Control Design for Mixing in Incompressible Flows

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Outline

- Mixing phenomena
- What is "good mixing"?
- Advective mechanisms for fluidic transport and mixing
- Measures for qualifying mixing
- Control for optimal mixing via flow dynamics (open- and closed-loop controls)

Mixing phenomena

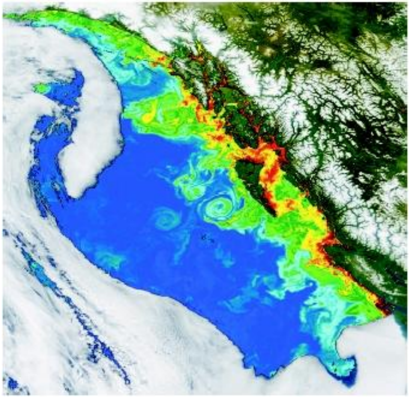
Mixing is to disperse one material or field in another medium. It occurs in many natural phenomena and industrial applications.

Mixing in painting

Mixing in baking

Mixing phenomena

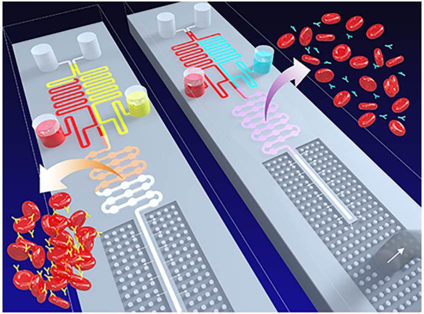
Spreading of a pollutant in the atmosphere



Mixing of temperature, salt, and nutrient in ocean*.

*http://www.waterencyclopedia.com/Mi-Oc/Ocean-Mixing.html

Mixing phenomena



- Microfluidic devices have allowed to make significant progress in biomedical diagnostics study, development of microfluidic and nanofluidic biosensors, in DNA analysis, chemical synthesis and genomics study, etc.
- Controllable and fast mixing is critical for practical development of microfluidic and lab-on-chip devices*.

*https://www.elveflow.com/microfluidic-reviews/microfluidic-flow-control/microfluidic-mixers-a-short-review/

"Good mixing": stirring + diffusion

- Mixing means a physical process where both the *stirring* (or *advective mechanism*) and the *diffusion* occur simultaneously.

*Y.-K. Suh and S. Kang, A review on mixing in microfluidics, Micromachines, 1(3),82–111, 2010.

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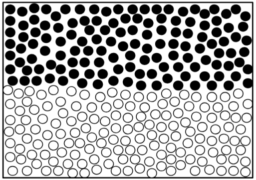
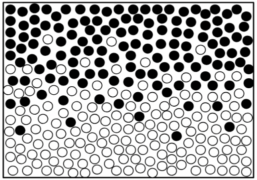
- *Stirring* means the advection of material blobs subjected to mixing without diffusive action.
- *Diffusion* is the averaged effect of small scale random (Gaussian) particle motions.



(a)



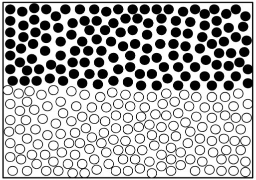
(b)

Cartoon illustration of the exchange of molecules across an interface between two different fluids activated by the molecules' random motion; (a) before starting the exchange, (b) instantaneous state during the exchange*

*Y.-K. Suh and S. Kang, A review on mixing in microfluidics, Micromachines, 1(3),82–111, 2010.

Diffusive mixing

- In the region near the interface, molecules on both sides have different properties, and so random molecular motion results in permeation of molecules from one side to the other. Such permeation is called *diffusion*.
- The flux of one species through the interface is proportional to the gradient of the concentration of the species (so-called Fick's law), and the proportional constant is defined as *molecular diffusivity*.



