Chaotic Advection in a Three-dimensional Volume-preserving Potential Flow

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Abstract

While mixing and particle transport in 2D incompressible flows are well-understood, much less is known about 3D incompressible flows. This is because the addition of a third dimension adds to the topological complexity, and more importantly, the link between 2D incompressible flows and Hamiltonian systems that proved so fruitful breaks down for 3D flows. Therefore, there is a need for fundamental studies on 3D fluid transport and mixing, with applications in groundwater flows, micro-fluidics, industrial mixers and biological flows.

Here fluid transport and mixing is studied using a model fluid flow, the 3D Reoriented Potential Mixing (3DRPM) flow, as a case study to reveal novel transport mechanisms and associated coherent structures that are generic to 3D volume-preserving flows. The 3DRPM flow consists of a periodically reoriented dipole flow, and is a 3D analogue of the 2D RPM flow that has been studied in the past.

In the 3DRPM flow it is found that there are a number of competing transport mechanisms, that together drive a transition from 1D to 3D particle transport. Periodic points and lines play an important role for all volume-preserving flows, revealing regions of chaos and impenetrable barriers to transport. Here it is shown that degenerate/parabolic periodic points are particularly important, as they represent bifurcations in flow stability. Conversely, discontinuous deformations are an unexpected consequence of dipole reorientation, akin to slip deformations seen in shear-banding materials, and occur even though the steady dipole flow is smooth. This has a significant impact on the transport behaviour of particles, and can either enhance or impede the rate of mixing. The combination of smooth and discontinuous deformations is generic to a wide range of systems, including flows with extraction and reinjection of fluid, granular flows, and deformations of shear-banding materials. Here it is shown that discontinuous deformations can destroy impenetrable barriers to transport, allowing greater freedom for particle transport. In 3D systems they can create a novel mechanism for fully 3D transport that is similar in effect to Resonance Induced Dispersion.
Declaration

I hereby declare that this thesis contains no material which has been accepted for the award of any other degree or diploma at any university or equivalent institution and that, to the best of my knowledge and belief, this thesis contains no material previously published or written by another person, except where due reference is made in the text of the thesis.

This thesis includes one original paper published in peer reviewed journals. The core theme of the thesis is mixing and chaos in fluid flows. The ideas, development and writing up of all the papers in the thesis were the principal responsibility of myself, the candidate, working within the Department of Mechanical and Aerospace Engineering under the supervision of Prof. Murray Rudman.

The inclusion of co-authors reflects the fact that the work came from active collaboration between researchers and acknowledges input into team-based research.

In the case of Chapter 5, my contribution to the work involved the following:

<table>
<thead>
<tr>
<th>Thesis chapter</th>
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I have not renumbered sections of published papers.

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The undersigned hereby certify that the above declaration correctly reflects the nature and extent of the student and co-authors’ contributions to this work.

**Main supervisor signature:** [Signature]  **Date:** 19/04/2016
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*foosball
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Chapter 1

Introduction

Understanding the mechanisms that drive material transport is central to many physical processes and engineering applications. In fluid flows, mixing can be achieved by repeated stretching and folding, and this commonly occurs in turbulent flows (high Reynolds number $Re$), due to the temporal nature of the velocity field. However, mixing is not limited to turbulent flows as many believe, and can be achieved in laminar flows (low $Re$) that are carefully engineered. This creates the ability to mix rapidly and efficiently at low Reynolds numbers, which is vital to many applications where turbulence is not possible. For instance, when the length scales are very small, such as in the growing field of micro-fluidics, where the goal is to mimic laboratory experiments on a device the size of a microchip [NW05]. Other applications of laminar mixing are industrial mixers that are designed to mix highly viscous materials, where achieving sufficient velocity to induce turbulence would be inefficient compared to the mixing that can be achieved by a well designed laminar mixer [WO04]. Turbulence also might not be possible if the fluid carries fragile suspended particles, such as DNA, that would be damaged by the high stresses imposed by a turbulent velocity field [PHU13]. Finally, flows with long length scales but longer time scales, i.e. low velocity, are laminar, and include porous media flows with applications in groundwater flows [TLM+12]. In this case fluid mixing is required to promote the spread of reagents to treat contaminated aquifers, as well as enhancing heat extraction from groundwater used by geothermal power stations by homogenising the distribution of heat.

Transport of material can be categorised as either mixing or non-mixing, depending on whether the material, or some passive tracer such as concentration or heat, becomes homogenised over time. In a given system, it is possible that there will be both regions of mixing and non-mixing, and in applications it is important to know if mixing will occur, and its extent. In some applications rapid, efficient and uniform
mixing is desired, such as enhancement of heat extraction from groundwater. On the other hand, there are applications where trapping certain regions of fluid is desired, to keep them segregated from the rest of the domain. It is therefore useful to be able to determine the transport dynamics of a flow before it is implemented in applications. As an example, consider the stirring of two viscous fluids such as honey and melted chocolate using a spoon. The choice of stirring method will have a significant effect on how long it takes for the fluids to mix. Some stirring methods will have non-mixing regions, meaning the fluids will only mix at the rate of diffusion, and a homogenised mixture could take years to produce. However, a small change in the stirring protocol could be enough to remove these non-mixing regions and yield rapid mixing. Through the use of simulations and dynamical systems theory, it is possible to determine whether a given stirring protocol will yield efficient mixing prior to its implementation in applications, saving considerable time and money.

The aim of this study is to elucidate the competing particle transport mechanisms and their associated structures that yield different modes of particle transport in fluid flows, in particular volume-preserving potential flows, and flows with extraction and reinjection of fluid. This is achieved by using model 2D and 3D fluid flows as case studies, whose Lagrangian transport topologies readily generalise to other systems. This thesis begins with a review of the relevant literature in Chapter 2, followed by a description of the 2D and 3D model flows studied in Chapter 3, the 2D and 3D Reoriented Potential Mixing (RPM) flows. Then the computational and analytical methods used are presented in Chapter 4. At this point the main results sections begin, first, the impact of discontinuous deformation on fluid transport and mixing in 2D systems is discussed in Chapter 5. It is shown that discontinuous deformations are generic to extraction-reinjection systems, and this significantly changes the possibilities for particle transport. Next, the transport topologies that occur in the 3DRPM flow are considered in Chapter 6 using bifurcation analysis of periodic-point structures. This is followed by a study of the mechanisms that drive the transition from 1D to 3D particle transport in the 3DRPM flow in Chapter 7, where it is shown that the discontinuous deformations produced by fluid extraction and reinjection produce a novel mechanism for 3D particle transport. Finally, the key conclusions of this thesis and future research directions are discussed in Chapter 8.
Chapter 2

Literature Review

Dynamical systems theory is the natural language of particle transport and mixing in fluid flows. Since its application to fluid flows over three decades ago, the signatures of chaotic particle transport have been found in biological flows [LNHG01], geo- and astro-physical flows [NS99, Wig05], and industrial and microfluidic flows [WO04, NW05]. This approach, termed chaotic advection, has uncovered the fundamental mechanisms which control fluid mixing and transport in natural and engineered systems, and its popularity has grown significantly over the last 30 years, as shown by the growth in yearly publication and citation figures (Fig. 2.1).

Fluid flows through porous media have widespread applications in engineering and science, ranging from biological tissue engineering and biofilms [Vaf11] to contaminant removal in groundwater [MBHS86]. Darcy’s Law governs flow through porous media, with a velocity field given by

\[ \mathbf{v} = -\frac{K}{\mu} \nabla P(\mathbf{x}) \]  

(2.1)

where \( K \) is the permeability of the porous media, \( \mu \) is the fluid viscosity and \( \nabla P \) is the pressure gradient. The corresponding advection equation

\[ \frac{dx}{dt} = \mathbf{v}(\mathbf{x}, t) \]  

(2.2)

describes the motion of passive fluid particles in the flow. Eq. (2.1) can be treated as a dynamical system, however this approach has not been widely adopted in engineering literature. Conversely, porous media flows are rarely studied in dynamical systems literature, and most studies only consider 2D flows which do not accurately represent physically interesting systems.

Following a brief introduction to the relevant background material in §2.1, the literature related to chaotic advection and groundwater flows is discussed. Individual studies can be classified according to the dimensionality of the fluid flow studied,
either 2D or 3D, and the methodology employed, either analytical or experimental. These categories will be reviewed extensively in §2.2 and §2.3. It will be shown that 2D incompressible flows are well understood due to their correspondence to Hamiltonian systems, and there is therefore a wealth of theory and numerical techniques that can be used to understand the transport of fluid particles within them. On the other hand, there is a lack of theory and a lack of knowledge in the mechanisms for 3D transport of fluid particles in 3D incompressible flows, which are more physically relevant.

