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COMPUTATIONAL CHARACTERIZATION OF FLUID MIXING IN INCOMPRESSIBLE FLOWS

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Abstract. We propose a computational methodology for characterizing fluid mixing in incompressible flows. Principal to the characterization is defining a mixing measure that will resolve the mixing process both in space and time. We base the mixing measure on rigorous notions, *mixing* and *correlation sequences*, known from dynamic system theory and suggest a suitable approximation. Moreover we consider the situation when the generating velocity field is not known a priori but rather from numerical data. Finally we peruse an error analysis considering the total error with contributions from: (1) the approximation of the mixing measure, (2) the computation of the mixing measure and (3) the approximate velocity field. We obtain an upper error bound for the mixing measure that in principle could be used for rigorous computational characterization of the mixing process.

Key Words: mixing, shadowing, finite elements, flow simulation

2000 Mathematics Subject Classification: 37A25, 37C50, 76M10

1. Introduction

We face the problem of mixing two miscible fluids on a time scale where diffusion is negligible. In order to obtain this we will have to displace the fluids by means of a velocity field that is sufficiently irregular. In the engineering literature such process is commonly refereed to *mixing by chaotic advection* and for further references we refer to the survey articles [1, 2, 21] or the book [20]. The problem has recently be revived spurred by the development of micro fluidics see the book [15] for a general reference and the review articles [14, 19] on mixing in micro fluid systems.

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Considering mixing as a relaxation process going from an unmixed state to a homogeneous (mixed) state and characterizing this relaxation we will need a measure that will resolve the mixing process in space and time. For example: the mixing could be nonuniform in space and we may be interested in resolving these spatial variations; or a process may be mixing although at a small rate, too small to be use full in an engineering application. There seems to be no consensus on what mixing measure to use. The mixing measures suggested in the literature varies and are in many case heuristical cf. [20, 3, 12].

In dynamic system theory mixing has a precise meaning, see for example [16, 25] or the survey article [24]. Related to mixing in this context is the *correlation sequence* which we use as a mixing measure in this work. Since the correlation sequence in principle is intractable we propose a computable approximation and analyze the error in this approximation. Moreover we consider a situation where the velocity field generating the mixing process is not a priori known in close for but rather from computed data to some model, e.g., the Stokes equations or possibly the Navier-Stokes equations or any other fluid model. This aspect is also included in the error analysis The provided error bound for the mixing measure could in principle be used for a rigorous computational characterization of the mixing process so that the error is controlled and made small.

1.1. **Assumptions.** Let $\Omega \subset \mathbf{R}^d$ for $d = 2, 3$ be an open set with boundary $\partial\Omega$. We assume that the fluids are contained in Ω and imposed by a Lipschitz continuous velocity field $f : \Omega \to \mathbf{R}^d$. Then f generates a flow $[0, t] \times \Omega \ni (t, x) \mapsto u(t, x) \in \mathbf{R}^d$, describing the motion of a fluid particles in Ω, as solutions to the system of ordinary differential equations

$$\partial_t u(t, x) = f(u(t, x)), \quad t > 0; \quad u(0, x) = x. \tag{1.1}$$

We also assume that f is differentiable and that the fluids are incompressible in the sense that

$$\nabla \cdot f(x) = 0 \quad \forall x \in \Omega. \tag{1.2}$$

Let ν be the outward normal to $\partial\Omega$. We assume that $\nu(x) \cdot f(x) = 0$ for a.e. $x \in \partial\Omega$, that is, there is no flow through $\partial\Omega$. Imposing some additional constraints on Ω and f we distinguish two types of flows.

(1) The flow $u(t, x)$ is said to be *confined* if Ω is bounden.

Let $\Gamma \subset \Omega$ with $\dim \Gamma = d-1$ such that $\partial\Gamma \subset \partial\Omega$ and $\Gamma + np \in \Omega$ for a scalar $p \in \mathbf{R}^d$ and any integer n.

(2) The flow $u(t,x)$ is said to be *space periodic* if $f|_\Gamma = f|_{\Gamma+np}$ and $\nu(x) \cdot f(x) \leq 0$ for a.e. $x \in \Gamma$.

1.2. **Considerations.** We ask to what extent the mixing process could be computationally characterized in the sense that computed predictions are accurate. Suppose we compute a mixing measure, of our choice, that reflects the amount of mixing in Ω generated by f. Then we also would like to estimate the error in the computed measure and make it small. Accurate predictions of this kind is inherently difficult since mixing is only obtained if f is sufficiently irregular meaning that the flow generated by f will have to be hyperbolic which loosely involves that the flow have to have enough contractive and expensive directions, see [16, 25] for a more precise statement of hyperbolicity. Such systems are dynamically unstable, sensitive to perturbations, which renders the computation delicate.