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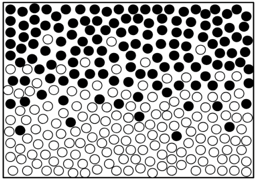

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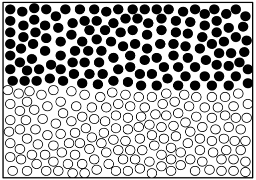

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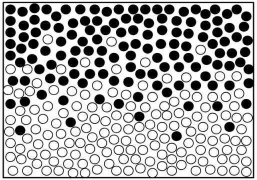

(b)

- Diffusive mixing can be made effective if there are sufficiently small blobs of one fluid immersed in a region of the other fluids; when the length-scale of these blobs reaches the diffusive length-scales, these blobs diffusive into the outer fluid, resulting in good mixing. If the blobs are too big, diffusive mixing is inefficient.

Mixing via an advection-driven diffusion process

To summarize,

- "Good mixing" of low-diffusivity materials occurs in two stages: stirring in the first stage and diffusion in the second stage*.
- The advective strategy (such as chaotic stretching and folding) should lead to fluid blobs or filaments, whose shapes are able to enhance diffusive mixing.

*S. Balasuriya, Dynamical systems techniques for enhancing microfluidic mixing, J. Micromech. Microeng., 25(9),094005, 2015.

Advective mechanisms for fluidic transport and mixing

In this talk, we focus on

- Advection dominant case (molecular diffusion is negligible).

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Advective mechanisms for fluidic transport and mixing

In this talk, we focus on

- Advection dominant case (molecular diffusion is negligible).
- It is possible to utilize purely advective mechanisms to create an additional fluid velocity to obtain complicated mixing (chaotic mixing) in fluids in which the velocity field is completely regular*.
- Time-variation in the velocity may generate chaotic transport, which in practice can be achieved by either *active* or *passive* approaches.

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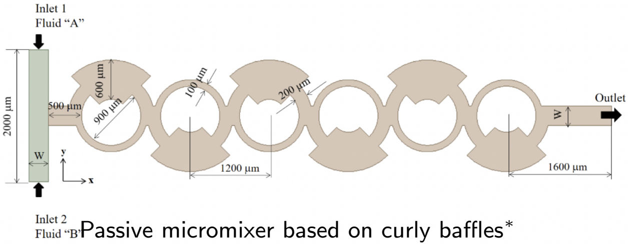
Advective mechanisms: active approaches

- 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.

Measures for qualifying mixing

Consider that the fluid trajectories are given by the solutions of the ordinary differential equation

$$\frac{dX(t,t_0;x)}{dt} = v(t, X(t,t_0;x)), \tag{1}$$

$$X(t_0,t_0;x) = x \in \mathbb{R}^d, \;\; d \geq 1. \tag{2}$$

- Equation (1) is the *Lagrangian specification* of the flow field, representing the rate of change of position of each fluid particle given by its velocity.
- Solving (1)-(2), the Lagrangian trajectories of the particles in the fluid can be determined.
- The conditions

$$\nabla \cdot v = 0, \quad i.e., \quad \partial_{x_1} v_1 + \partial_{x_2} v_2 = 0 \; (d = 2),$$

are equivalent to imposing that for each time t, t_0 the map $X(t,t_0;\cdot)\colon \mathbb{R}^d \to \mathbb{R}^d$ is area preserving.

Measures for qualifying mixing

- 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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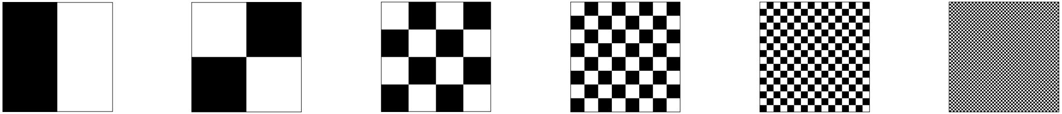