Following the discussion of 2D and 3D systems, studies that consider particle transport in the presence of discontinuous deformations will be reviewed in §2.5, because discontinuous deformations are generic to systems with extraction and reinjection of fluid, such as the model flows considered in this study. Then the idea of ‘twist’ and ‘twistless tori’ is introduced in §2.6, in particular the non-standard bifurcations that can result from there presence, which occur in the model flows studied here. Finally, the relevant theory of volume-preserving flows and maps is discussed and a method for creating explicitly volume-preserving numerical integration schemes is introduced in §2.7. This method is later adapted to the 3D model fluid flow considered in this study.
2.1 Background

In 1984, Aref coined the term ‘chaotic advection’ describing the phenomenon of deterministic chaos in Lagrangian particle transport [Are84]. While others had already noticed this phenomenon of mixing through a process of stretching and folding [Eck48, Wel55, BBTV79], Aref’s study sparked interest in the fluid mechanics community. A flow is said to exhibit chaotic advection if pairs of nearby fluid particles diverge exponentially in time, and the study of chaotic advection has led to fundamental changes in the way mixing is viewed [Are02]. Chaotic advection can be present in both laminar and turbulent flows, but it is most clearly illustrated in laminar flows where the flow is simple from an Eulerian viewpoint. Before Aref’s study, it was widely believed that the stretching and folding that leads to the filamental structures such as in Figure 2.2 could only be generated by turbulent flows, but Aref showed that this can be caused by simple laminar flows which are completely deterministic.

In all fluid flows, the motion of a fluid particle is described by the advection
2.1. BACKGROUND

Equation (2.2) where $v$ is the velocity of the particle. The trajectory of a particle initially located at $x_0$ is given by the solution of (2.2) combined with the initial condition $x(0) = x_0$, and the position of the particle after time $t$ can be written as $x(t) = \Phi_t(x_0)$. In the context of dynamical systems, this map $\Phi_t : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is known as the ‘flow’ associated with the system (2.2); it is a diffeomorphism (differentiable with differentiable inverse). In this study the focus is on fluid flows that are incompressible, i.e. $\nabla \cdot v = 0$, and in this case the map $\Phi_t$ is volume-preserving by Liouville’s Theorem (see §2.7 for a proof).

One of the keys in the development of chaotic advection theory was to view the advection equation (2.2) as a dynamical system, for which there is a vast amount of theory [KH96, Ott02]. In this context, an important result for chaotic advection and mixing is the Poincaré–Bendixson Theorem, stating that at least three degrees of freedom are necessary for the advection equation (2.2) to be non-integrable and allow chaotic particle trajectories. This criterion can only be met for 2D flows when the velocity field is time-dependent, for instance Aref’s blinking vortex flow [Are84] (Fig. 2.2), and any higher dimensional system can exhibit chaotic advection providing particles have sufficient freedom.

The fundamental concepts and theory describing the link between dynamical systems and chaotic advection in fluid flows can be found in the books by Ottino [Ott89] and Wiggins [Wig03]. Both books emphasise the importance of periodic points in governing the overall behaviour of a system. For a time-periodic fluid flow with period $T$, a point $x$ is periodic if a particle initially located at that point will return to its starting position after some number of flow periods, i.e. $\Phi_{nT}(x) = x$. On the other hand, for a discrete map $\Lambda : \mathbb{R}^d \rightarrow \mathbb{R}^d$, a periodic point satisfies $\Lambda^N(x) = x$ for some number of iterations $N$. There is thus a correspondence between periodic points with period $nT$ in a continuous fluid flow and period-1 points of the map $\Phi_{nT}$. These periodic points can be classified according to the stability of the orbits of nearby points. If all points in the vicinity of the periodic point remain close to the periodic point, then the point is called elliptic, otherwise the point is called hyperbolic. Elliptic points are surrounded by toroidal orbits that form impenetrable barriers to mixing, whereas hyperbolic points are necessary for chaos. The full impact of periodic points will be discussed in more detail in §4.3.

\*Note that this is different to the use of the term ‘flow’ used in fluid mechanics literature, which means the system as a whole. In general ‘fluid flow’ or ‘flow’ will be used here in the fluid mechanics sense to describe the system as a whole, and refer to the map $\Phi_t$ when discussing the dynamical systems flow.
2.2 Transport in 2D area-preserving fluid flows

Studies on 2D fluid flows have formed the bulk of the literature on chaotic advection and mixing. They can be divided into studies that use numerical and analytical methods, and those that use experimental methods.

2.2.1 Analytical and numerical techniques

Aref’s article [Are84] showed that the 2D blinking vortex flow exhibits chaotic advection for certain values of the system parameters, making use of the connection between 2D incompressible flows and Hamiltonian dynamical systems as a means to predict and describe chaotic fluid flow. This approach has since been exploited in a large number of studies on chaos and mixing in 2D flows ([CCTT87, RKLW90, LMT+09, LRM+10, TLM+12, MLTO07, BAS00, Fin01, TF06, CS09, Thi10, Ber78, BM77, CSFS06, JA88]). Formally, the 2D advection equation can be written as

\[
\frac{dx}{dt} = \frac{\partial \psi}{\partial y}, \quad \frac{dy}{dt} = -\frac{\partial \psi}{\partial x} \tag{2.3}
\]

where \( \psi \) is the stream-function of the flow. The equation (2.3) also describes the system as a one degree of freedom Hamiltonian system*, with Hamiltonian \( \psi \). Such Hamiltonian systems have been studied in detail, and the well-developed theory can be directly applied to 2D incompressible fluid flows. Therefore, almost everything is known about chaotic advection in 2D systems.

One of the key theoretical results is the Kolmogorov–Arnold–Moser (KAM) Theorem [Ber78] that describes the resonant breakup of tori surrounding an elliptic periodic point under perturbation. The tori that are ‘most rational’ i.e. whose winding number is of the form \( m/n \) and \( n \) is small are the first to breakup. This breakup is governed by the Poincaré–Birkhoff Fixed Point Theorem [Ott89]. Before the breakup every point on the torus with winding number \( m/n \) is a period-\( n \) point, but after the breakup only an even number \( 2kn \) will remain, and they will alternate between elliptic and hyperbolic type. These new elliptic points are also surrounded by tori that are also subject to the KAM and Poincaré–Birkhoff theorems, leading to self-similar fractal structures. Analysis of periodic points creates a kinematic template for a fluid flow, and has become a standard tool for analysing 2D systems [CCTT87, RKLW90, LMT+09, LRM+10, TLM+12, MLTO07].

*Note that a \( d \)-degree of freedom Hamiltonian system is represented by \( d \) position coordinates \( p_1, \ldots, p_d \) and \( d \) momentum coordinates \( q_1, \ldots, q_d \) meaning that it represents a \( 2d \)-dimensional system.
For applications where mixing is desirable, the presence of hyperbolic points is necessary for chaos. It is therefore desirable to find values of the system parameters such that particle transport is dominated by hyperbolic points and where non-mixing regions surrounding elliptic points are negligible. On the other hand, it may be desirable to isolate regions of space that don’t mix, for example to trap contaminants in groundwater. Such systems would require the existence of an elliptic point in the trapping region, and sufficiently large KAM tori enclosing the region.

Another common analytical method is the use of stroboscopic maps to create Poincaré sections, providing a qualitative measure of chaos. In a time periodic flow a snapshot of particle positions after each period of the flow is taken. From a few initial particles, a picture is built up by combining a large number of these snapshots, this is known as a Poincaré section, as it sections the flow in the time dimension. Poincaré sections have become a standard qualitative tool for detecting chaotic and non-mixing regions for both 2D and 3D flows, and can be seen in almost all studies on chaotic advection and mixing.

Another standard technique in the analysis of chaotic advection is the computation of Lyapunov exponents, which quantify the rate of stretching of material lines. In a chaotic region material lines are stretched exponentially in time, the exponent of the rate of stretching is the Lyapunov exponent [Ott89, Wig03]. A greater Lyapunov exponent results in more rapid stretching of fluid elements and thus faster mixing. It is common for studies to use Poincaré sections as a qualitative means of detecting chaos and then to compute the corresponding Lyapunov exponent to quantify the rate of stretching and mixing.

While there are few gaps in the knowledge of 2D flows with chaotic advection, the theory and tools developed have provided a starting point for 3D studies.

### 2.2.2 The 2DRPM flow

As previously discussed, porous media flows have many applications, including contaminant extraction from groundwater. In Metcalfe et al. [MLTO07] it is shown that Darcy’s Law (2.1) is satisfied by potential flows, and hence potential flows such as the 2D dipole flow are representative of homogeneous porous media flows.