In practice we will not know the flow $u(t,x)$ a priori in a closed form and in order to study the properties of the flow we may instead analyze a limited number of numerically computed orbits $u_k(t,x_j)$ for $j = 1, 2, \ldots, I$, and where k denote the time discretization. Moreover in many situations we may not even know f a priori in a closed form but it will rather be defined from a model, for example, a partial differential equation, and we will have to use approximate data f_h for f where h denote the space discretization. Now let $u_k(t,x)$ be a computed orbit to (1.1) with right hand side $f = f_h$. Then the error

$$e(t,x) := u_k(t,x) - u(t,x), \tag{1.3}$$

will depend on the discretization-error associated with the numerical method use to compute $u_k(t,x)$ and the error in the velocity field $e_f := f_f - f$. Since (1.1) probably is dynamically unstable we will only be able to compute $u_k(t,x)$ with small $e(t,x)$ for a rather small time. However, if the system is sufficiently hyperbolic we may argue by shadowing, that is, provided $u_k(t,x)$ is computed accurately enough and provided e_f is small enough there is an exact orbit $u(t,y)$ such that $\|u_k(t,x) - u(t,y)\|$ is small for $t \in [0,T]$ [7, 8, **?**]. The overall idea is to use this kind of argument in order to control the error in a computed mixing measure.

1.3. **Notions form dynamic system theory.** Within the realm of dynamic system theory mixing has a precise meaning. For a probability

space $(X, \mathcal{M}, \mu)$ a measure preserving bijective mapping $T : (X, \mathcal{M}, \mu) \to (X, \mathcal{M}, \mu)$ is called *mixing* if

$$\forall\, A, B \in \mathcal{M} \quad \mu(A \cap T^n B) \to \mu(A)\mu(B) \quad \text{as} \quad n \to \infty, \tag{1.4}$$

for discrete time systems;

$$\forall\, A, B \in \mathcal{M} \quad \mu(A \cap T^t B) \to \mu(A)\mu(B) \quad \text{as} \quad t \to \infty, \tag{1.5}$$

for continuous time systems. We remark that T is measure preserving if for every $A, B \in \mathcal{M}$, $\mu(T^{-1}A) \in \mathcal{M}$ and $\mu(T^{-1}(A)) = \mu(A)$, see for example [9, 25].

Generally mixing is also defined for measure preserving maps that is only surjective but then we must replace $\mu(A \cap T^n B)$ by $\mu(T^{-n}(A) \cap B)$ in the definition, and likewise for the time continuous case, [9, 25].

Related to mixing is the decay of correlations between the sets $A, B \in \mathcal{M}$ defined by the *correlation sequence*

$$C_n(A, B) = \mu(A \cap T^n B) - \mu(A)\mu(B) \tag{1.6}$$

for discrete time systems;

$$C_t(A, B) = \mu(A \cap T^t B) - \mu(A)\mu(B) \tag{1.7}$$

for continuous time systems, see for example [4, 25]. The asymptotic behavior will indicate whether the mapping is mixing and also on the rate. The decay may be exponential $C_n(A, B) \sim e^{-\alpha n}$ or polynomial $C_n(A, B) \sim n^{-\alpha}$ for some $\alpha > 0$ and likewise for $C_t(A, B)$.

1.4. **Computability.** In practice some of the notions in Section 1.3 are too general and intractable. We will have to approximate $\mathcal{M}$, which in our case is a Borel σ-algebra on $X = \Omega$. It seems natural to replace $\mathcal{M}$ by a family of partitions $\{\mathcal{U}_h\}_{h>0}$ where $\mathcal{U}_h$ is the class of finite number of disjoint sets U_i such that $\bigcup_i U_i = \Omega$ and where h denote the size of the largest set in $\mathcal{U}$, that is, $h = \max_i \operatorname{diam} U_i$. In principle any type of partition will suffice although if Ω is a polyhedral domain it is convenient to let $\{\mathcal{U}_h\}_{h>0} = \{\mathcal{T}_h\}_{h>0}$ be a family of quasi uniform triangulation, see for example [11].

The size h will determine the resolution of the approximation and could for example be motivated by some physical length scale, that is, form the Einstein relation we get $h \sim (\tau D)^{1/2}$ where τ is typical time scale and D is the diffusion constant.

In order to investigate whether a mapping is mixing we may consider the correlation sequence $C_n(A,B)$ (or $C_t(A,B)$) for $A, B \in \mathcal{U}_h$ and for some finite n. We will have to evaluating the measure $\mu(A \cap T^n B)$ (or $\mu(A \cap T^t B)$) which is inherently difficult since the mapping probably is dynamically unstable and even though B may have a simple geometry $T^n B$ will be severely deformed. It is plausible to assume that we only know $T^n x_j$ for $x_j \in B$ and a limited number $j = 1, \dots, M$. It then seems viable to evaluate $\mu(A \cap T^n B)$ by a simple Monte Carlo method. We will discuss this kind of implementation in more detail in the sections below where the measure is explicitly stated.

1.4.1. *Monte Carlo integration.* For further reference we now briefly recall Monte Carlo method, see for example [17]. Consider integrable functions f and g on $A \in \mathcal{M}$ such that $g \geq 0$ and

$$\int_A g(x)\, dx = 1,$$

and independent random variables $\{x_j\}_{j=1}^M$ that is $g(x)\, dx$ distributed on A. Then

$$\int_A f(x)g(x)\, dx = \frac{1}{M}\sum_{j=1}^{M} f(x_j) + R_M(\sigma), \tag{1.8}$$

where $R_M(\sigma)$ is a residual that must be interpreted statistically in the sense that R_M is normal distributed with standard deviation $\sigma/\sqrt{M}$ where

$$\sigma^2 = \int_A f(x)^2\, dx - \left(\int_A f(x)\, dx\right)^2$$

is the variance. In practice we may estimate this variance by the empirical variance

$$\hat{\sigma}^2 = \frac{1}{M-1}\sum_{i=1}^{M}(x_i - \bar{x})^2$$

where $\bar{x}$ is the mean of $\{x_j\}_{j=1}^M$.

