - θ: mass concentration or density distribution
  - v: incompressible velocity field with no-penetration BC, that is, $\nabla \cdot v = 0, \quad v \cdot n|_\Gamma = 0$.
  - $\|\theta(t)\|_{L^p} = \|\theta_0\|_{L^p}$, $p \in [1, \infty]$, $t > 0$.

Mix-norm: how to quantify mixing

For mean-zero $f \in L^2(\mathbb{T}^d)$ with Fourier coefficients $\{\hat{f}_k\}_{k\in\mathbb{Z}^d}$, its Sobolev norm and negative Sobolev norm (in L^2-sense) on $\mathbb{T}^d := [0,1)^d$ are defined as

$$\|f\|_{H^s}^2 := \sum_{k\in\mathbb{Z}^d} (1+|k|^2)^s |\hat{f}_k|^2 \quad \text{and} \quad \boxed{\|f\|_{H^{-s}}^2 := \sum_{k\in\mathbb{Z}^d} \frac{|\hat{f}_k|^2}{(1+|k|^2)^s}}, \quad s>0.$$



$|\hat{f}_k|$ in decreasing magnitude

- $\|f\|_{L^2}^2 = \sum_{k\in\mathbb{Z}^d} |\hat{f}_k|^2$ conserves
- Mixing pushes $\theta(t)$ to high frequencies by creating finer-scale oscillations
- High modes suppressed by $(1+|k|^2)^s$ denominator
- **Mix-norm**: any negative Sobolev norm $H^{-s}, s>0$ that quantifies the weak convergence, can be used as a mix-norm*
- Vanishing norm indicates perfect mixing

*Mathew-Mezic-Petzold '05, Lin-Thiffeault-Doering '10, Thiffeault '11, etc.

Optimal mixing via stirring strategies

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  - First-order necessary optimality conditions
  - Numerical experiments

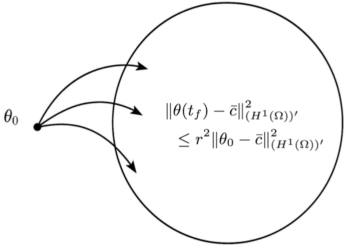
Optima mixing based on Least Action Principle (LAP)

- **Minimize**

$$J(v) = \frac{1}{2}\int_0^{t_f}\int_\Omega \theta(x,t)|v(x,t)|^2\,dxdt, \qquad (P)$$

for a given $t_f > 0$, subject to

$$\begin{cases} \frac{\partial\theta}{\partial t} + v\cdot\nabla\theta = 0, \\ \nabla\cdot v = 0 \quad \text{with} \quad v\cdot n|_\Gamma = 0, \\ \theta(0) = \theta_0 \quad \text{and} \\ \|\theta(t_f) - \bar{\theta}\|_{(H^1(\Omega))'} \le r\|\theta_0 - \bar{\theta}\|_{(H^1(\Omega))'}, \end{cases}$$



Point-to-set map

where $\bar{\theta} = \frac{1}{|\Omega|}\int_\Omega \theta_0(x)dx = \frac{1}{|\Omega|}\int_\Omega \theta(x,t)dx, t > 0.$

- The dual norm $\|\cdot\|_{(H^1(\Omega))'}$ is employed to quantify mixing, where $(H^1(\Omega))'$ is the dual space of $H^1(\Omega)$.

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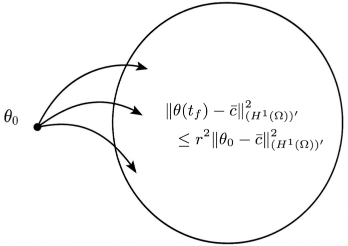

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- The dual norm $\|\cdot\|_{(H^1(\Omega))'}$ is employed to quantify mixing, where $(H^1(\Omega))'$ is the dual space of $H^1(\Omega)$.
- Consider

$$(-\Delta + I)\eta = \theta, \quad \frac{\partial\eta}{\partial n}|_\Gamma = 0 \implies \|\theta\|_{(H^1(\Omega))'} = \|\eta\|_{H^1(\Omega)}.$$

Cellular flows based finite dimensional control design

- Let $\Omega = (0,1)^2$. Consider that the flow velocity is induced by a set of finite basis flows

$$v(x,t) = \sum_{i=1}^{N} u_i(t) b_i(x),$$

where $b_i(x), i = 1, 2, \ldots, N$, are the cellular flows generated by the Hamiltonians $H_i = \sin(i\pi x_1)\sin(i\pi x_2)$

$$b_i = \nabla^{\perp} H_i(x_1, x_2) = (-\partial_{x_2} H_i, \partial_{x_1} H_i)^T = i\pi \begin{bmatrix} -\sin(i\pi x_1)\cos(i\pi x_2) \\ \cos(i\pi x_1)\sin(i\pi x_2) \end{bmatrix},$$

and the temporal coefficients $u_i(t), i = 1, 2, \ldots, N$, serve as the control inputs.