Mix-norm: negative Soblev norm

- **Mix-norm**: consider the 1D periodic interval $[0, 1]$. Define

$$d(\theta, x, w) = \frac{1}{w} \int_{x-w/2}^{x+w/2} \theta(y)\, dy$$

for all $x, w \in [0, 1]$. The mix-norm $M(\theta)$ is then obtained by averaging d^2 over x and w:

$$M^2(\theta) = \int_0^1 \int_0^1 d^2(\theta, x, w)\, dx\, dw$$

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For a density field with a Fourier expansion $\theta(x) = \sum_{\mathrm{k}} \hat{\theta}_{\mathrm{k}} e^{i2\pi(\mathrm{k}\cdot x)}$,

$$\|\theta\|_{H^{-1/2}} = \left(\sum_{\mathrm{k}} \frac{1}{(1+\|\mathrm{k}\|^2)^{1/2}} |\hat{\theta}_{\mathrm{k}}|^2\right)^{1/2}, \quad \|\mathrm{k}\|^2 = k_1^2 + \cdots + k_d^2.$$

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- Assume that $\Omega = \mathbb{T}^d = [0,1]^d$ is a d-dimensional torus and initial distribution has zero mean, that is, $\int_{\mathbb{T}^d} \theta_0 \, dx = 0$.
- For an $s \in \mathbb{R}$, define the homogeneous Sobolev norm of index s by

$$\|\theta\|_{\dot{H}^s}^2 := \sum_{\mathrm{k}\in\mathbb{Z}^2, \mathrm{k}\neq 0} \|\mathrm{k}\|^{2s} |\hat{\theta}_{\mathrm{k}}|^2,$$

where $\hat{\theta}_0 = 0$ for mean-zero functions.

*M. C. Zelati, G. Crippa, G. Iyer, and A. L. Mazzucato, Mixing in incompressible flows: transport, dissipation, and their interplay, Notices of the AMS, 71(5), 593–604, 2024.

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- Therefore, mixing of θ is equivalent to

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- In fact, for any $s < 0$ the quantity $\|\theta\|_{\dot{H}^s}$ can be used as a measure of how “mixed” the distribution is at time t.

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- In a general bounded domain Ω, we employ Sobolev norm for the dual space $(H^1(\Omega))'$ of $H^1(\Omega)$ for quantifying mixing, which is defined by

$$\|f\|_{(H^1(\Omega))'} = \sup_{\phi \in H^1(\Omega)} \frac{|\int_\Omega f \phi \, dx|}{\|\phi\|_{H^1}}, \quad f \in (H^1(\Omega))'.$$

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Mixing modeled by transport equation

Recall that the total rate of change of the function $\theta(t, x(t))$ as the fluid parcels moving through a flow field can be described by the *Eulerian specification* of v, which is given 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 sufficiently regular boundary Γ.

- θ: mass concentration or density distribution
- v: incompressible velocity field with no-penetration BC, that is,

$$\nabla \cdot v = 0, \quad v \cdot n|_\Gamma = 0.$$

- $\|\theta(t)\|_{L^p} = \|\theta_0\|_{L^p}, \ p \in [1, \infty], \ t > 0.$

Some known results and open questions

$$\frac{\partial \theta}{\partial t} + v \cdot \nabla \theta = 0, \quad \nabla \cdot v = 0, \quad x \in \Omega,$$
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  1. if $s < 1$: perfect mixing in finite time, i.e., there is a time t^* such that $\lim_{t \to t^*} \|\theta(t, \cdot)\|_{H^{-1}} = 0$;
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- Elgindi-Zlatoš '18: The answer is affirmative for

$$1 < s < \frac{1+\sqrt{5}}{2} < 2 \quad \text{and} \quad p \in \left[1, \frac{2}{2s + 1 - \sqrt{5}}\right).$$

Mixing via flow dynamics

Optimize mixing via active control of fluid dynamics

Mixing via flow dynamics

Consider the scalar field modeled by the transport equation

$$\frac{\partial \theta}{\partial t} + v \cdot \nabla \theta = 0,$$

which is advected by incompressible fluid flows. Specifically,

- mixing via Stokes flows ($\Omega \in \mathbb{R}^d$, $d = 2, 3$)

$$\frac{\partial v}{\partial t} - \nu \Delta v + \nabla p = 0, \quad \nabla \cdot v = 0,$$

  where p is the pressure and ν is the viscosity.