In the sequel we will set $f = \chi_A$, the characteristic function defined by

$$\chi_A(x) = \begin{cases} 1, & \text{if } x \in A, \\ 0, & \text{if } x \notin A. \end{cases} \tag{1.9}$$

1.5. **Error analysis.** We compute approximate orbits $u_k(t, x_j)$ to (1.1) for $t \in [0, T]$ and $x_j \in B$ and $j = 1, \ldots, M$ by a continuous finite element method. This involve partitioning $[0, T]$ into intervals $I_i = [t_{i-1}, t_i]$ for $i = 1, 2, \ldots, N$ such that $0 = t_0 < t_1 < \ldots < t_N = T$ and set $k_i = t_{i-1} - t_i$. Let $P_q(I_i)$ denote the polynomials of degree less or equal to q on I_i and set

$$V_q([0, T]) := \{v \in C^0([0, T]) : v|_{I_i} \in P_q(I_i), \text{ for } i = 1 \ldots N\}$$

which is the finite element space of piecewise continuous polynomials of degree q.

For $q \geq 1$ we now obtain the finite element formulation to (1.1) with $f = f_h$ and approximate velocity field. Find $u_k \in V_q([0, T])^d$ with $u_k(t, 0) = x$ such that

$$\int_0^T (\partial_t u_k - f_h(u_k)) \cdot v \, dt = 0 \quad \forall v \in V_{q-1}([0, T])^3, \tag{1.10}$$

This is the continuous Galerkin method of order q, referred to as the cG(q) method in [10, p. 210]. There will be $N(q + 1) - 1$ nodes in the interval $[0, T]$, where the piecewise polynomials are evaluated.

We will now assume that $u_k(t, x)$ is computed sufficiently accurate and that e_f is sufficiently small. A precise statement of this could be found in [10] for general finite element approximations and particularly in the percent situation in [**?**]. The condition requiring $u_k(t, x)$ to be computed sufficiently accurate could be translated to $u_k(t, x)$ being a *pseudo orbit* cf. [16, 22]. We will use this notion in the sequel and in addition, when it is not explicitly stated, always assume that e_f is sufficiently small.

If Ω is sufficiently hyperbolic for (1.1) then every pseudo orbit will be shadowed by an exact orbit at least for some finite time $t \in [0, T]$, cf. [8, 7, **?**] and the book [22]. This implies that $\|u_k(t, x) - u(t, y)\|$ could be made small for $t \in [0, T]$.

Now for every pseudo orbit $u_k(t, x_j)$ for $t \in [0, T]$ and $x_j \in B$, $j = 1, \ldots, M$, we assume that there is another orbit $u(t, y_j)$ where $y_j \in \widetilde{B}$ such that

$$\|u_k(t, x_j) - u(t, y_j)\| \leq \varepsilon_j, \tag{1.11}$$

and we set

$$\varepsilon = \max_j \varepsilon_j. \tag{1.12}$$

In order to better characterize $\widetilde{B}$ we extend the notation given above and assume $u_k(t,x)$ is a pseudo orbit for all $x \in B$ and set

$$\widetilde{B} = \bigcup_{x\in B} \mathcal{B}(x,\varepsilon), \tag{1.13}$$

where $\mathcal{B}(x,\varepsilon)$ is the ball or radius ε about x.

2. Mixing in confined incompressible flows

Let $u(t,x)$ be a confined incompressible flow as defined in Section 1.1. For an open set $A \subseteq \Omega$ we define the measure as the volume of A normalized with the volume of Ω

$$\mu(A) = c_0^{-1} \int_A dx = c_0^{-1}|A|. \tag{2.1}$$

where

$$c_0 = \int_\Omega dx = |\Omega|,$$

is the volume of Ω. Then $(\Omega, \mathcal{M}, \mu)$ is a probability space.

Now let $T^t(\cdot)$ be defined by the flow $u(t,\cdot)$. Since u is a flow and f is incompressible T is bijective and measure preserving, that is, $|A| = |T^t A|$ for every $A \in \mathcal{M}$ or in other words we say that T^t preserve volume. Hence mixing according to (1.5) and the correlation sequence (1.7) are well defined in this case.

2.1. Computational characterization.

Let $u_k(t,x_j)$ for $t \in [0,T]$ and $x_j \in B$ be pseudo orbits defining the mapping T_k^t and approximate $\mathcal{M}$ with a partition $\mathcal{U}_h$ as defined in Section 1.4.

In order to approximately compute (1.7) we let $\{x_j\}_{j=1}^M$ be independent random variables uniformly distributed on B. Now $\{T_k^t x_j\}_{j=1}^M$ will be independent random variables $T_k^t x\, dx$ distributed on $T_k^t B$ and we compute $|A \cap T_k^t B|$ by the Monte Carlo method. Set $f(x) = \chi_A(x)$ and $g(x) = |T_k^t B|^{-1}$ in (1.8) and we obtain

$$|A \cap T_k^t B| = \int_{T_k^t B} \chi_A(x)\, dx \approx |T_k^t B| M^{-1} \sum_{j=1}^M \chi_A(T_k^t x_j).$$

It may seem tempting to set $|T_k^t B| = |B|$ but since T_k^t in general is not measure preserving we can not do so. Instead we evaluate $|T_k^t B|$ by Mote

Carlo integration and by a change of variables we obtain

$$|T_k^t B| = \int_{T_k^t B} dx = \int_B |\det(\nabla T_k^t x)|\, dx \approx |B| M^{-1} \sum_{j=1}^{M} |\det(\nabla T_k^t x_j)|,$$

where we note that $|\det(T_k^t x)| = 1$ if is T_k^t is measure preserving, that is, if f_h is incompressible [6, p. 10].