- It is clear that

$$\nabla \cdot b_i = 0 \quad \text{and} \quad b_i \cdot n|_{\Gamma} = 0.$$

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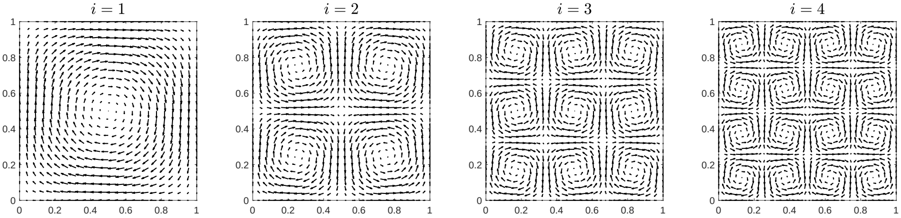
- It is clear that

$$\nabla \cdot b_i = 0 \quad \text{and} \quad b_i \cdot n|_{\Gamma} = 0.$$

- It can be shown that as long as N is large enough, the desired degree of mixing can be achieved by the final time $t_f > 0$.

Cellular flows and their linear combination

- Cellular flows $b_i = i\pi\left(-\sin(i\pi x_1)\cos(i\pi x_2), \cos(i\pi x_1)\sin(i\pi x_2)\right)^T, i = 1, 2, \ldots, N.$



Cellular flows on the unit square

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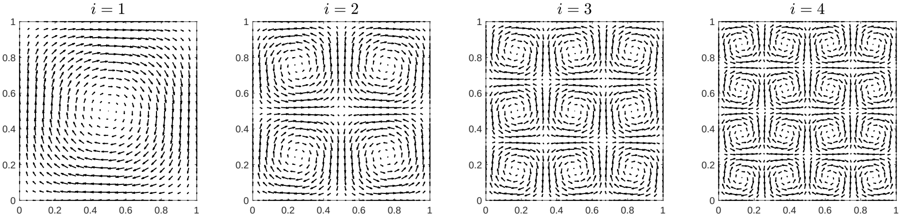

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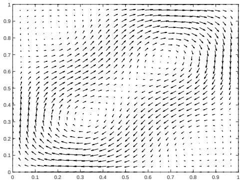

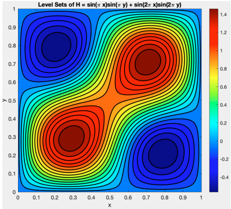

Combination of cellular flows $b_1 + b_2$ on the unit square

Mixing with cellular flows

- Let $\gamma \colon [0, \infty) \to [0, +\infty)$ be a continuous and decreasing function vanishing at infinity. The velocity field b is *mixing* with rate $\gamma(t)$ if for every $\theta_0 \in H^1(\mathbb{T}^2)$ with zero streamlines-average we have the following estimate*

$$\|\theta(t)\|_{H^{-1}} \leq \gamma(t)\|\theta_0\|_{H^1}, \quad \forall t \geq 0.$$

*E. Bruè, M. C. Zelati, and E. Marconi, Enhanced dissipation for two-dimensional hamiltonian flows, Archive for Rational Mechanics and Analysis, 248 (2024).

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- For cellular flows $b(x_1, x_2) = \nabla^\perp \sin(x_1)\sin(x_2)$,

$$\gamma_N(t) \leq \frac{C(\epsilon)}{t^{1/3-\epsilon}}, \quad \forall \epsilon > 0, \quad C(\epsilon) > 0 \quad \text{constant depends on } \epsilon.$$