The 2D steady dipole flow does not have the three degrees of freedom necessary for chaos. Therefore, Metcalfe et al. added time-dependency to the system by periodically reorienting the dipole, creating the possibility of chaotic advection. This system became known as the ‘Reoriented Potential Mixing’ (RPM) flow. The 2D RPM flow has been subject to further study [LMT+09, LRM+10, TLM+12], with a common emphasis on finding and classifying the periodic points so as to classify the
transport properties of the system. Lester et al. [LMT+09] showed that an optimal choice of system parameters exists to achieve the most efficient mixing, whereas Trefry et al. [TLM+12] focused on both mixing and isolating regions in the presence of a cross-flow. In [TLM+12] it is conjectured that the 3D analogue of the RPM flow, extending the domain to the unit sphere, would behave in a similar manner to its 2D counterpart, with the existence of optimal system parameters for mixing as well as isolated non-mixing regions. This 3D analogue is the model 3D flow that is studied here.

2.3 Transport in 3D volume-preserving fluid flows

Even though almost everything is known about transport and chaos in 2D flows, there is still a vast gap in the understanding of particle transport in 3D fluid flows, which are more relevant to physical systems. In particular, the possible mechanisms for 3D particle transport are not well understood. Here 3D transport does not simply refer to particles being contained in a 3D domain, but rather that particles are free to move throughout a 3D volume. In some cases particles are not free to move three-dimensionally, when they are trapped to 1D curves or 2D surfaces, and in these cases transport is described as 1D and 2D respectively.

In 2010, Wiggins [Wig10] highlighted the need for further study on 3D systems. He pointed out that while a large number of studies had considered 2D incompressible flows, little work had been done in three dimensions, and most of the 3D studies that existed considered a spatially periodic flow that could be reduced to the 2D time-periodic case. This is evident in the number of publications (grey bars in Fig. 2.1) and citations (black line) on chaotic advection with the terms ‘three-dimensional’ or ‘3D’ in their title, making up less than 6% of the total publications (47 out of 828)∗. Wiggins posed the natural question: “how does the dynamical systems approach generalize to three dimensions?” In some cases the theory carries over, for instance the homoclinic theorem is valid for any number of dimensions [Ott89], and so the presence of homoclinic/heteroclinic connections is still a necessary and sufficient condition for local chaos. However, the connection between Hamiltonian systems and 2D incompressible flows that formed the basis for many of the results in two dimensions breaks down at stagnation points of 3D flows [Baj94] because Hamiltonian systems must have an even number of dimensions. As a re-

∗There will be studies on 3D systems that do not include these terms in their title, so the actual number will be greater. However, due to their rarity and general interest, studies on 3D systems typically make a note of this in their title, so this number should be relatively accurate
2.3. TRANSPORT IN 3D VOLUME-PRESERVING FLUID FLOWS

As a result, the understanding of 3D systems is much less than for two dimensions. For instance, the KAM Theorem which provides a description of the flow topology near an elliptic periodic point cannot be directly applied to 3D systems. Cheng et al. [CS90] proved a 3D analogue of the KAM Theorem, though with the loss of the Hamiltonian analogy additional conditions are required for the theory to be valid.

In addition to lack of theory, there is an increase in the topological complexity of 3D systems, for instance periodic points need not be isolated, and can instead form periodic lines∗. Furthermore, the points on the periodic line may not all be elliptic or hyperbolic, but can be a mixture of the two. The critical points where the stability changes from elliptic to hyperbolic have been linked to interesting transport phenomena [SCvH04], and will be discussed later.

As previously discussed, potential flows are useful in modelling flow through porous media, and many of these applications will be 3D systems. However, there have been few studies that have considered mixing in 3D potential flows. A key difference between potential flows and inviscid or Stokes flows is that potential flows are irrotational, meaning steady 3D potential flows can stretch but not fold fluid elements. Thus in steady 3D potential flows homoclinic/heteroclinic connections between stable and unstable manifolds, which are hallmarks of chaos, cannot form [Spo94].

With all these factors considered, it is clear that studies of the fundamental transport properties of 3D unsteady potential flows are needed.

2.3.1 Mechanisms for 3D transport

3D fluid flows are most interesting when the transport of fluid particles is truly 3D. Otherwise particles are confined to 1D curves or 2D surfaces, and there are either 2 or 1 coordinates (in an appropriately chosen coordinate system) that are unchanged by the flow. Ignoring one of the coordinates that is unchanged, what remains is a 2D area-preserving flow that can be treated as a one degree of freedom Hamiltonian system, which is well understood. Therefore, studies have focused on the mechanisms that generate 3D transport, often using perturbations away from a base state with 1D or 2D transport. The underlying mechanisms that drive 3D transport are in general not well understood. The mechanisms known as ‘resonance induced dispersion’ [CFP94, CFP99, VWG07, VWG08, VA12, Mei12] and ‘resonance induced merger’ [SCvH04, SCvH06a, SCvH06b, PSC10] have been discovered and studied, but it is likely that there are other mechanisms.

∗Note that the term periodic line is used in the literature to refer to curves as well.
Studies of Resonance Induced Dispersion (RID) show that in some systems under small perturbation there exist regions of space known as ‘resonances’ that allow particles to jump between the 1D streamlines of the unperturbed flow. Typically particles spend a long time on one of the 1D streamlines, and can be kicked to a new streamline after visiting the resonance. The transitions between the streamlines allow particles to undergo 3D transport, and potentially visit the entire domain, even though they spend the majority of their time travelling on 1D curves. Cartwright et al. [CFP94, CFP99] studied RID in the spherical Couette flow, and Vainchtein et al. [VWG07, VWG08, VA12] studied RID in a perturbed Stokes Taylor–Couette flow. In both systems it is possible to make a change of coordinates of the form $$(x,y,z) \leftrightarrow (I_1,I_2,\theta)$$ such that the advection equation (2.2) becomes

$$\frac{dI_1}{dt} = \epsilon v_1(I_1,I_2,\theta), \quad \frac{dI_2}{dt} = \epsilon v_2(I_1,I_2,\theta), \quad \frac{d\theta}{dt} = \omega(I_1,I_2) + \epsilon g(I_1,I_2,\theta)$$

(2.4)

with $\epsilon \ll 1$. The regions where $\omega(I_1,I_2)$ is $O(\epsilon)$ define the resonances. In regions away from the resonance the ‘action’ variables $I_1,I_2$ change slowly compared to the ‘angle’ variable $\theta$, and the particle trajectory lives close to a curve with constant $I_1,I_2$. In these situations the system can be averaged over the period of the fast variable $\theta$, and cast as a Hamiltonian system

$$\frac{dI_1}{dt} = \epsilon \frac{\partial \Phi}{\partial I_2}, \quad \frac{dI_2}{dt} = -\epsilon \frac{\partial \Phi}{\partial I_1},$$

(2.5)

where $\Phi$ is an adiabatic invariant, i.e. not exactly conserved, but approximately conserved. On the other hand, in regions close to a resonance this averaging is not valid, because the angle $\theta$ slows down and varies at the same rate as the two slow variables $I_1,I_2$. In these resonance regions particles are able to move to a new curve with constant $I_1,I_2$ before leaving the resonance, and as the particles repeatedly visit the resonances 3D chaos is created. Determining whether RID will occur and where the resonances are located is relatively simple if the system can be transformed into the coordinates $I_1,I_2,\theta$ satisfying (2.4). However, an analytic expression for this coordinate transformation is generally not possible in most scenarios, making detection of resonances and RID a difficult task.

The second mechanism for 3D transport, Resonance Induced Merger (RIM), has been uncovered in a series of papers studying the flow generated by sliding plates over the ends of a fluid filled cylinder [SCvH04, SCvH06a, SCvH06b, PSC10]. These studies show that in the non-inertial limit particles are confined to 2D spheroids, but at a critical value of the Reynolds number some of the spheroids merge, connected by localised tubes, allowing 3D transport. This mechanism is similar to RID in that they both occur at resonances where the angle coordinates slow to the same
rate as the action coordinate. More specifically, in the presence of inertia the closed orbits near an elliptic segment of a period-1 line coalesce and form concentric tubes. These tubes merge with the spherical adiabatic shells at resonances associated with critical points of the period-1 line where the stability of points changes from elliptic to hyperbolic, called parabolic or degenerate points. At sufficiently high Reynolds numbers the invariant spheroids become adiabatic invariants, i.e. particles loosely adhere to them, allowing slow 3D transport. However, the transverse transport through a merging tube is several orders of magnitude faster than the transverse transport on an adiabatic surface, meaning RIM significantly enhances 3D transport. A common feature of RID and RIM is that the fast 3D transport takes place only in small regions of the domain. So far RID and RIM are the only known mechanisms for 3D transport in low Reynolds number flows, and finding other mechanisms is central to understanding chaos in 3D flows.

In summary, the theory of 3D flows is lacking, due to the loss of the Hamiltonian analogy and the added geometric complexity of 3D systems. Mechanisms for 3D transport are the key to understanding routes to chaos in 3D systems. The mechanisms known as RID and RIM have been identified and studied but the classification of all possible mechanisms is far from complete. Furthermore, the study of fundamental transport properties of 3D potential flows has been neglected in the literature.