Hence we define the following approximation to the correlation sequence (1.7) for $A, B \in \mathcal{U}_h$

$$C_{k,t}^M(A,B) = |B| M^{-2} \sum_{i=1}^{M} |\det(\nabla T_k^t x_i)| \sum_{j=1}^{M} \chi_A(T_k^t x_j) - |A||B| \tag{2.2}$$

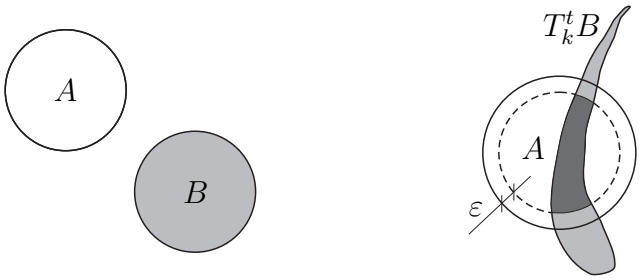

Figure 2.1: (left) $A, B \subset \Omega$ at $t = 0$. **(right)** Intersection $A \cap T_k^t B$ and the ε-shell inside A.

2.2. **Error analysis.** As outlined in Section 1.5 we assume that to every pseudo orbit $u_k(t,x)$ there is an exact orbit $u(t,y)$ such that (1.11) is satisfied and that ε in (1.12) is small. Then for $A, B \in \mathcal{U}_h$ and $\widetilde{B}$ as defined in (1.13) we argue that

$$|A \cap T_k^t B| - |A \cap T^t \widetilde{B}| \leq \varepsilon |\partial A \cap T_k^t B| \leq \varepsilon |\partial A|$$

where $\varepsilon|\partial A \cap T_k^t B|$ is the measure of the points $T_k^t x \in T_k^t B$ such that $\operatorname{dist}(T_k^t x, \partial A) \leq \varepsilon$, Figure 2.1, and in the same way

$$|B| - |\widetilde{B}| \leq \varepsilon |\partial B|,$$

and hence we may estimate

$$\big| |A \cap T_k^t B| - |A||B| - C_t(A, \widetilde{B}) \big| \leq \varepsilon \big(|\partial A| + |A||\partial B| \big).$$

Now with the estimate above and for $A, B \in \mathcal{U}_h$ and $\widetilde{B}$ as defined in (1.13) we estimate the error in the approximate correlation sequence (2.2)

$$|C^M_{k,t}(A,B) - C_t(A,\widetilde{B})| \leq \varepsilon\big(|\partial A| + |A||\partial B|\big) + R, \tag{2.3}$$

where R must be interpreted statistically as explained in Section 1.4.1.

3. Mixing in periodic channel flows

Let $u(t,x)$ be a space periodic incompressible flow as defined in Section 1.1. For an open set $A \subseteq \Gamma$ we define the measure as the flow through A normalized with the flow trough Γ

$$\mu(A) = c_0^{-1} \int_A f \cdot \nu \, dx, \tag{3.1}$$

where

$$c_0 = \int_\Gamma f \cdot \nu \, dx,$$

is the total flow through Γ. Then $(\Gamma, \mathcal{M}, \mu)$ is a probability space.

Now for $u(0,x) \in \Gamma$ let t be such that $u(t,x) \in \Gamma + p$ and let $T : \Gamma \to \Gamma$ be the mapping defined by $T := u(t,x) - p$. We note that since u is a flow and f is incompressible T is bijective and measure preserving. Iterating $T^n(x) = T \circ T^{n-1}(x)$ with $T^0(x) = x$ we obtain the Poincaré map for which mixing according to (1.4) and the correlation sequence (1.6) are well posed in this case.

3.1. **Computational characterization.**

We need define an approximate measure based on the f_h instead of f. For an open set $A \subseteq \Gamma$ set

$$\mu_h(A) = c_{h0}^{-1} \int_A f_h \cdot \nu \, dx, \tag{3.2}$$

where

$$c_{h0} = \int_\Gamma f_h \cdot \nu \, dx.$$

Let $u_k(t, x_j)$ for $t \in [0,T]$ and $x_j \in B$ be pseudo orbits defining the mapping T_k^n and approximate $\mathcal{M}$ with a partition $\mathcal{U}_h$ of Γ as defined in Section 1.4.