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*Hou-Li '05, Chae '06, Danchin-Paicu '11, Lai-Pan-Zhao '11, Larios-Lunasin-Titi '13, H.-Kukavica-Zane '13, '15, '16, H. *et. al* '18, etc.

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- mixing via Navier-Stokes flows ($\Omega \in \mathbb{R}^d, d = 2$)

  $$\frac{\partial v}{\partial t} - \nu \Delta v + v \cdot \nabla v + \nabla p = f(\theta), \quad \nabla \cdot v = 0,$$

  where $f(\theta)$ stands for the local forces (such as buoyancy, i.e., $f(\theta) = \theta \vec{e}$, where $\vec{e}$ is a unit vector in the direction of buoyancy)*.

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Example: Boundary control for mixing in Stokes flows

Consider

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

where the velocity field is govern by

$$\frac{\partial v}{\partial t} - \nu \Delta v + \nabla p = 0, \quad \nabla \cdot v = 0, \quad v \cdot n|_\Gamma = 0.$$

Motivated by the observation that moving walls accelerate mixing compared to fixed walls with no-slip boundary condition*, we consider the Navier slip boundary control for mixing †

$$v \cdot n|_\Gamma = 0 \quad \text{and} \quad (2\nu n \cdot \mathbb{D}(v) \cdot \tau + kv \cdot \tau)|_\Gamma = g \cdot \tau.$$

- n and τ are the outward unit normal and tangential vectors to the boundary Γ
- $\mathbb{D}(v) = \frac{1}{2}(\nabla v + (\nabla v)^T)$: deformation tensor
- $k > 0$: coefficient of friction
- g: control input function

*Chakravarthy-Ottino '96, Thiffeault-Gouillart-Dauchot '11, etc.

†H., AMO' 18, 20; H.-Wu, SICON' 18, JDE' 19; H.-Rautenburg-Zheng' 23 JDE; Zheng-H.-Wu, CMAME '23

Control for mixing via flow dynamics

Rewrite the flow-transport system into an abstract Cauchy problem

$$\begin{cases} \partial_t \theta = -v \cdot \nabla \theta, \\ \partial_t v = Av + N(v) + F(\theta) + Bu, \qquad (M) \\ (\theta(0), v(0)) = (\theta_0, v_0). \end{cases}$$

- $A = \nu \mathbb{P} \Delta$: Stokes operator associated with the appropriate boundary conditions, where

  $$\mathbb{P}\colon L^2(\Omega) \to V_n^0 = \{v \in L^2(\Omega)\colon \operatorname{div} v = 0,\ v \cdot n|_\Gamma = 0\}$$

  is the Leray projector;
- $N(v) = -\mathbb{P}(v \cdot \nabla v)$ (which is set to be zero for Stokes flows)
- $F(\theta) = \mathbb{P} f(\theta)$: local force of interest
- u: control input (stirring)
- B: control input operator

Problem formulation: optimal nonlinear control

- **Minimize**

$$J(u) = \frac{\alpha}{2}\|\theta(T)\|^2_{(H^1(\Omega))'} + \frac{\beta}{2}\int_0^T \|\theta\|^2_{(H^1(\Omega))'}\, dt + \frac{\gamma}{2}\|u\|^2_{U_{ad}}, \quad (P),$$

for a given $T > 0$, subject to

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  where $\alpha, \beta \geq 0$ and $\gamma > 0$ are the state and control weight parameters, respectively, and U_{ad} stands for the set of admissible controls.

- Introduce η such that

$$(-\Delta + I)\eta = \theta, \quad \frac{\partial\eta}{\partial n}|_\Gamma = 0.$$

- Let $\Lambda = (-\Delta + I)^{1/2}$. Then

$$\|\theta\|_{(H^1(\Omega))'} = \|\Lambda^{-1}\theta\|_{L^2(\Omega)} = \|\Lambda\eta\|_{L^2(\Omega)} = \|\eta\|_{H^1(\Omega)}.$$

Challenges in analysis and computation

- *Nonlinearity:* The nonlinear coupling due to advection essentially leads to a nonlinear control and non-convex optimization problem.
- *Zero diffusivity:* Differentiability leads to a high-order regularity required for the velocity field.
- *Boundary control*:*
  1. Creation of vorticity on the domain boundary;
  2. Compatibility conditions may come into play even in the case of non-smooth solutions.