2.4 Experimental studies

There have been a number of important experimental studies conducted on chaotic advection in both quasi-2D [OLRS88, CRO86, CCTT86, LO89, MLO+10b, MLO+10a] and 3D [FKO98, FKMO00, SCvH04] fluid flows. These studies provide proof that the phenomena predicted by theoretical and numerical studies are realistic and demonstrable, and were the first illustration of the applicability of dynamical systems ideas to mixing. Many of these experimental studies relate to, or have lead to, the creation of industrial mixers for fluids where turbulence is not possible, e.g. high viscosity, small length scales, fragile suspended particles.

A common experimental technique is to insert a blob of fluorescent dye into the flow and track its position with time. Measuring the evolution of the interfacial area provides an estimate of the Lyapunov exponent. These dye trace experiments can be directly compared with the path of a grid of particles with the same initial location as the blob of dye, known as a dye trace simulation. Experimental studies have shown that even though simulations are normally highly idealised (e.g. physical
effects such as inertia and diffusion are neglected), the gross features of a system are often accurately represented by numerical approximation.

Of particular interest is the experimental study conducted by Metcalfe et al. [MLO+10a] creating a realisation of the 2D RPM flow. Dye traces were performed for several values of the system parameters, and compared with numerical and theoretical results. It was found that the experimental results agreed well with the numerical and theoretical results, which proved the viability of the flow as a batch mixer, and validated the existing numerical findings [MLTO07, LMT+09] as well as results in subsequent papers [TLM+12, LRM+10].

2.5 Transport in the presence of discontinuous deformations

The studies discussed so far have only been concerned with particle transport when the deformation of fluid is smooth. In these cases stretching and folding of fluid is the primary mechanism for mixing. However, there also exist systems, including the model fluid flows considered here, in which transport is governed by a combination of both smooth deformations and discontinuous ‘cutting and shuffling’ (CS) deformations. Examples include geological faults, avalanching in granular matter [OK00, MS96], and shear banding in colloidal suspensions, plastics, polymers and alloys [Olm08, LLLLC12]. In the discussion of particle transport and mixing in the presence of discontinuous deformations, studies can be grouped into those that consider CS-only systems, i.e. systems where the only deformations are cutting and rearranging of material, and those that consider systems with combined CS and SF, which are most relevant to this study.

2.5.1 CS-only systems

Most of the studies to date have considered CS-only systems. These have been collectively termed *piecewise isometries* [Goe03] as the deformation at every point that is not affected by the discontinuous deformation is an isometry, i.e. composed of a solid-body rotation and a translation (no stretching or contraction). These piecewise isometries have been linked to fields as diverse as digital filters [Ash97, Dav95], granular flows [COL10, CLO11, JLO+10, KCOL12, Stu12] and kicked harmonic oscillators [SHM01], and it is often found that transport structures have a pattern similar to Fig. 2.3 which arises from the so-called tangent map or outer billiards map [Hug12, Hug13].
In terms of mixing capabilities, the Lyapunov exponent is zero in all CS-only maps as there is no stretching or contraction of material. This means the exponential increase in particle separation that characterises chaos is not possible, and so-called ‘strong mixing’ [Stu12] cannot occur. However, through repeated cutting and shuffling, material can still be mixed, and CS-only systems are able to produce ‘weak mixing’, which is a stronger condition than simply being ergodic.

2.5.2 Combined CS and SF systems

While there have been several studies on CS-only systems, there have been few that have considered systems with transport driven by both CS and SF. Of particular interest is the study based on the Pulsed Source Sink (PSS) flow conducted by Jones and Aref [JA88], showing that periodic extraction from a sink and reinjection at a source can produce discontinuous deformations of fluid. While the presence of discontinuous deformations was noted, the full impact of discontinuous deformations on particle transport was not uncovered, with the primary focus being the structures created by smooth deformations that do not interact with the discontinuous deformations. Since [JA88] there have been numerous other studies on fluid flows based on the periodic extraction and reinjection of fluid [Col04, CSFS06, BGCR10, BO07, HSW07], and in each of these cases discontinu-
uous deformations will occur by essentially the same process as in the PSS flow. However, none of these studies make note of the discontinuous deformations that exist in the flows, and neglect the consequences of combined CS and SF.

There is therefore a need for study of the Lagrangian transport structures that can occur in systems that combine CS and SF transport mechanisms. This is addressed later in this study, where it is shown that the periodic reorientation of the dipole flow in the 2D RPM flow and its 3D analogue produces discontinuous deformations that have a significant impact on transport organisation.

2.6 Twist and twistless tori

The study of so-called non-monotonic twist maps began in 1984 with the study by Howard and Hohs [HH84] and has since been explored in numerous studies [BVOB+10, DDL00, DMS00, DI05, DM12, HH95, Mor00, Sim98, WAFM05] focusing on the non-standard bifurcation phenomena that can occur surrounding elliptic periodic points. These bifurcation phenomena will also be shown to occur in the model 2D and 3D fluid flows considered here, caused by the presence of ‘twistless tori’, and these bifurcations play a significant role in the overall organisation of particle transport.

Following the work of Dullin et al. [DMS00] the idea of twist around an elliptic fixed point is introduced. For area-preserving 2D maps (such as the Poincaré section of a 2D Hamiltonian flow) with an elliptic fixed point the Birkhoff normal form is

\[ J \mapsto J, \quad \theta \mapsto \theta + 2\pi \Omega(J). \]  

(2.6)

Here \( J \) is the action coordinate, and can be thought of as the radius of each KAM-torus surrounding the elliptic fixed point, or the parameter describing the one-parameter family of KAM-tori, and \( \theta \) is the angle coordinate, describing the position on each KAM-torus. The quantity \( \Omega(J) \) is the rotation number or winding number of each torus, and its derivative

\[ \tau(J) = \frac{d\Omega}{dJ} \]  

(2.7)

is called the twist. An assumption of the KAM theorem is that the rotation number \( \Omega(J) \) is a monotonic function of \( J \), i.e. either uniformly increasing (\( \tau(J) > 0 \)) or decreasing (\( \tau(J) < 0 \)). However, it is possible that there will be local maxima and minima of the rotation number \( \Omega(J) \), corresponding to tori with twist \( \tau = 0 \), called twistless tori. The KAM-theorem and its corollaries do not apply to twistless tori, allowing different bifurcation phenomena in their local vicinity than is normally expected, such as reconnection bifurcations, an example of which is shown in
Fig. 2.4. These bifurcations occur when the rotation number of the twistless torus approaches a rational number $m/n$ from above. Letting $J^*$ denote the action coordinate corresponding to the twistless torus, i.e. $\tau(J^*) = 0$, when $\Omega(J^*) = m/n + \epsilon$ as in Fig. 2.5(a) there are two tori with action coordinates $J^*-\delta_1$ and $J^*+\delta_2$ with rotation numbers equal to $m/n$ (assuming without loss of generality that $\Omega''(J) = \tau'(J) < 0$ as in Fig. 2.5). These tori will experience classical KAM break-up into chains of elliptic and hyperbolic periodic points with period $n$, as in Fig. 2.4(a). As the bifurcation parameter is increased, moving from (a) to (d) in Fig. 2.4, the rotation number of the twistless torus $\Omega(J^*)$ approaches $m/n$, resulting in the two chains of period-$n$ points converging towards the twistless torus. When they meet the chains braid together as in Fig. 2.4(b) before annihilating each other in a series of saddle–centre bifurcations (Fig. 2.4(c,d)).

The prototypical example frequently used for the study of twistless tori and their impacts on transport is the Standard Non-twist Map (SNM) [SJCL+09], given by

$$
\begin{align*}
x_{n+1} &= x_n + f(y_{n+1}) \mod 1 \\
y_{n+1} &= y_n - b \sin(2\pi x_n),
\end{align*}
$$

(2.8)
where \( f(y) = a(1 - y^2) \) is the twist function. Since \( f(y) \) is non-monotonic a twistless torus occurs where \( f'(y) = 0 \), i.e. \( y = 0 \). The rotation number of the twistless torus \( \Omega \) is determined by the parameters \( a \) and \( b \), producing reconnection bifurcations that occur along the meander seen in Fig. 2.6(a,b), which forms a barrier to transport that separates the domain. For fixed \( b \) the parameter \( a \) acts as a perturbation parameter leading to the breakup of the meanders and chaotic transport. This is clearly seen in Fig. 2.6(c) where the last surviving meander (shown in black) forms a barrier between the blue and red initial conditions. However, even once the last meander has broken up, as in Fig. 2.6(d), Szezech et al. [SJCL+09] observe that the transmissivity across the last remaining meander is non-monotonically dependent on the parameter \( a \). For instance in Fig. 2.6(d) the transmissivity is very small, which is said to be caused by the ‘sticky’ cantori regions associated with chains of elliptic points that occur along the last meander. Therefore, the remnants of the last remaining meander can still act as an inhibitor to transverse transport even once it has been broken by the perturbation.
2.6. Twist and Twistless Tori

Figure 2.6: (a,b) Poincaré sections for the SNM (2.8) for $b = 0.6$ and (a) $a = 0.364$ (b) $a = 0.354$. (c,d) Phase portraits for the SNM for $b = 0.6$ and (c) $a = 0.8000$ (d) $a = 0.8063$. The red (blue) points represent orbits whose initial conditions were chosen above (below) the last meander, shown as the black line in (c). Reproduced with permission from J. D. Szezech Jr, I. L. Caldas, S. R. Lopes, R. L. Viana, and P. J. Morrison. Transport properties in nontwist area-preserving maps. Chaos, 19(4):043108, 2009 [SJCL+09], Copyright 2009 AIP Publishing LLC.