In order to approximately compute (1.6) we let $\{x_j\}_{j=1}^M$ be independent random variables $f_h(x) \cdot \nu \, dx$ distributed on B. Now $\{T_k^n x_j\}_{j=1}^M$ will be independent random variables $f_h(T_k^n x) \cdot \nu \, dx$ distributed on $T_k^n B$ and we

compute $\mu_h(A \cap T_k^n B)$ by the Monte Carlo method. Set $f(x) = \chi_A(x)$ and $g(x) = \mu_h(T_k^n B)^{-1}$ in (1.8) and we obtain

$$\mu_h(A \cap T_k^n B) = \int_{T_k^n B} \chi_A(x) f_h \cdot \nu \, dx \approx \mu_h(T_k^n B) M^{-1} \sum_{j=1}^{M} \chi_A(T_k^n x_j).$$

Since T_k^n in general is not μ_h measure preserving we can not set $\mu_h(T_k^n B) = \mu_h(B)$. Instead we evaluate $\mu_h(T_k^n B)$ by mote carlo integration and by a change of variables we obtain

$$\int_{T_k^n B} f_h \cdot \nu \, dx = \int_B f_h \cdot \nu |\det(\nabla T_k^n x)| \, dx \approx \mu_h(B) M^{-1} \sum_{j=1}^{M} |\det(\nabla T_k^n x_j)|,$$

where we note that $|\det(T_k^n x)| = 1$ if f_h is incompressible [6, p. 10].

Hence we define the following approximation to the correlation sequence (1.7) for $A, B \in \mathcal{U}_h$

(3.3)

$$C_{k,n}^M(A, B) = \mu_h(B) M^{-2} \sum_{i=1}^{M} |\det(\nabla T_k^n x_i)| \sum_{j=1}^{M} \chi_A(T_k^n x_j) - \mu_h(A)\mu_h(B)$$

3.2. **Error analysis.** As outlined in Section 1.5 we assume that to every pseudo orbit $u_k(t, x)$ there is an exact orbit $u(t, y)$ such that (1.11) is satisfied and that ε in (1.12) is small. Then for $A, B \in \mathcal{U}_h$ and $\widetilde{B}$ as defined in (1.13) we argue in the same way as we did in Section 2.2 and obtain

$$|\mu(A \cap T_k^n B) - \mu(A)\mu(B) - C_n(A, \widetilde{B})| \leq \varepsilon\big(\mu(\partial A) + \mu(A)\mu(\partial B)\big).$$

In order to make the connection to the approximate correlation function (3.3) we first note that for any $A \in \mathcal{U}_h$

$$|\mu_h(A) - \mu(A)| = \int_A (f_h - f) \cdot \nu \, dx \leq |A| e_f,$$

and thus we arrive at the following estimate. For $A, B \in \mathcal{U}_h$ and $\widetilde{B}$ as defined in (1.13)

$$|C_{k,n}^M(A, B) - C_n(A, B)| \leq \varepsilon\big(\mu(\partial A) + \mu(A)\mu(\partial B)\big) + C e_f + R, \tag{3.4}$$

where the constant $C = C(A, B)$ and where R must be interpreted statistically as explained in Section 1.4.1.

4. Numerical experiments

We only consider two examples of space periodic flows.

Inspired by [23] where laminar fluid mixing was experimentally studied in small channels we set up the following model. Let $\Omega \subset \mathbf{R}^3$, be a polyhedral domain with periodic boundaries Γ_A and Γ_B, see Figures 4.1 and 4.2, and consider the Dirichlet Stokes problem with periodic boundary conditions in dimensionless form

$$\begin{aligned} -\Delta U + \nabla P &= 0 \quad \text{in } \Omega, \\ \nabla \cdot U &= 0 \quad \text{in } \Omega, \\ U &= 0 \quad \text{on } \partial\Omega \setminus (\Gamma_A \cup \Gamma_B), \\ U|_{\Gamma_A} &= U|_{\Gamma_B}, \\ P|_{\Gamma_A} &= P|_{\Gamma_B} + R_P, \end{aligned} \tag{4.1}$$

where $U = (U_1, U_2, U_3)$ is the unknown velocity field, P the unknown pressure and R_P is a constant modelling the pressure drop.

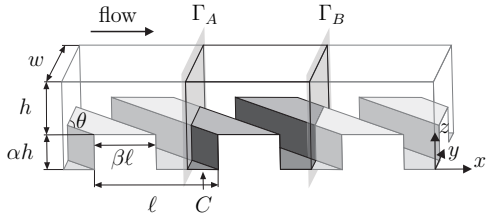

Figure 4.1: Three juxtaposed Ridge Domains. The shaded planes Γ_A and Γ_B are periodic boundaries. We choose the following values for the parameters: $\ell = w = 1$, $h = 0.3$, $\theta = 45°$, $\alpha = 2/3$, $\beta = 0.5$, and the length of the unit cell is $= 1$.

From [5] and [18] we know that $U \in W^{2,4/3}(\Omega)^3 \cap W_0^{1,3}$ and thus U is continuous although not Lipschitz continuous. There will be singularities in ∇U and P along the edges and vertices of Ω. However, if we let $\Omega' \subset \Omega$ such that $\text{dist}(\Omega', \partial\Omega)$ is not too small, then we may argue that U is Lipschitz continuous in Ω' by an interior estimate as in for example [13, Theorem 4.2, p. 209]. Thus when we compute orbits using $f = U$ (or in practice $f = U_h$) in (1.1) we only consider orbits that are not too close to $\partial\Omega$.