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  3. Optimal open-loop control requires solving the state equations forward in time, coupled with the adjoint equations backward in time together with a nonlinear optimality condition.

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Construction of feedback laws based on model predictive control (MPC)

- Consider mixing via Stokes flows ($N(v) = 0, F(\theta) = 0$)

$$\begin{cases} \partial_t \theta = -v \cdot \nabla \theta, & \theta(0) = \theta_0, \\ \partial_t v = Av + Bu, & v(0) = v_0, \\ (-\Delta + I)\eta = \theta, & \frac{\partial \eta}{\partial n}\big|_\Gamma = 0. \end{cases}$$

- **Instantaneous control design** is closely tied to receding horizon control (RHC) or model predictive control (MPC) with finite time horizon*.

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- **Instantaneous control design** is closely tied to receding horizon control (RHC) or model predictive control (MPC) with finite time horizon*.
- **One-step MPC:** consider a uniform partition of $[0, T]$ and let $h = \frac{T}{n}$ for $n \in \mathbb{N}$. Using semi-implicit Euler's method (I) in time for discretizing the state equations in t gives

$$\begin{cases} \theta^{i+1} = \theta^i - hv^{i+1} \cdot \nabla \theta^i, \\ v^{i+1} = v^i + hAv^{i+1} + Bu^{i+1} \\ (-\Delta + I)\eta^{i+1} = \theta^{i+1}, \quad \frac{\partial \eta^{i+1}}{\partial n}|_\Gamma = 0, \end{cases} \tag{3}$$

where $\theta^i = \theta(\cdot, t_i)$, $v^i = v(\cdot, t_i)$, and $u^i = u(\cdot, t_i)$, $i = 0, 1, \ldots, n-1$.

- Consider now the cost functional for one time step

$$J(u^{i+1}) = \frac{1}{2}\|\Lambda \eta^{i+1}\|^2_{L^2} + \frac{\gamma}{2}\|u^{i+1}\|^2_{U_{ad}}, \quad \Lambda = (-\Delta + I)^{1/2}.$$

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Construction of feedback laws (cont'd)

- Let (ρ^{i+1}, w^{i+1}) be the adjoint state of (θ^{i+1}, v^{i+1}). Applying the Euler-Lagrange method leads to

$$\rho^{i+1} = \eta^{i+1} = (-\Delta + I)^{-1}\theta^{i+1}, \quad (I - hA)w^{i+1} = h\mathbb{P}(\theta^{i}\nabla\rho^{i+1}), \tag{4}$$

and the optimality condition

$$\gamma u^{i+1} + B^{*}w^{i+1} = 0. \tag{5}$$

The optimality system (3)–(5) admits a unique solution due to the quadratic cost functional and the uniqueness of (3).

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- Compute $(u^{i+1}, v^{i+1}, \theta^{i+1})$ recursively by setting $u_0^i = 0$, which turns out to be the semi-implict time discretization of the closed-loop system

$$\begin{cases} \partial_t \theta = -v \cdot \nabla \theta, \quad \theta(0) = \theta_0, \\ \partial_t v = Av + Bu, \quad v(0) = v_0, \\ u = -\gamma^{-1} hBB^*(I - hA)^{-1}\mathbb{P}(\theta \nabla \eta) \quad \text{(sub-optimal)}. \end{cases}$$

Well-posedness and stability of the closed-loop system

- The closed-loop system reads (H.-Rautenberg-Zheng, JDE '23)

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  where $\eta = (I - \Delta)^{-1}\theta$, γ and h are the fixed parameters.