2.6.1 Twist in 3D Volume-Preserving Maps

For 3D systems, twist has been considered by Dullin and Meiss [DM12] for 1-action maps, i.e. those of the form

\[
\begin{align*}
I' &= I + \epsilon f(I, \theta_1, \theta_2), \\
\theta_1' &= \theta_1 + \Omega_1(I) + \epsilon g_1(I, \theta_1, \theta_2) \mod 1, \\
\theta_2' &= \theta_2 + \Omega_2(I) + \epsilon g_2(I, \theta_1, \theta_2) \mod 1,
\end{align*}
\]

where $I$ is the ‘slow’ action variable and $\theta_1, \theta_2$ are the ‘fast’ angle variables. In 1-action systems with no perturbation, i.e. $\epsilon = 0$, particles are trapped on the isosurfaces of the action variable $I$, which are 2-tori. If $\Omega_1(I), \Omega_2(I)$ are both irrational, then each particle orbit will densely cover the torus. On the other hand, if one of $\Omega_1(I), \Omega_2(I)$ is rational, then each particle orbit will densely fill a closed curve on the 2-torus, and if they are both rational, then each orbit on the 2-torus is periodic, and
returns to its initial position after some number of iterations (the lowest common
denominator of $\Omega_1$ and $\Omega_2$). These cases when one or both of $\Omega_1(I), \Omega_2(I)$
are rational are called resonances, where one or both of the angle variables slow to
the same rate as the action variable, and the tori in their vicinity are the first to be
destroyed when the perturbation $\epsilon$ is added [Mei12]. These resonances occur where
the image of the frequency map
\[
I \mapsto (\Omega_1(I), \Omega_2(I)), \tag{2.10}
\]
crosses the ‘resonance web’, as in Fig. 2 in [DM12], and result in different behaviour
depending on whether the resonance crossing is transverse or tangent. When the
resonance crossing is tangent, and only one of the angle variables is resonant, then
it is possible to average over the fast angle variable, reducing the system to a 2D
Hamiltonian system. For this 2D system, the resonant torus is a twistless torus,
that can produce reconnection bifurcations in 3D, as shown in Fig. 2.7.

For 1-action maps twist can be defined as the derivative of the frequency map
eq (2.10) with respect to the action variable $I$. On the other hand, for 2-action
maps, with 2 slow action variables and 1 fast angle variable, twist is more difficult
to define as there are an infinite number of directional derivatives that could be
used. This will be discussed in more detail in §6, where period-tripling bifurcations
that generically produce twistless tori in 2D systems are observed in a 3D model
fluid flow, and produce a twistless tube in a 2-action region.
2.7 Volume-preserving maps, flows and integration

Central to all the discussion in this chapter is the concept of a volume-preserving flow map, i.e. a map of the form $\Pi : X \subset \mathbb{R}^d \rightarrow \mathbb{R}^d$ such that $\text{vol}(\Pi(S)) = \text{vol}(S)$ for any set $S \subset X$. The theory of volume-preserving maps has been developed for centuries, and in this section the key results applicable to this study are detailed. In particular, Liouville’s Theorem shows that the solutions of incompressible fluid flows are volume-preserving maps. However, when considering complex flow topologies (or even some seemingly simple ones) it is not always possible to find analytic expressions for their solution, and numerical integration schemes are required to find approximate solutions. Integration schemes that do not explicitly preserve volume can introduce artificial attractors to conservative systems, significantly changing the behaviour of particle transport. Therefore, it is desirable to use explicitly volume-preserving numerical integration schemes, which have been developed using the theory of volume-preserving maps and symplectic maps.

Now considering general volume-preserving maps, the following lemma provides an equivalent condition for a map to be volume-preserving.

**Lemma 1.** A map $\Pi : X \subset \mathbb{R}^d \rightarrow \mathbb{R}^d$ is volume-preserving if and only if $|\det M| = 1$, where $M$ is the Jacobian of $\Pi$, i.e. $M = (\partial \Pi_i / \partial x_j) = d\Pi/dX$.

**Proof.** This follows immediately from the change of variables theorem which asserts that for a suitable domain $V \subset \mathbb{R}^d$,

$$\text{vol}(V) = \int_V d\mathbf{x}, \quad \text{and} \quad \text{vol}(\Pi(V)) = \int_V |\det M|d\mathbf{x}. \quad (2.11)$$

Now, considering the advection equation (2.2) as a dynamical system in Cartesian coordinates. For each initial condition $\mathbf{X}$ the solution to (2.2) is a map $\Phi_t(\mathbf{X})$, satisfying $\Phi_0(\mathbf{X}) = \mathbf{X}$ and $d\Phi_t(\mathbf{X})/dt = \mathbf{v}(\Phi_t(\mathbf{X}), t)$.

**Lemma 2.** If $\mathbf{v}$ is incompressible, i.e. $\nabla \cdot \mathbf{v} = 0$, then the Jacobian of the map $\Phi_t : X \rightarrow X \subset \mathbb{R}^d$ has determinant 1 for all values of $t$.

**Proof.** By definition, $\Phi_t$ satisfies

$$\frac{d\Phi_t(\mathbf{X})}{dt} = \mathbf{v}(\Phi_t(\mathbf{X})). \quad (2.12)$$

Therefore, the Jacobian of each side is

$$\frac{d}{d\mathbf{X}} \left( \frac{d\Phi_t(\mathbf{X})}{dt} \right) = \frac{d}{d\mathbf{X}} \left( \mathbf{v}(\Phi_t(\mathbf{X})) \right) = \frac{d\mathbf{v}(\Phi_t(\mathbf{X}))}{d\Phi_t(\mathbf{X})} \cdot \frac{d\Phi_t(\mathbf{X})}{d\mathbf{X}}. \quad (2.13)$$
Reversing the order of differentiation in the first term and writing \( M_t = d\Phi_t(X)/dX \), the Jacobian of \( \Phi_t \), yields

\[
\frac{d}{dt}M_t = \nu' (\Phi_t(X)) \cdot M_t. \tag{2.14}
\]

Assuming that \( M_t \) is invertible, each side is multiplied by \( M_t^{-1} \) on the right, and the trace is

\[
\text{Tr} \left( \frac{dM_t}{dt} \cdot M_t^{-1} \right) = \text{Tr} (\nu' (\Phi_t(X))) = \nabla \cdot \nu = 0. \tag{2.15}
\]

Jacobi’s formula for the derivative of a determinant gives

\[
0 = \text{Tr} \left( \frac{dM_t}{dt} \cdot M_t^{-1} \right) = \frac{d}{dt} \text{det} M_t \tag{2.16}
\]

and thus \( \text{det} M_t \) is a constant for all \( t \). Furthermore, \( M_0 = \Phi'_0(X) = I \) since \( \Phi_0(X) = X \), and it follows that \( \text{det} M = 1 \) for all \( t \).

From the previous two lemmata, Liouville’s Theorem follows immediately:

**Theorem 1. Liouville’s Theorem:** If \( \nu \) is incompressible then the corresponding map \( \Phi_t \) is a volume-preserving map.

Since all Hamiltonian flows are incompressible, it follows from Liouville’s Theorem that they are also volume-preserving. This provides a large class of volume-preserving flows. In the next section the concept of ‘symplectic’ maps is introduced, providing a stronger criterion than volume-preservation, and later it will be seen that the advection maps \( \Phi_t \) corresponding to Hamiltonian flows are also symplectic.