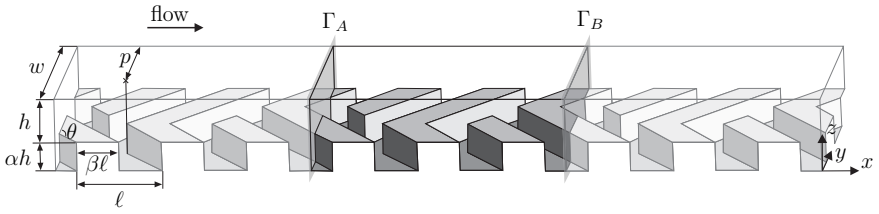

Figure 4.2: Three juxtaposed Herringbone Domains. The shaded planes Γ_A and Γ_B are periodic boundaries. We choose the following values for the parameters: $\ell = 2/3$, $w = 1$, $h = 1/5$, $\theta = 45°$, $\alpha = 2/3$, $\beta = 9/16$, $p = 2/3$, and the length of the unit cell is $= 14/9$.

We refer to the domains in Figures 4.1 and 4.2 as the Ridge Domain and the Herringbone Domain respectively, the names are quoted from [23]. Accurate solutions to (4.1) in the two domains are computed by a finite element method, Hood-Taylor P_2P_1 on fine triangulations. We illustrate the solutions in Figure 4.3 and 4.4.

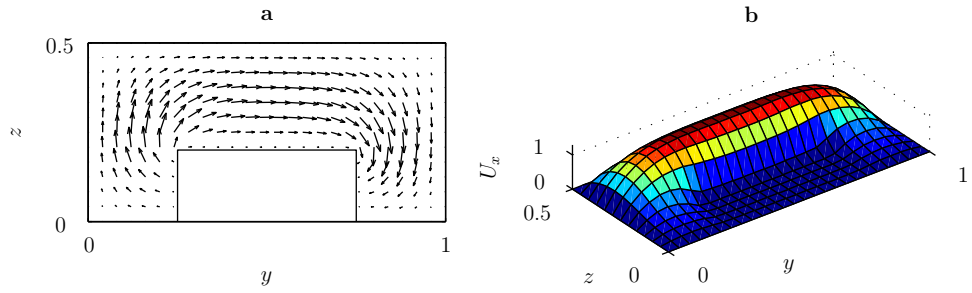

Figure 4.3: Velocity field for (4.1) solved in the Ridge Domain, Figure 4.1, at $x = 0.0$. **(a)** The y and z components of the velocity field. **(b)** The x component of the velocity field.

4.1. **Decay of correlations and Poincaré sections.** We identified Γ_A and Γ_B which are equal boundaries in (4.1) with Γ as defined in Section 1.1. Since Γ is a polygon we choose to partition it into a regular triangulation $\mathcal{T}$.

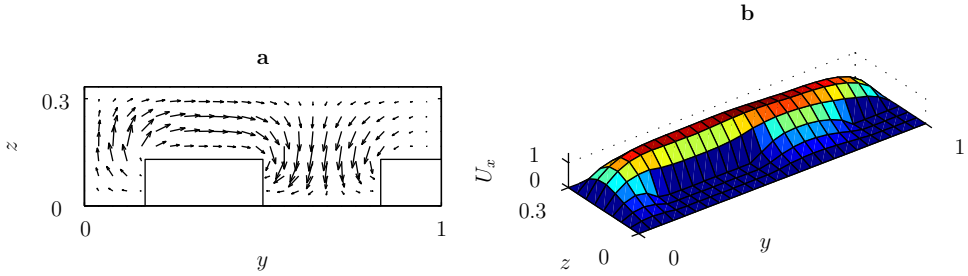

Figure 4.4: Velocity field for (4.1) solved in the Herringbone Domain, Figure 4.2, at $x = 0.0$. **(a)** The y and z components of the velocity field. **(b)** The x component of the velocity field.

In order to examine the approximate correlation sequence (3.3) we choose one $B \in \mathcal{T}_S$ and three $A = A_i \in \mathcal{T}_i$, $i = 0, 1, 2$ such that $A_2 \subset A_1 \subset A_2$ and where $\mathcal{T}_{1,2}$ are defined by uniformly refining $\mathcal{T}_0 = \mathcal{T}$ two or four times, thus $\operatorname{diam} A_0 > \operatorname{diam} A_1 > \operatorname{diam} A_2$. In this case $\mathcal{T}_S$ is part of the triangulation use to solve (4.1) and hence is not commensurate with $\mathcal{T}$, which is just a coincidence and not important for the conclusions. We illustrate $\mathcal{T}_0$ and A_i and B in Figures 4.5 and 4.6 and the triangles A_i and B are explicitly specified in Tables 4.1 and 4.2.

We may think of this numerical experiment as modelling a mixing process where one fluid flowing through B is suppose to mix with another fluid flowing through $\Gamma \setminus B$. The approximate correlation sequence will reflect the amount of mixing in A_i as a function of number of iterates n and $\operatorname{diam} A_i$ will reflect the length scale on which we resolve the mixing process, cf., the discussion in Section 1.4.

As outlined in Section 3.1 we let $x_j \in B$ for $j = 1, \ldots, M$ be $U_h\, dx$ distributed random variables for a relatively large number $M = 80964$ for the Ridge Domain and $M = 73445$ for the Herringbone Domain. We compute orbits to (1.1) for these initial data points using the simple cG(1) method described in Section 1.5, with $f = U_h$ where U_h now is the computed solution to (4.1) . The time steps k_i for $i = 1, 2, \ldots, N$ is chosen adaptively so that the local residual is less than a relatively small tolerance, for more details see [10].

