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A transfer operator based computational study of mixing processes in open flow systems

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We study mixing by chaotic advection in open flow systems, where the corresponding small-scale structures are created by means of the stretching and folding property of chaotic flows. The systems we consider contain an inlet and an outlet flow region as well as a mixing region and are characterized by constant in- and outflow of fluid particles. The evolution of a mass distribution in the open system is described via a transfer operator. The spatially discretized approximation of the transfer operator defines the transition matrix of an absorbing Markov chain restricted to finite transient states. We study the underlying mixing processes via this substochastic transition matrix. We conduct parameter studies for example systems with two differently colored fluids. We quantify the mixing of the resulting patterns by several mixing measures. In case of chaotic advection the transport processes in the open system are organized by the chaotic saddle and its stable and unstable manifolds. We extract these structures directly from leading eigenvectors of the transition matrix.

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1 Transfer-operator and its numerical approximation in open systems

Let $T : (A, \mathcal{B}(A)) \rightarrow (X, \mathcal{B}(X))$ be a measurable and nonsingular transformation that maps an initial particle in $A \subset X \subset \mathbb{R}^d$ to its new position after a given timestep τ (open system). The evolution of the mass distribution f over A under T can be described by an affine operator: $L_1(A) \rightarrow L_1(A)$, defined by $\mathcal{P}_A f + \varsigma$, where \mathcal{P}_A is the conditional Perron-Frobenius operator [1] and ς describes the new mass that is released into the system after time-step τ . The linear operator $\mathcal{P}_A : L^1(A) \rightarrow L^1(A)$ is defined by

$$\int_B \mathcal{P}_A f d\mu = \int_{T^{-1}B} f d\mu \quad \text{for all } B \in \mathcal{B}(A).$$

Using Ulam's method [2], a spatially discretized approximation of \mathcal{P}_A is given by the substochastic matrix P with entries estimated as

$$P_{ij} = \frac{\mu(B_i \cap T^{-1}(B_j))}{\mu(B_i)},$$

where $\{B_1, B_2, \dots, B_n\}$, is a fine partition of A and μ is the Lebesgue measure on A . The evolution of the mass distribution vector v over A can now be described as an affine transformation $vP + \sigma$, where σ is the discrete source that is injected into the system after time-step τ . Under the assumption that all particles can finally leave A and that the source σ is constant, the matrix P defines the transition matrix of an absorbing Markov chain restricted to finite transient states. Assuming that the underlying velocity field in our system is time-periodic with period τ , then the Markov chain is time-homogeneous and the mass distribution converges to the invariant mass distribution $v_{\text{inv}} = \sigma(I - P)^{-1}$ (fixed point of the affine transformation) [3].

2 Mixing in open systems: Example set-up

Let a system with domain X contain an inlet and an outlet flow region, X_1 and X_3 , as well as a mixing region X_2 (see Fig.1). Two types of particles in the system are advected by velocity field

$$u(x, y, t) = \begin{cases} u_w(x, y), & \text{for } (x, y) \in X_1 \cup X_3 \\ u_w(x, y) + u_m(x, y, t), & \text{for } (x, y) \in X_2 \end{cases},$$

where u_w is a constant homogeneous velocity field and u_m is the velocity field of a time-periodic mixer.

Here, as velocity field of the time-periodic mixer we use the well-known periodically perturbed double gyre flow [4], whose phase portrait contains two counter-rotating gyres separated by a periodically moving separatrix.

In the outlet region a "periodic" pattern is formed after some time, which we want to quantify with respect to the mixing quality. Therefore, we consider the open subsystem with domain A containing an inlet flow region A_{in} , the mixing region A_{mix} and an outlet flow region A_{out} , which fully describes the pattern.

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We partition the domain A in 49152 square boxes and calculate the transition matrix P . As constant source we use a signed mass distribution σ , describing the two types of particles.