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Mixing with cellular flows

Proposition 1.* Given $N \in \mathbb{Z}^+$, consider the cellular flow $b_N(x_1, x_2) = \nabla^\perp H_N$ in domain $\Omega = (0,1)^2$. For $\theta_0 \in H^1(\Omega)$ with $\theta_0 \notin \ker(b_N \cdot \nabla)$ we have the following estimate

$$\|\theta(t_f) - \bar{\theta}\|_{(H^1(\Omega))'} \leq \gamma(t)\|\theta_0 - \bar{\theta}\|_{H^1(\Omega)}, \quad t \geq 0, \tag{1}$$

where

1. if $H_N = \sin(N\pi x_1)\sin(N\pi x_2)$, then for every $\epsilon > 0$ the mixing rate $\gamma_N(t)$ satisfies
$$\gamma_N(t) \leq \frac{C_1(\epsilon)}{(N^2 t)^{\frac{1}{3}-\epsilon}}; \tag{2}$$
2. if $H_N = \frac{1}{N\pi}\sin(N\pi x_1)\sin(N\pi x_2)$, then for every $\epsilon > 0$ the mixing rate $\gamma_N(t)$ satisfies
$$\gamma_N(t) \leq \frac{C_2(\epsilon)}{(N^{\frac{3}{2}} t)^{\frac{1}{3}-\epsilon}}, \tag{3}$$

where $C_1(\epsilon) > 0$ and $C_2(\epsilon) > 0$ in (2) and (3), respectively, are constants depending on ϵ and the initial condition θ_0.

*W. Hu, H.-N. Wu, and M.-J. Lai, Cellular flow control design for mixing based on the least action principle, arXiv:2510.22703.

Feasibility of the constraint set

- **Theorem on Feasibility.** For given $t_f > 0$, set

$$\frac{C_2(\epsilon)}{(N^{\frac{3}{2}} t_f)^{\frac{1}{3}-\epsilon}} \leq r \frac{\|\theta_0 - \bar{\theta}\|_{(H^1(\Omega))'}}{\|\theta_0 - \bar{\theta}\|_{H^1(\Omega)}}, \quad 0 < r < 1,$$

If N is chosen to satisfy

$$N \geq \left\lceil \left(\frac{C_2(\epsilon)\|\theta_0 - \bar{\theta}\|_{H^1(\Omega)}}{r\|\theta_0 - \bar{\theta}\|_{(H^1(\Omega))'}} \right)^{\frac{2}{1-3\epsilon}} \frac{1}{t_f^{\frac{2}{3}}} \right\rceil,$$

where $\lceil \cdot \rceil$ stands for the celling function, then the desired degree of mixing can be achieved by the final time $t_f > 0$. In other words, the problem is feasible.

Existence of a global optimal control

- Let $\vec{u}(t) = [u_1(t), u_2(t), \ldots, u_N(t)]^T$ and $\vec{b}(x) = [b_1(x), b_2(x), \ldots, b_N(x)]^T$.
- Further let $m(x,t) = \vec{u}^T(t)\vec{b}(x)\theta(x,t)$. Clearly, for any control $\vec{u}(t) \in (L^2(0,t_f))^N$,

$$\nabla \cdot \left(\frac{m}{\theta}\right) = 0 \quad \text{and} \quad \frac{m}{\theta} \cdot n|_\Gamma = 0.$$

- Our point-to-set optimal control problem can be rewritten as

$$\min \quad J(m,\theta) = \frac{1}{2}\int_0^{t_f}\int_\Omega \frac{|m(x,t)|^2}{\theta(x,t)}\, dxdt$$

$$\text{subject to} \begin{cases} \frac{\partial\theta}{\partial t} + \nabla \cdot m = 0, \\ \theta(0) = \theta_0 \quad \text{and} \quad \|\theta(t_f) - \bar{\theta}\|_{(H^1(\Omega))'} \le rC_0, \quad 0 < r < 1, \end{cases}$$

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where $C_0 := \|\theta_0 - \bar{\theta}\|_{(H^1(\Omega))'}$.

- **Convex problem (Optimal Transport: Benamou–Brenier Formulation)**
  - Jointly convex in (m, θ)
  - Existence of a global optimal control (not necessarily unique)

First-order necessary optimality conditions

Using the Euler-Lagrangian approach, we can derive the optimality conditions:

1. **State Equation**:

$$\partial_t \theta + \sum_{i=1}^{N} u_i (b_i \cdot \nabla \theta) = 0, \quad \theta(x,0) = \theta_0(x),$$

2. **Adjoint Equation**:

$$-\partial_t \rho - \sum_{i=1}^{N} u_i (b_i \cdot \nabla \rho) = \frac{1}{2} \sum_{i=1}^{N} |u_i b_i|^2, \quad \rho(t_f) = -2\lambda(-\Delta + I)^{-1} \theta(t_f);$$