We remark that a complete characterization of the correlation sequence (1.6) involves examining all combinations of $A, B \in \mathcal{T}_h$. Such general

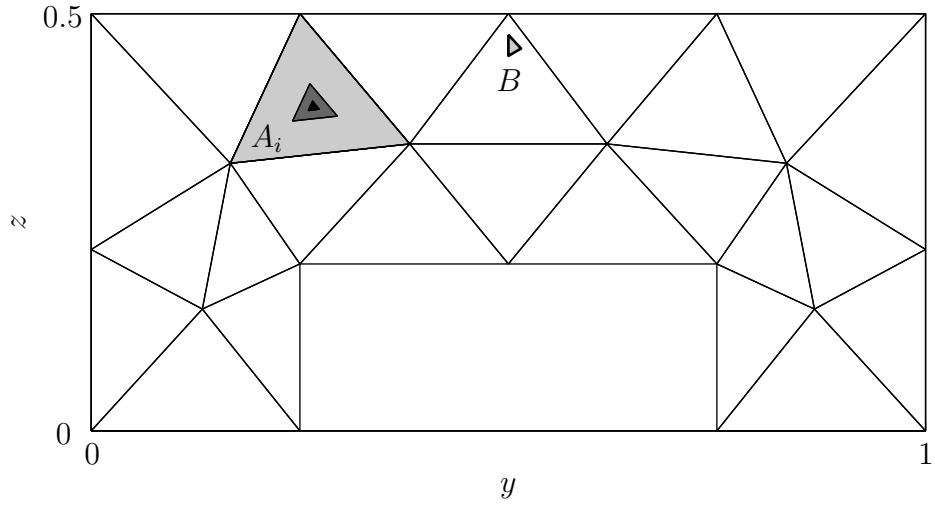

Figure 4.5: Partition of Γ for the Ridge Domain in terms of a triangulation $\mathcal{T}_0$. Shaded triangles illustrates B and A_i, $i = 1, 2, 3$, where $A_{2,3}$ are defined by refining A_1 two or four times picking the central triangle.

Table 4.1: A_i and B for the Ridge Domain where a_0, a_1 and a_2 denote the (x, y)-coordinates of vertices.

	a_0	a_1	a_2
B	(0.499997, 0.474672)	(0.499994, 0.449343)	(0.515248, 0.458255)
A_0	(0.381751, 0.344022)	(0.250000, 0.500000)	(0.166667, 0.320676)
A_1	(0.262104, 0.416175)	(0.241271, 0.371343)	(0.295042, 0.377180)
A_2	(0.259922, 0.384010)	(0.273365, 0.385470)	(0.265131, 0.395218)

analysis would be computationally challenging since the amount of work will grow quadratically in the number of triangles in $\mathcal{T}_h$. A general characterization of this kind is beyond the scoop of this work.

Instead of the complete characterization of the correlation sequence we may plot the Poincaré sections for orbits starting in B see Figures 4.7 and 4.8. This will give qualitative information of the mixing in the entire

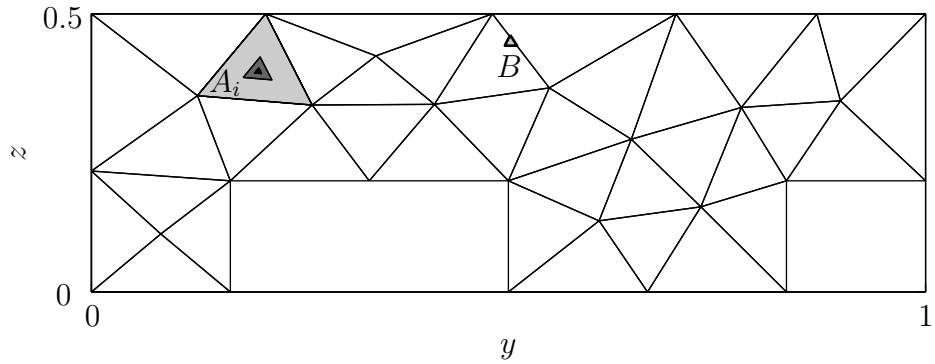

Figure 4.6: Partition of Γ for the Herringbone Domain in terms of a triangulation $\mathcal{T}_0$. Shaded triangles illustrates B and A_i, $i = 1, 2, 3$, where $A_{2,3}$ are defined by refining A_1 two or four times picking the central triangle.

Table 4.2: A_i and B for the Herringbone Domain where a_0, a_1 and a_2 denote the (x, y)-coordinates of vertices.

	a_0	a_1	a_2
B	$(0.502007, 0.510363)$	$(0.495657, 0.295325)$	$(0.510363, 0.295325)$
A_0	$(0.209104, 0.333333)$	$(0.127166, 0.235331)$	$(0.264605, 0.224165)$
A_1	$(0.182010, 0.257040)$	$(0.216370, 0.254248)$	$(0.202495, 0.281541)$
A_2	$(0.204311, 0.261769)$	$(0.200842, 0.268592)$	$(0.195721, 0.262467)$

domain Γ and from such plots we may readily identify regions with either poor or good mixing.

Figure 4.7: Poincaré sections for the flow on the Ridge Domain. 80964 orbits stating in B are included in the data.

Figure 4.8: Poincaré sections for the flow on the Herringbone Domain. 73445 orbits stating in B are included in the data.