### 2.7.1 Symplectic maps

In order to provide the definition for a symplectic map, it is necessary to introduce some new notations. For Hamiltonian systems it is customary to denote a set of coordinates for \( \mathbb{R}^{2d} \) as \( \{q_1, \ldots, q_d, p_1, \ldots, p_d\} \). The \( q_i \) are thought of as position coordinates and the \( p_i \) as momentum coordinates. Let \( \xi = (\xi_{q_1}, \ldots, \xi_{q_d}, \xi_{p_1}, \ldots, \xi_{p_d}) \) and \( \eta = (\eta_{q_1}, \ldots, \eta_{q_d}, \eta_{p_1}, \ldots, \eta_{p_d}) \) be two vectors in \( \mathbb{R}^{2d} \). For each \( i = 1, \ldots, d \) the quantity \( \omega_i(\xi, \eta) \) is defined as

\[
\omega_i(\xi, \eta) = \xi_{q_i} \eta_{p_i} - \xi_{p_i} \eta_{q_i}. \tag{2.17}
\]

This is the same as the oriented area of the orthogonal projection of the parallelogram spanned by \( \xi \) and \( \eta \) in the \((q_i, p_i)\)-plane. Here oriented refers to the fact that \( \omega_i \) can be positive or negative according to the right hand rule. Now consider the bilinear form

\[
\omega(\xi, \eta) = \sum_{i=1}^{d} \omega_i(\xi, \eta), \tag{2.18}
\]
which can be written more simply as

$$\omega(\xi, \eta) = \xi^T \mathcal{J} \eta,$$

where $\mathcal{J} = \begin{pmatrix} I_d & 0 \\ 0 & -I_d \end{pmatrix}$,

(2.19)

where $I_d$ is the $d \times d$ identity matrix. With these definitions, a matrix $A$ is said to be \textit{symplectic} if it preserves the bilinear form $\omega$, i.e.,

$$\omega(A\xi, A\eta) = \omega(\xi, \eta)$$

(2.20)

for all vectors $\xi, \eta$. This condition can also be expressed as

$$\xi^T A^T \mathcal{J} A \eta = \xi^T \mathcal{J} \eta.$$  

(2.21)

Since this must be true for all vectors $\xi, \eta$, an equivalent condition for a matrix to be symplectic is that

$$A^T \mathcal{J} A = \mathcal{J}.$$  

(2.22)

In terms of maps $\Pi : \mathbb{R}^{2d} \rightarrow \mathbb{R}^{2d}$, they are said to by symplectic if their Jacobian matrix $(\partial \Pi_i / \partial x_j)$ is a symplectic matrix. The following theorem relates symplectic and volume-preserving maps:

\textbf{Theorem 2.} If a map $\Pi : \mathbb{R}^{2d} \rightarrow \mathbb{R}^{2d}$ is symplectic, then it is also volume-preserving\(^*\).

\textit{Proof.} By definition the Jacobian matrix $M = \Pi'$ satisfies

$$M^T \mathcal{J} M = \mathcal{J}.$$  

(2.23)

Computing the determinant of both sides yields

$$\det(M) \det(\mathcal{J}) \det(M) = \det(\mathcal{J}) = (-1)^d.$$  

(2.24)

It follows immediately that $|\det(M)| = 1$, and so from Lemma 1 $\Pi$ is a volume-preserving map. \hfill \Box

\(^*\)In 2D the converse is also true, i.e. if a map is volume-preserving then it is also symplectic, but the converse is not true in general.

Next, it is shown that Hamiltonian systems provide examples of symplectic maps.
2.7.2 Hamiltonian systems

Recall that a Hamiltonian system with \(d\)-degrees of freedom can be expressed as

\[
\frac{dq_i}{dt} = \frac{\partial H(q,p)}{\partial p_i}, \quad \text{and} \quad \frac{dp_i}{dt} = -\frac{\partial H(q,p)}{\partial q_i},
\]

where \(H : \mathbb{R}^{2d} \to \mathbb{R}\) is the Hamiltonian of the system. This can also be written as

\[
\frac{dx}{dt} = J\nabla H(x)
\]

where \(x = (q_1, \ldots, q_d, p_1, \ldots, p_d)\). As before, \(\Phi_t(X)\) is used to denote the solution of this system from the initial point \(X\), satisfying \(\Phi_0(X) = X\) and \(d\Phi_t(X)/dt = v(\Phi_t(X)) = J\nabla H(\Phi_t(X))\).

**Theorem 3.** For a Hamiltonian system with \(d\)-degrees of freedom, the map \(\Phi_t : \mathbb{R}^{2d} \to \mathbb{R}^{2d}\) is a symplectic map for all \(t\).

**Proof.** Let \(M\) denote the Jacobian of \(\Phi_t\). The aim is to show that \(M^TJM = J\).

First, since \(d\Phi_t(X)/dt = J\nabla H(\Phi_t(X))\), the Jacobian of each side is given by

\[
\frac{d}{d\bar{X}} \left( \frac{d\Phi_t(X)}{dt} \right) = \frac{d}{d\bar{X}} \left( J\nabla H(\Phi_t(X)) \right) = JH_{XX}(\Phi_t(X)) \frac{d\Phi_t(X)}{d\bar{X}}.
\]

Here \(H_{XX}\) denotes the symmetric Hessian matrix of second partial derivatives of \(H\), \(\left( \frac{\partial^2 H}{\partial X_i \partial X_j} \right)\). Reversing the order of differentiation for the first term yields

\[
\frac{dM}{dt} = JH_{XX}M.
\]

Consider the matrix \(R = M^TJM\). It will be shown that \(R = J\) by showing that its time derivative is zero and noting that \(R(0) = M^T(0)JM(0) = I^TJI = J\) as \(M(0) = d\Phi_0(X)/dX = I\). The time derivative of \(R\) is given by

\[
\frac{dR}{dt} = \frac{dM^T}{dt}JM + M^TJ\frac{dM}{dt}
\]

\[
= M^TH_{XX}^TJM + M^TJH_{XX}M
\]

\[
= M^T(H_{XX}M - H_{XX}M) = 0,
\]

where it has been recognised that \(J^TJ = I\) and \(J^2 = -I\). Thus \(R\) is a constant matrix identically equal to \(J\), and so

\[
M^TJM = J
\]

as required. \(\square\)

Therefore not only are all Hamiltonian systems volume-preserving, but they are also symplectic.
2.7.3 Volume-preserving integration schemes in Cartesian coordinates

To ensure that volume is strictly preserved when tracking particles in a conservative system it is necessary to use an explicitly volume-preserving integration scheme. These schemes prevent the introduction of artificial attractors to conservative systems.

2D flows

As previously discussed, in order for a numerical method to be volume-preserving its Jacobian must have determinant 1. As a non-example, consider the Euler scheme

\[ x' = x + hv(x, t) \]  

where \( x = x(t) \) and \( x' = x(t + h) \). The Jacobian is defined as \( J = (\partial x'_i / \partial x_j) \), and can also be written \( d\mathbf{x}'/d\mathbf{x} \). Therefore the Jacobian of the Euler method is

\[ J = I + hF \]  

where \( F \) is the matrix \((\partial v_i / \partial x_j)\). So in general \( \det J \) is not equal to 1, and the Euler method is not an explicitly volume-preserving method.

On the other hand, the Crank–Nicolson method,

\[ x' = x + hv \left( \frac{x + x'}{2}, t + \frac{h}{2} \right) \]  

has Jacobian

\[ J = I + (h/2)(F + FJ) \]  

Rearranging gives

\[ J = (I - hF/2)^{-1}(I + hF/2) \]  

and so

\[ \det J = \frac{1 + h \text{Tr}(F)/2 + h^2 \det(F)/4}{1 - h \text{Tr}(F)/2 + h^2 \det(F)/4} \]  

Since \( \mathbf{v} \) is incompressible, if follows that \( \text{Tr}(F) = \nabla \cdot \mathbf{v} = 0 \), which yields \( \det J = 1 \), showing that the Crank–Nicolson method is area preserving. Indeed, it can be shown that the Crank–Nicolson method is symplectic. This method is second order accurate in time, meaning the local error in \( x' \) is order \( h^3 \).

Both the Euler method and Crank–Nicolson methods are examples of Runge–Kutta methods, and it has been demonstrated that some but not all Runge–Kutta
methods are explicitly volume preserving. Considering a general \( s \)-stage Runge–Kutta method\(^*\)

\[
k_i = v \left( x + h \sum_{j=1}^{s} a_{ij} k_j, t + c_i h \right), \quad i = 1, \ldots, s,
\]

\[
x' = x + h \sum_{i=1}^{s} b_i k_i,
\]

with Butcher tableau

\[
\begin{array}{c|cc}
  c & A \\
  \hline
  b^T \\
\end{array}
\]

a sufficient condition for the method to be volume-preserving is found by considering

the \( s \times s \)-matrix \( \mathcal{M} = (m_{ij}) \) where

\[
m_{ij} = b_i a_{ij} + b_j a_{ji} - b_i b_j.
\]

**Theorem 4.** If the matrix \( \mathcal{M} = 0 \), then the corresponding Runge–Kutta method (2.37) is symplectic (and hence volume-preserving).