3. **Optimality Condition**:

$$\vec{u}(t) = \boldsymbol{M}^{-1}(t) \boldsymbol{p}(t), \quad \text{where}$$

   - $\boldsymbol{M}(t) \in \mathbb{R}^{N \times N}$ is a matrix with entries $M_{ij}(t) := \int_\Omega \theta b_i \cdot b_j \, dx$,
   - $\boldsymbol{p}(t) \in \mathbb{R}^N$ is a vector with entries $p_i(t) := \int_\Omega (b_i \cdot \nabla \rho) \theta \, dx$;

4. **Final Time Constraint** :

$$\|\theta(t_f) - \bar{\theta}_0\|^2_{(H^1(\Omega))'} \leq r^2 C_0^2;$$

5. **Complementary Slackness**:

$$\lambda \left(\|\theta(t_f) - \bar{\theta}_0\|^2_{(H^1(\Omega))'} - r^2 C_0^2 \right) = 0, \quad \lambda \geq 0.$$

Numerical implementation

- The optimality system can be solved via a **fixed-point iteration**:

$$(u^{k+1}, \lambda^{k+1}) = (F_1(u^k, \lambda^k), F_2(u^k, \lambda^k))$$

where F_1 encodes 1–3 and F_2 incorporates 4–5. Specifically, λ^{k+1} can be updated by the following iteration

$$\lambda^{k+1} = \max\left\{\lambda^k + \beta^k\left(\|\theta^k(t_f)\|^2_{(H^1(\Omega))'} - r^2 C_0^2\right), 0\right\},$$

where $\beta^k > 0$ is a step-size parameter.

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where $\beta^k > 0$ is a step-size parameter.

- At convergence, we recover

$$\lambda^* = \max\left\{\lambda^* + \beta\left(\|\theta^*(t_f)\|^2_{(H^1(\Omega))'} - r^2C_0^2\right), 0\right\}$$

for some $\beta > 0$, which implies $\lambda^* \geq 0$ and

$$\begin{cases} \text{If } \|\theta^*(t_f)\|^2_{(H^1(\Omega))'} - r^2C_0^2 < 0, \text{ then } \lambda^* = 0, \\ \text{If } \lambda^* > 0, \text{ then } \|\theta^*(t_f)\|^2_{(H^1(\Omega))'} - r^2C_0^2 = 0, \end{cases}$$

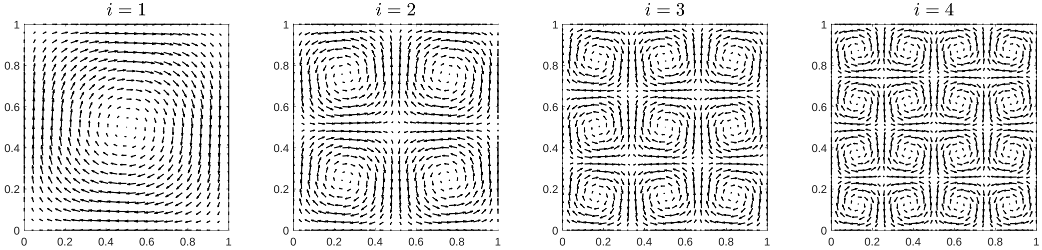
- $u^k \to (\theta^{k+1}, \eta^{k+1}) \to \lambda^{k+1} \to \rho^{k+1} \to u^{k+1}$.

Numerical experiments on a unit square

Recall the cellular flows on a unit square $\Omega = (0,1)^2$

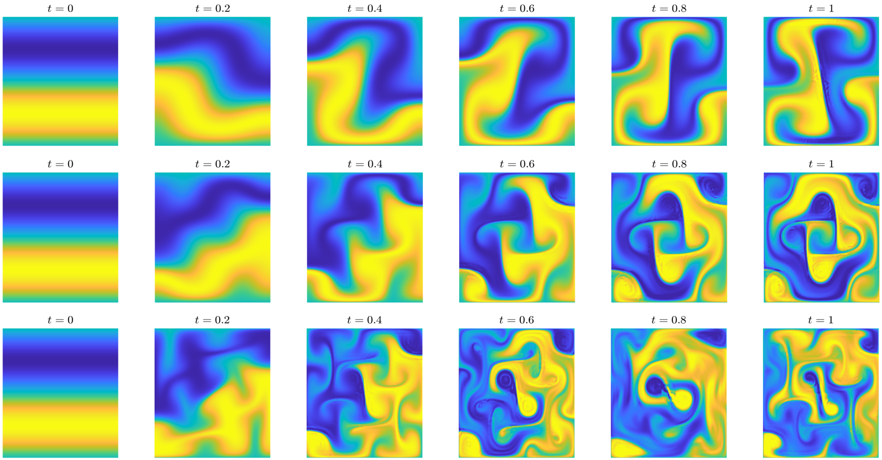
$$b_i(x_1, x_2) = i\pi \begin{bmatrix} -\sin(i\pi x_1)\cos(i\pi x_2) \\ \cos(i\pi x_1)\sin(i\pi x_2) \end{bmatrix}, \quad i = 1, 2, \ldots, N,$$