Finally, we plot the correlation sequence in Figure 4.9 and normalized the data in the following way,

$$\widehat{C}_{k,n}^{N} = \left| \frac{C_{k,n}^{N}}{\mu(A)\mu(B)} \right|. \tag{4.2}$$

4.2. **Discussion.** We stress that the treatment of the examples in this Section are not meant to be exhaustive in characterizing the mixing properties of Ridge Domain and Herringbone Domain. We rather meant to indicate how the proposed mixing measure work in practice. The over all impression form the Poincaré mapping, Figures 4.7 and 4.8, are still in qualitative agreement with the experiments [23]. However the correlation sequences in Figure 4.9 are not obviously interpreted, the simulations must for example be run over larger time intervals in order to see whether the decay rate is exponential or potential. Although increase the resolution, decreasing the size of A_i, we can see a clear difference between the Ridge Domain and the Herringbone Domain as when the correlation sequences start to decay.

5. Conclusions

We have outlines a methodology for computationally characterizing fluid mixing in incompressible flows. This methodology could in principle be used for rigorous computational characterization of fluid mixing in the sense that error in the mixing measure is controlled and made small. We have not attempt to to achieve this during the cause of this work.

However we remark that in order to obtain such result we will have to control all sort of errors: the error in the velocity field $e_f = f_h - f$, discretization error associated with the numerical method use to compute $u_k(t, x)$, and the error approximating the mixing measure. Of these the most difficult to control is the error in the computed velocity field e_f. This type of error control is vital research field and is rather involved to implement.

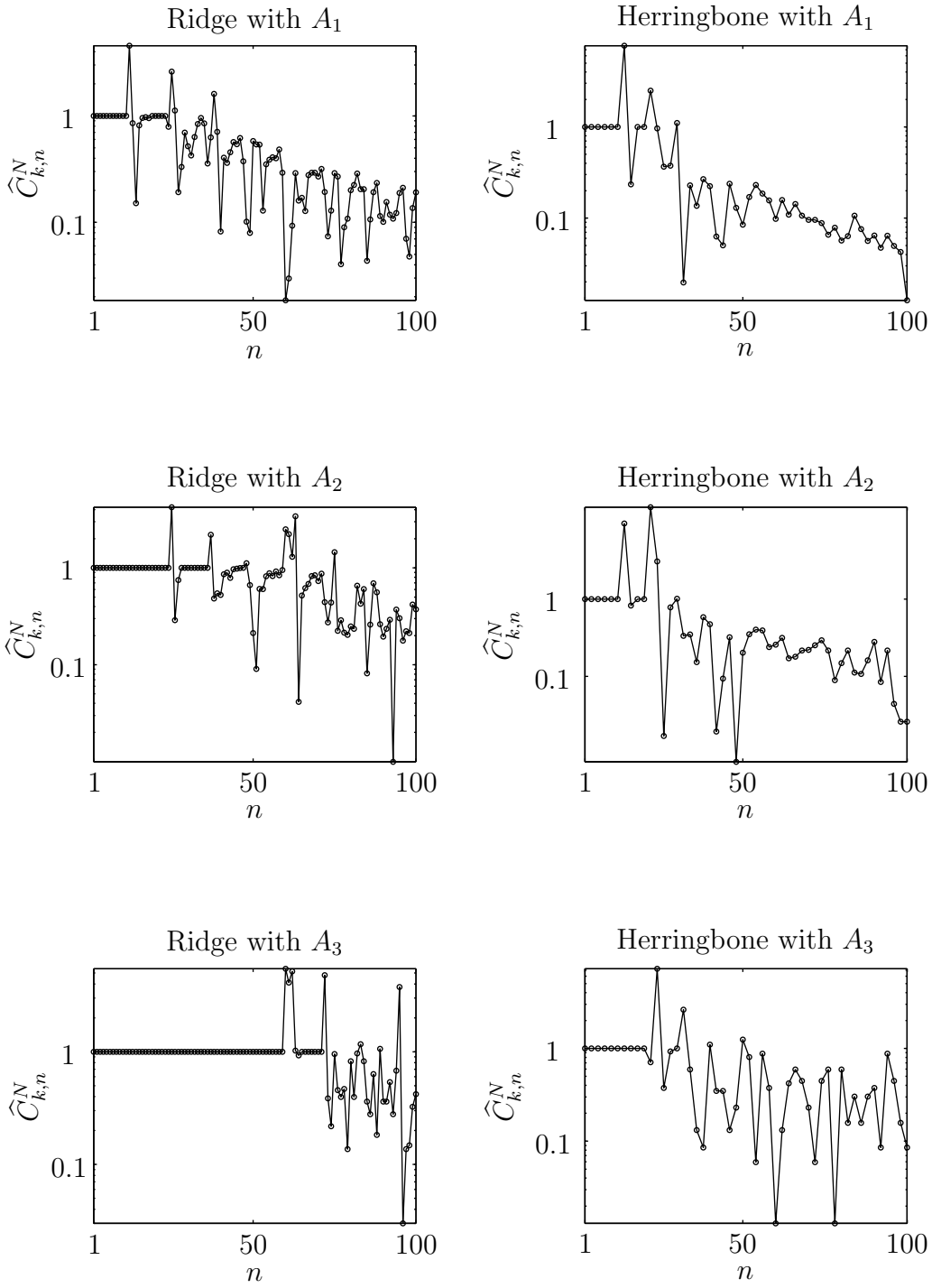

Figure 4.9: The correlation sequence for the Ridge Domain and Herringbone Domain and differen A_i.

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