- Let $B = \mathbb{P}I$ (internal control). Then

$$\partial_t v = Av - \gamma^{-1} h(I - hA)^{-1}\mathbb{P}(\theta \nabla \eta).$$

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- Let $B = \mathbb{P}I$ (internal control). Then

$$\partial_t v = Av - \gamma^{-1} h(I - hA)^{-1}\mathbb{P}(\theta\nabla\eta).$$

- **Well-posedness:** For $(\theta_0, v_0) \in (L^\infty(\Omega) \cap H^1(\Omega)) \times V_n^2(\Omega)$, there exists a unique solution (θ, v) satisfying

$$(\theta, v) \in L^\infty(0, T; L^\infty(\Omega) \cap H^1(\Omega)) \times L^\infty(0, T; V_n^2(\Omega)) \cap L^2(0, T; V_n^3(\Omega))$$

  for any $T > 0$.

Well-posedness and stability (cont'd)

- Applying energy estimates yields

$$\frac{d}{dt}\text{ Total Energy} = \frac{d}{dt}\|\theta\|^2_{(H^1(\Omega))'} + \frac{\gamma}{\delta}\frac{d}{dt}\|v\|^2_{H^1(\Omega)} \leq -C\|v\|^2_{H^1(\Omega)} < 0.$$

- **Long-time behavior:**
  1. $\|v\|_{L^2}, \|\nabla v\|_{L^2}, \|Av\|_{L^2}, \|\partial_t v\|_{L^2} \to 0$ as $t \to +\infty$;
  2. $\|\theta\|_{(H^1(\Omega))'} \to c_0$ as $t \to \infty$, and $c_0 < C(\eta_0, v_0)$;
  3. $\|u\|_{L^2} \to 0$ as $t \to +\infty$.

Well-posedness and stability (cont'd)

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  3. $\|u\|_{L^2} \to 0$ as $t \to +\infty$.
- **Polynomial decay:**
  - Using C_0-semigroup theory and nonlinear analysis, we can show that there exist constants $a, b, c > 0$ such that

$$\|v\|_{L^2} = O\left(\frac{1}{t^a}\right), \quad \|\theta - \bar{\theta}\|_{(H^1(\Omega))'} = O\left(\frac{1}{t^b}\right), \quad \text{and} \quad \|u\|_{L^2} = O\left(\frac{1}{t^c}\right), \quad t \to \infty,$$

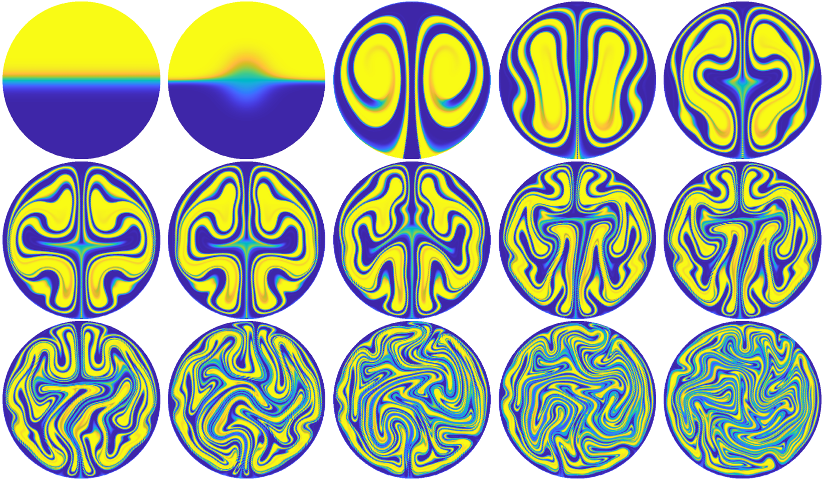
where $\bar{\theta} = \frac{1}{|\Omega|}\int_\Omega \theta\, dx$, if we make ansatz on the decay rates of high-order norms of v.