**Proof.** See [SS88]. \( \square \)

As a specific example, the class of Gauss–Legendre Runge–Kutta schemes are all symplectic. The Gauss-Legendre method of order two has Butcher tableau

\[
\begin{array}{c|cc}
  \frac{1}{2} & \frac{1}{2} \\
  \hline
  1 \\
\end{array}
\]

which can be seen to be the Crank–Nicolson method eq. (2.33). The fourth order method has Butcher tableau

\[
\begin{array}{c|ccc}
  \frac{1}{2} - \frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\
  \frac{1}{2} + \frac{\sqrt{3}}{6} & \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \\
  \frac{1}{2} & \frac{1}{2} \\
\end{array}
\]

and in general the Gauss–Legendre method based on \( s \) points has order \( 2s \).

Note that the requirement that \( \mathcal{M} = 0 \) dictates that any symplectic Runge–Kutta scheme must be implicit, adding computational expense to solve the implicit equations at each step numerically via Newton or Picard iterations.

Therefore, symplectic integration schemes such as the Gauss–Legendre Runge–Kutta methods are explicitly volume-preserving. However, these only apply to even dimensional systems. In the next section a method that produces volume-preserving integration in 3D flows is discussed. This method is used in this study to track particles in a 3D model flow, the details of which are contained in \( \S \) 4.1.2.

\(^*\)Note that the coefficients \( a_{ij} \) may be non-zero for \( j \geq i \), in these cases the method is implicit, and Picard or Newton iterations are required to obtain a numerical solution.
3D flows

Since 3D systems in general cannot be cast as Hamiltonian systems, applying the symplectic techniques described in the previous section will not produce volume-preserving numerical integration. For example, considering the Crank–Nicolson scheme in three-dimensions, using the same argument as before combined with the fact that $\text{Tr}(F) = 0$ for incompressible flows yields

$$\det J = \frac{1 + h^2 Q(F)/4 - h^3 \det(F)/8}{1 + h^2 Q(F)/4 + h^3 \det(F)/8} = 1 + O(h^3) \quad (2.42)$$

where $Q(F) = F_{11}F_{22} + F_{22}F_{33} + F_{11}F_{33} - F_{12}F_{21} - F_{23}F_{32} - F_{13}F_{31}$. So the Crank–Nicolson method is not volume-preserving in all dimensions.

Finn and Chacón [FC05] have introduced a method to overcome these obstacles and create explicitly volume-preserving schemes in 3D. Since the velocity $v$ is incompressible, it can be written as $v = \nabla \times A$ for some vector potential $A : \mathbb{R}^3 \to \mathbb{R}^3$. It follows that

$$\nabla \times A = \nabla \times (A_x \hat{e}_x + A_y \hat{e}_y + A_z \hat{e}_z) = \nabla A_x \times \hat{e}_x + \nabla A_y \times \hat{e}_y + \nabla A_z \times \hat{e}_z, \quad (2.43)$$

which provides a natural way to split the flow into three incompressible 2D flows

$$v_1 = \nabla A_x \times \hat{e}_x, \quad v_2 = \nabla A_y \times \hat{e}_y, \quad v_3 = \nabla A_z \times \hat{e}_z. \quad (2.44)$$

If $N_1(h)$ is a symplectic integration method for the flow $dx/dt = v_1$, then it follows that it is area preserving in the $yz$-plane and so it is explicitly volume-preserving. Therefore any method of the form $N = N_3(h) \circ N_2(h) \circ N_1(h)$ is an explicitly volume-preserving method for the overall system. The method can also be symmetrized to increase accuracy and maintain volume preservation as

$$N = N_1(h/2) \circ N_2(h/2) \circ N_3(h) \circ N_2(h/2) \circ N_1(h/2). \quad (2.45)$$

2.7.4 Volume-preserving integration schemes in curvilinear coordinates

Directly applying the method for Cartesian coordinates to curvilinear coordinates will fail as ‘rectangular’ regions in the curvilinear coordinates, i.e. regions of the form $a_i < \xi_i < b_i$, $i = 1, 2, 3$, do not have equal volume when the ‘rectangle’ is translated. This can be overcome by scaling by the Jacobian of the coordinate transformation, as shown by Finn and Chacón [FC05], and summarised here.

The method proceeds as follows:
Write \( \mathbf{v} \) in contravariant form as
\[
\mathbf{v} = v^1 \nabla \xi^2 \times \nabla \xi^3 + v^2 \nabla \xi^3 \times \nabla \xi^1 + v^3 \nabla \xi^1 \times \nabla \xi^2.
\] (2.46)

The \( v^i \) are given by \( v^i = \mathbf{J} \mathbf{v} \cdot \nabla \xi^i \) where \( \mathbf{J} \) is the Jacobian of the coordinate transformation\(^*\), \( \mathbf{J} = (\nabla \xi^1 \cdot \nabla \xi^2 \times \nabla \xi^3)^{-1} = |\det(\partial \xi^i/\partial x^j)| \).

The equations of motion then become
\[
\frac{d\xi^i}{dt} = \mathbf{v} \cdot \nabla \xi^i = \frac{v^i}{\mathbf{J}},
\] (2.47)

It follows that \( \nabla \cdot \mathbf{v} = (1/\mathbf{J}) \sum_i \partial v^i / \partial \xi^i \), and so if \( \mathbf{v} \) is incompressible then the formal divergence of \( \sum \partial v^i / \partial \xi^i \) is also zero.

Also, since \( \mathbf{v} = \nabla \times \mathbf{A} \) for some vector potential \( \mathbf{A} \), this can be written in covariant form
\[
\nabla \times \mathbf{A} = \nabla \times \left( \sum_i A_i \nabla \xi^i \right) = \sum_i \nabla A_i \times \nabla \xi^i,
\] (2.48)
and it follows that
\[
v^i = \mathbf{J} \mathbf{v} \cdot \nabla \xi^i = \mathbf{J} \left( \sum_i \nabla A_i \times \nabla \xi^i \cdot \nabla \xi^i \right) = \epsilon^{ijk} \frac{\partial A_k}{\partial \xi^j},
\] (2.49)
therefore \( \mathbf{v} \) in contravariant form is obtained as the formal curl of \( \mathbf{A} \).

Introducing the new independent variable \( \lambda \) such that \( dt/d\lambda = \mathbf{J} \), the equations of motion become \( d\xi^i / d\lambda = v^i \), and in rectangular \((\xi^1, \xi^2, \xi^3)\)-space, the divergence is zero and \( \mathbf{v}' = (v^1, v^2, v^3) \) is obtained as the curl of \( \mathbf{A} \). Applying the same argument as in the Cartesian case, volume-preserving integrators are produced in the rectangular \((\xi^1, \xi^2, \xi^3)\)-space.

**End result:** integrating the \( d\xi^i / d\lambda = v^i \), where \( dt/d\lambda = \mathbf{J} \), as if they are rectangular produces volume-preserving integration in curvilinear coordinates.

This is the approach used in the following analysis to ensure that volume is explicitly conserved in volume-preserving systems.

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*Here this refers to the scalar, not the matrix as before. The term is used interchangeably in the literature.*
Chapter 3

The 2D and 3D Reoriented Potential Mixing Flows

In this chapter the 2D and 3D Reoriented Potential Mixing (RPM) flows are described. These flows form the basis of this study, and consist of periodically reoriented dipole flows in 2D and 3D respectively. These particular flows have been chosen since they approximate flow in porous media, where the singularities at the dipole mimic valved wellbores used in groundwater applications.

3.1 The (2D)RPM flow

The 2DRPM flow is a 2D incompressible potential (Darcy) flow that has been studied both numerically [LMT+09, LRM+10, MLTO07] and experimentally [MLO+10b, MLO+10a] in the context of chaos and mixing in groundwater flow [TLM+12].

3.1.1 2D steady dipole flow

First the 2D steady dipole flow is described, which under periodic reorientation forms the 2DRPM flow. As described by Lester et al. in [LMT+09], the 2D dipole flow is an incompressible potential flow with potential function

\[ \phi(r) = \log \left( \frac{|r - y^+|}{|r - y^-|} \right) \]  

(3.1)

where \( y^{\pm} \) denote the poles at \((x, y) = (0, \pm 1)\). In polar coordinates \((r, \theta)\) this is

\[ \phi(r, \theta) = \frac{1}{2} \log \left( \frac{r^2 - 2r \sin \theta + 1}{r^2 + 2r \sin \theta + 1} \right). \]  

(3.2)
From this potential \( \phi \) the velocity field is found as \( \mathbf{v} = \nabla \phi \). Alternatively, the velocity field can be found using the streamfunction

\[
\psi(r, \theta) = \arctan \left( \frac{2r \cos \theta}{1 - r^2} \right)
\]

(3.3)
as \( \mathbf{v} = \nabla \times \psi \hat{e}_z \) where \( \hat{e}_z \) is the unit vector in the \( z \) direction. The contours of this streamfunction \( \psi \) (black) and potential \( \phi \) (dashed orange) are shown in Fig. 3.1. Particles follow streamlines given by the contours of the streamfunction, moving from the source (red) to the sink (blue). The potential, velocity and streamfunction provided here are valid for the unbounded domain \( \mathbb{R}^2 \), and the unbounded flow possesses a separating streamline coinciding with the unit circle. This study and the preceding studies on the 2DRPM flow primarily consider the flow restricted to the unit disk \( \mathcal{D} \), creating a bounded flow domain with a free-slip boundary condition. As the separating streamline is circular, when the dipole is reoriented the system domain is unchanged.