2.1 Mixing measures

We consider the following mixing measures: the sample variance (as measure of the intensity of segregation), the mean length scale (as measure of the scale of segregation) [5, 6] and the mix variance (a multiscale measure of mixing that considers a concentration field to be well-mixed if its averages over arbitrary open sets are uniform) [7]. In Fig.2 we show the results of a parameter study. We vary the double gyre parameter ϵ , which controls the maximum displacement of the separatrix, and apply the different mixing measures to the invariant mass distribution v_{inv} restricted to the outlet region A_{out} . The mixing measures show peaks in the mixing quality for similar parameter values. Three corresponding mass distributions on A_{out} are included in the figure. In further parameter studies, the mixing variance has been shown to be robust to numerical changes in the calculation of P . For future work, spectral mixing measures that take into account information on two types of fluid could be useful.

2.2 Organizing structures

Most fluid material has a transient behavior and leaves the open system relatively fast, but some material intersects with its original domain. This region is a chaotic saddle. Particles near the stable manifold of a chaotic saddle stay longer in the system and follow the unstable manifold of a chaotic saddle on their way out [8].

In Fig.3a we follow a bulb of particles at time $t = 0$ (cyan and blue) to $t = 10$ (pink and orange). The cyan particles remain in the system after 10 time steps (colored in pink). This reveals the unstable manifold (pink) and the stable manifold (cyan). Instead of following particles, we can extract these structures now directly from the leading left and right eigenvectors of our substochastic transition matrix P . In Fig.3b-c the leading two left and the leading two right eigenvectors of the transition matrix P are shown. The support of a left eigenvector approximates an unstable manifold. The support of a right eigenvector approximates a stable manifold. The intersection of the support of the two left and right eigenvectors (dark blue) approximates two chaotic saddles (see Fig.3d). To optimize mixing, it would be interesting to study how these organizing structures can be manipulated.

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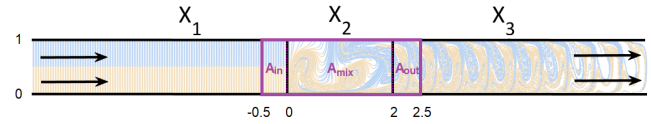


Fig. 1: Set-up of the double gyre mixer

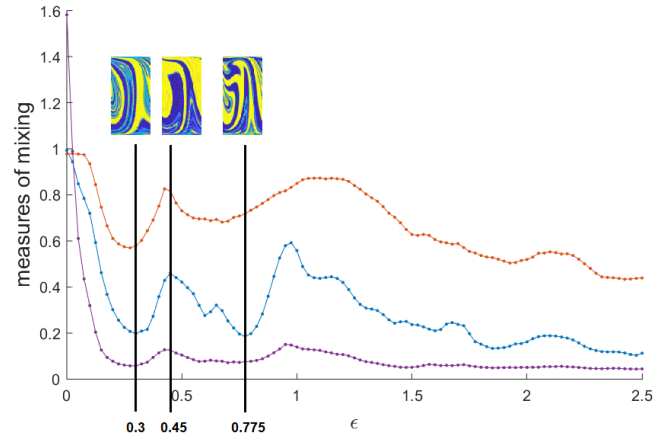


Fig. 2: Different measures of mixing applied to v_{inv} restricted to A_{out} . Red: sample variance, blue: relative mix variance, purple: mean length scale

Most fluid material has a transient behavior and leaves the open system relatively fast, but some material intersects with its original domain. This region is a chaotic saddle. Particles near the stable manifold of a chaotic saddle stay longer in the system and follow the unstable manifold of a chaotic saddle on their way out [8].

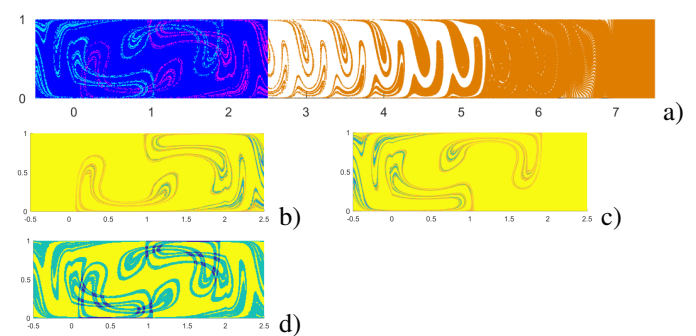


Fig. 3: **a** Evolution of a set of particles. Position of the particles after 0 (cyan and blue) and 10 (pink and orange) time steps. **b** Leading two left eigenvectors of the transition matrix P . **c** Leading two right eigenvectors. **d** Support of the leading two left and right eigenvectors.

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