Numerical implementation of the closed-loop system

Numerical schemes (H.-Wu-Zheng, CMAME '23; H.-Rautenberg-Zheng, JDE '23)

- Taylor-Hood finite element algorithm together with projection method and BDF2 time discretization for solving the Stokes equations
- Runge-Kutta Discontinuous Galerkin (RKDG) scheme with 3rd order accurate in time and piecewise quadratic in space for solving the transport equation

Numerical simulations: semi-implicit Euler's method I



$\theta_0 = \tanh(y/0.1)$. Evolution of θ for $\in [0, 2]$, $h = 0.1, \gamma =$1e-6

Mixing decay rate in time

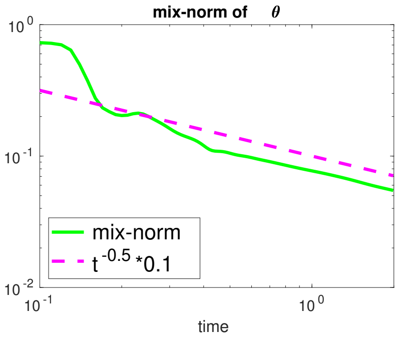
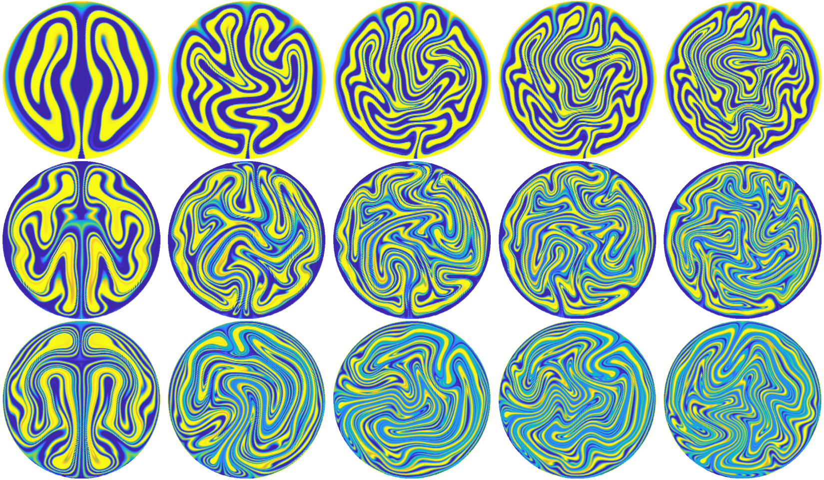


Fig. 14: Evolution of $(H^1(\Omega))'$-norm of the closed-loop solution θ over time

Semi-implicit Euler's method I with different h



Density snapshots of semi-implicit Euler method I. First row: $h = 0.01$. Second row: $h = 0.1$. Third row: $h = 1$. All the time frames are at $t = 1, 3, 5, 7, 10$.

Different discretization scheme

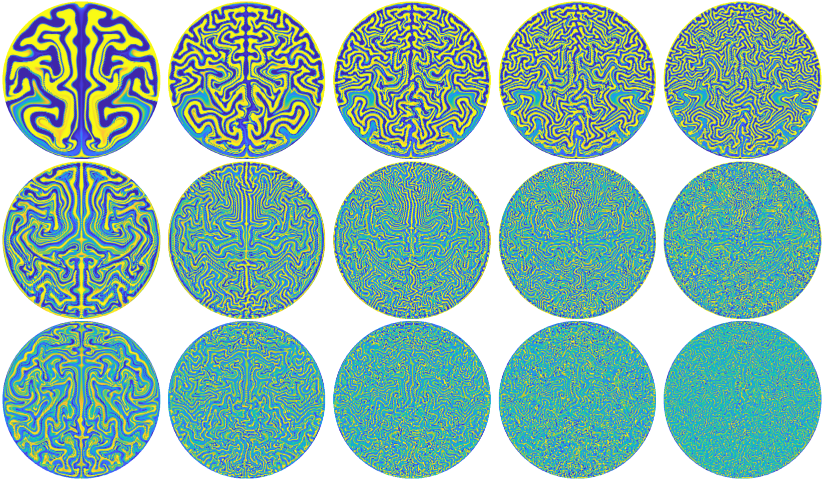
Using a different semi-implicit Euler method (II) in time for discretizing the state equations in t gives

$$\begin{cases} \theta^{i+1} = \theta^i - hv^{i+1} \cdot \nabla\theta^i, \\ v^{i+1} = v^i + hAv^i + Bu^{i+1} \\ (-\Delta + I)\eta^{i+1} = \theta^{i+1}, \quad \frac{\partial\eta^{i+1}}{\partial n}|_\Gamma = 0. \end{cases} \tag{6}$$