which are illustrated as follows:



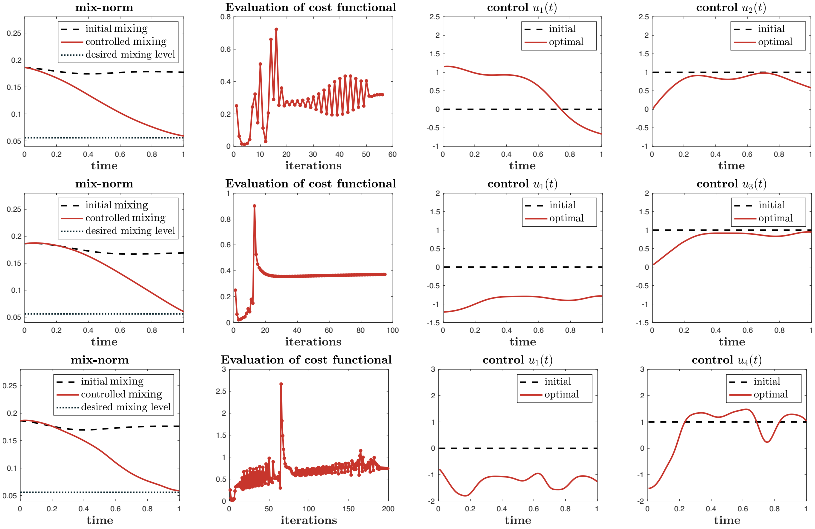
Cellular flows on a unit square

Numerical experiments: $\theta_0 = \sin(2\pi x_2) + 1$, $t_f = 1$ and $r = 0.3$



Top: b_1 & b_2; **Middle:** b_1 & b_3; **Bottom:** b_1 & b_4 with initial $u_1(t) \equiv 0$ and $u_i(t) \equiv 1$, $i = 2, 3, 4$.

Performance of optimal control on a unit square



Top: u_1 & u_2; **Middle:** u_1 & u_3; **Bottom:** u_1 & u_4.

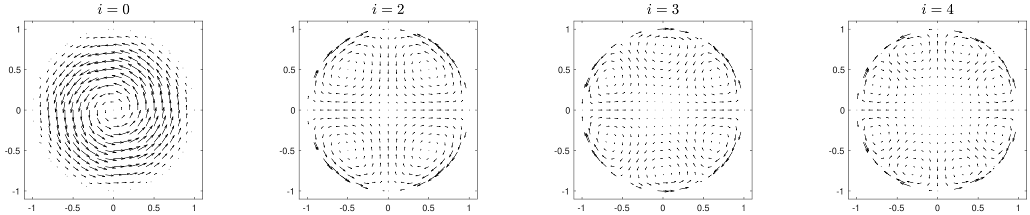
Numerical experiments on a unit disk

Consider the cellular flows on a unit disk $\Omega = \{(x_1, x_2) \in \mathbb{R}^2 : x_1^2 + x_2^2 \leq 1\}$.