Following similar procedures, one can show that (6) is the semi-implicit time discretization of the closed-loop system

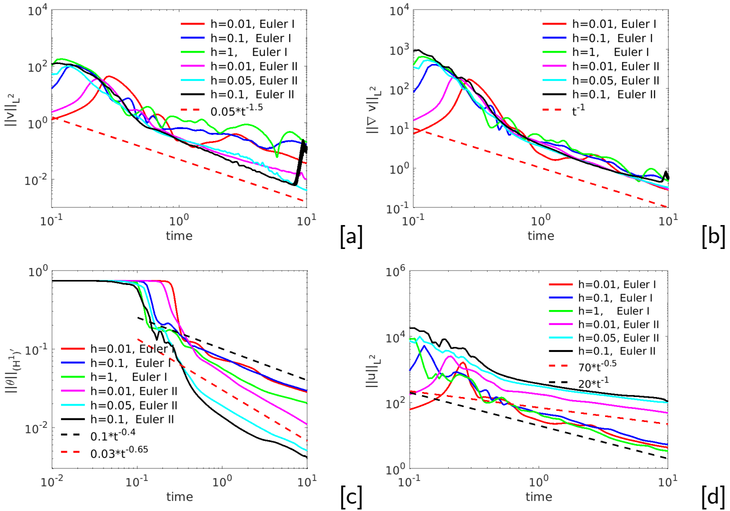
$$\begin{cases} \partial_t\theta = -v \cdot \nabla\theta, \quad \theta(0) = \theta_0, \\ \partial_t v = Av + Bu, \quad v(0) = v_0, \\ u = -\gamma^{-1} hBB^*\mathbb{P}(\theta\nabla\eta). \end{cases} \tag{7}$$

Semi-implicit Euler's method II with different h



Density snapshots of semi-implicit Euler method II. First row: $h = 0.01$. Second row: $h = 0.05$. Third row: $h = 0.1$. All the time frames are at $t = 1, 3, 5, 7, 10$.

Long-time behavior of the closed-loop system



[a]-[d]: Evolution of norms in time.

Questions

- Determine the velocity field that achieves mixing with no flow dynamics involved;
- Approximate the desired velocity field via active control of the flow dynamics.

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- Determine the velocity field that achieves mixing with no flow dynamics involved;
- Approximate the desired velocity field via active control of the flow dynamics.
- Consider

$$\begin{cases} \frac{\partial \theta}{\partial t} + v \cdot \nabla \theta = 0, \quad \theta(0) = \theta_0, \\ \nabla \cdot v = 0, \quad v \cdot n|_\Gamma = 0, \\ (-\Delta + I)\eta = \theta, \quad \frac{\partial \eta}{\partial n}|_\Gamma = 0. \end{cases}$$

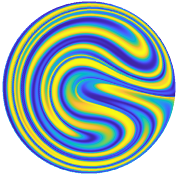
- Let $\theta_0 \in L^\infty(\mathbb{T}^2)$ with $\int_{\mathbb{T}^2} \theta_0 = 0$. Assume $v \in W^{s,p}(\Omega)$, uniformly in time, for some $s \geq 0$ and $1 \leq p \leq \infty$.

  1. If $s < 1$: for any $0 < t^* < \infty$, can we construct a feedback law

  $$v = F(\theta, \eta),$$

  such that $\lim_{t \to t^*} \|\theta(t, \cdot)\|_{H^{-1}} = 0$, i.e., perfect mixing in finite time can be achived?
  2. If $s \geq 1$: can we construct a feedback law such that exponential mixing is possible, i.e., there exist constants $M, \delta > 0$ such that

  $$\|\theta\|_{(H^1(\Omega))'} \leq M e^{-\delta t}, \quad t \geq 0\,?$$



Thank you for your attention!

Questions?