- Let (γ, ϕ) be polar coordinates and

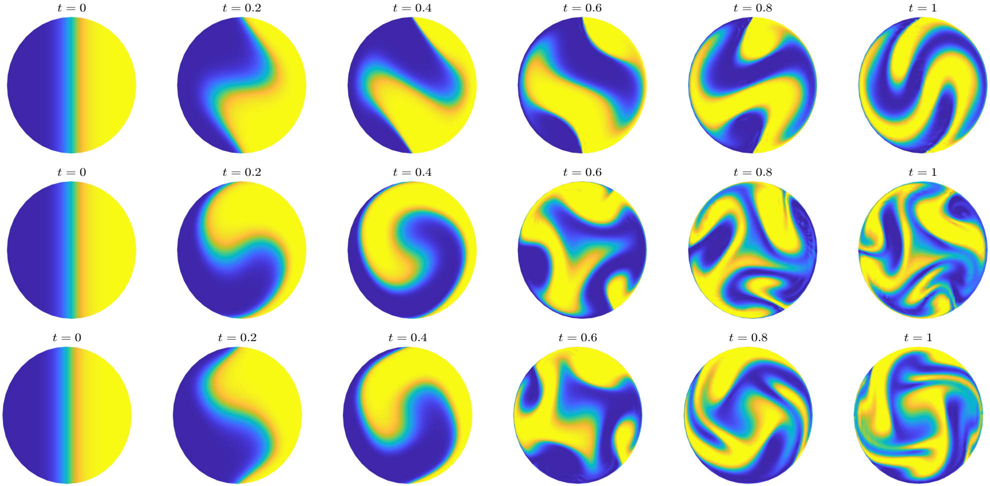
$$\psi_i(\gamma, \phi) = (1 - \gamma^2)\gamma^i \sin(i\phi),$$

  be a stream function with $i = 1, 2, \ldots$
- The corresponding velocity components are derived via $u_{\gamma_i} = \frac{1}{\gamma}\frac{\partial \psi_i}{\partial \phi}, \quad u_{\phi_i} = -\frac{\partial \psi_i}{\partial \gamma}$.
- For $i = 0$, we let $u_\gamma = 0$ and $u_\phi = 4\gamma(1 - \gamma^2)$.
- Converted to polar coordinates through the transform $b_i(x, y) = \begin{bmatrix} u_{\gamma_i} \cos\phi - u_{\phi_i} \sin\phi \\ u_{\gamma_i} \sin\phi + u_{\phi_i} \cos\phi \end{bmatrix}$.



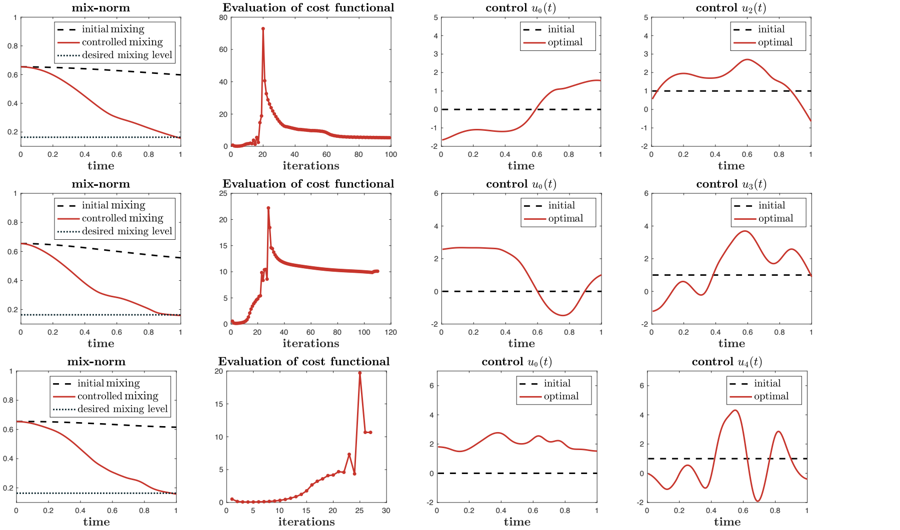
Cellular flows on a unit disk

Numerical experiments: $\theta_0 = \tanh(x_1/0.2) + 1$, $t_f = 1$ and $r = 0.25$



Top: b_0 & b_2; **Middle:** b_0 & b_3; **Bottom:** b_0 & b_4 with initial $u_0(t) \equiv 0$ and $u_i(t) \equiv 1$, $i = 2, 3, 4$

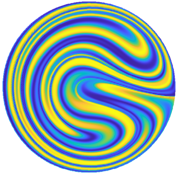
Performance of optimal control on a unit disk



Top: u_0 & u_2; **Middle:** u_0 & u_3; **Bottom:** u_0 & u_4.

Ongoing work

- Hybrid controls utilizing Hamiltonian flows and LAP for transport and mixing, which integrates the continuous- and discrete-time dynamics (e.g. switching, impulse controls with even-triggered strategies, and sliding mode control) in the design.
- Neural operator formulation of optimal mixing problems.



Thank you for your attention!

Questions?