The 2D dipole flow can be considered as either a closed or open system depending on the conditions imposed at the poles. If fluid is allowed to escape the domain via the sink while new fluid is injected at the source then the system is open, whereas reinjecting fluid that reaches the sink back at the source results in a closed system. In terms of practical implementation, the open system is easier to implement and is the subject of the experimental studies \([\text{MLO}^{+10b}, \text{MLO}^{+10a}]\). However, allowing particles to escape the domain means the loss of information of Lagrangian transport structures that exist in the the regions that are extracted. This loss of information...
3.1. THE (2D)RPM FLOW

Figure 3.2: The RPM flow. (a) Streamfunction contours with the dipole (blue/red) in its original (black) and rotated (dashed grey) positions. (b) Source (red) and sink (blue) positions and a typical particle trajectory in the flow with $(\Theta, \tau) = (2\pi/3, 0.1)$, starting at the star.

...can be countered by imposing a reinjection protocol across the dipole. In this study all fluid extracted from the sink is instantaneously reinjected at the source along the same streamline. An advantage of this protocol is that it preserves Lagrangian structures during the extraction/reinjection process. Other protocols have been considered by Lester et al. [LMT+09], leading to different Lagrangian behaviours.

The advection map after time $t$ is denoted $\hat{\Upsilon}_t$, and satisfies

$$\frac{d}{dt} \hat{\Upsilon}_t(x) = v(\hat{\Upsilon}_t(x)), \quad \hat{\Upsilon}_0(x) = x$$

for all $x \in D$. Since the velocity field $v$ is incompressible, it follows from Theorem 1 in §2.7 that the map $\hat{\Upsilon}_t$ is area-preserving.

3.1.2 The time-dependent flow

The 2D dipole flow is an example of a steady 2D incompressible flow that is therefore integrable and cannot produce chaos. In order to create the streamline crossings necessary for chaos the dipole is reoriented periodically. The reorientation protocol used for the 2DRPM flow consists of rotation of the dipole through an angle $\Theta$ at the end of each flow period $\tau$. This switching period $\tau$ is non-dimensionalised by scaling such that $\tau = 1$ corresponds to the emptying time of the domain $\mathcal{D}$. The dipole positions and corresponding streamlines are shown in Fig. 3.2(a) for $\Theta = 2\pi/3$, and a typical particle trajectory for $\tau = 0.1$ is shown in Fig. 3.2(b).

The velocity field $\hat{v}$ for the time-periodic flow can be approximated by the piecewise-steady velocity

$$\hat{v}(x, t) = v \left( R_{\left\lfloor \frac{t}{\tau} \right\rfloor \Theta} x \right)$$

where $R_{\alpha}$ denotes rotation through the angle $\alpha$ and $\lfloor a \rfloor$ is the floor of $a$, i.e. the greatest integer less than $a$. If the viscous time scale $1/\kappa$ is small, where $\kappa$ is the fluid...
kinematic viscosity, then transient effects associated with dipole reorientations (as quantified by the Strouhal number $St = Re/\tau$) may be ignored. Since it is assumed that the Reynolds number is negligible, the piecewise-steady velocity approximation is exact (except in the limit as $\tau \to 0$) [LMT+09]. The limit of $\hat{v}$ as $\tau \to 0$ can still be considered from a mathematical standpoint, and forms a useful basis for studying the flow at small values of $\tau$ where the approximation is valid. With this approximation the two parameters $\tau$ and $\Theta$ completely characterise the system. Large expanses of the parameter space $\{(\tau, \Theta) : \tau > 0, -2\pi < \Theta \leq 2\pi\}$ have been studied previously. However, an exception is the small scale structures for very small values of $\tau$, corresponding to rapid switching of the dipole, which are considered in detail in Chapter 5.

Using the piecewise-steady approximation the flow can be broken down into steady dipole advection, and dipole reorientation steps. If particles are tracked in the dipole frame rather than the laboratory frame, then the flow consists of steady dipole advection and particle rotation phases, and can be written as

$$\Upsilon_{\tau}^{\Theta}(x) = R_{-\Theta} \tilde{\Upsilon}_{\tau}(x). \quad (3.6)$$

Studying the flow in this dipole frame via the map $\Upsilon_{\tau}^{\Theta}$ has the advantage that its period is $\tau$, whereas in the laboratory frame the flow period is equal to the number of reorientations required to return the dipole to its initial position, which is 3 for $\Theta = 2\pi/3$ and infinite if the rotation angle $\Theta$ is incommensurate with $2\pi$, i.e. $\Theta/\pi$ is irrational. For more discussion of the different frames of reference see Appendix A.

### 3.1.3 Symmetries

Flow symmetries play an important role in the overall organisation of transport structures. Symmetries of the time-periodic flow can be derived from underlying symmetries of the steady flow and the reorientation protocol.

The steady dipole flow possesses two basic symmetries: reflection symmetry about the $y$-axis and a reflection reversal symmetry about the $x$-axis. Algebraically these can be written respectively as

$$\tilde{\Upsilon}_{t} = S_y \tilde{\Upsilon}_{t} S_y^{-1}, \quad (3.7)$$
$$\tilde{\Upsilon}_{t} = S_x \tilde{\Upsilon}_{t}^{-1} S_x^{-1}, \quad (3.8)$$

where $S_y$ is reflection about the $y$-axis, and likewise for $S_x$. These symmetries yield two symmetries for the map $\Upsilon_{\tau}^{\Theta}$. First, as a result of eq. (3.7)

$$\Upsilon_{\tau}^{\Theta} = R_{-\Theta} \tilde{\Upsilon}_{\tau} = R_{-\Theta} S_y \tilde{\Upsilon}_{\tau} S_y = S_y R_{\Theta} \tilde{\Upsilon}_{\tau} S_y = S_y \Upsilon_{\tau}^{-\Theta} S_y \quad (3.9)$$
since $R_{-\Theta}S_y = S_yR_{\Theta}$. Therefore, changing $\Theta$ to $-\Theta$ results in a reflection through the $y$-axis, but does not alter transport dynamics. This symmetry can be generalised to any 2D periodically reoriented flow where the base flow has two symmetries [Met10].

The map $\Upsilon^\Theta_\tau$ also possesses a reflection reversal symmetry, inherited from the reflection reversal symmetry of the dipole flow eq. (3.8) as follows,

$$\Upsilon^\Theta_\tau = R_{-\Theta} \hat{T}_\tau = R_{-\Theta}S_x \hat{T}_\tau S_x$$

where $S_1 = R_{-\Theta}S_x$. Direct computation shows that $S_1$ is the map that reflects a point through the plane $y = \tan(-\Theta/2)x$. Therefore structures in the Lagrangian topology must also evolve symmetrically about this line. This has a significant impact on the overall organisation of transport structures, for example it constrains all chains of periodic points to be distributed symmetrically about the symmetry plane.

### 3.1.4 The limit as $\tau \to 0$

A key topic in this study is the variation in particle transport behaviour as $\tau$ is varied while $\Theta$ is kept fixed. It has been found that in the limit as $\tau \to 0$ the flow becomes steady [LMT+09], and this forms the basis for low $\tau$ transport behaviour. As $\tau$ approaches zero, the frequency of dipole switching approaches infinity, and the flow becomes steady (no dependence on $\tau$). This limiting flow is equivalent to having the dipoles in all reorientation positions operating simultaneously. Thus the streamfunction (and Hamiltonian) is given by the average of all the reoriented streamfunctions

$$\tilde{\psi}(x) = \begin{cases} \frac{1}{n} \sum_{j=0}^{n-1} \psi(R_{n\Theta}x) & \text{for } \Theta = \frac{2\pi m}{n}, \\ \frac{1}{2\pi} \int_{-\pi}^{\pi} \psi(R_{\alpha}x) d\alpha & \text{for } \Theta/\pi \text{ irrational.} \end{cases}$$

As a result of the reflection reversal symmetry (3.10) $\psi(x) = -\psi(R_\pi x)$ and the streamfunction $\tilde{\psi}$ is identically zero in all cases except when $\Theta = 2\pi m/n$ and $n$ is odd. Intuitively, this is because when $n$ is even or $\Theta/\pi$ is irrational for every orientation of the dipole, a corresponding dipole with the opposite orientation also exists, and the average is zero. On the other hand, when $n$ is odd there is no cancellation of dipoles, yielding a net flow. In each case the velocity field $\bm{v}_0$ is given by $\bm{v}_0 = \nabla \times \tilde{\psi} \hat{e}_z$, and again is only non-zero when $\Theta = 2\pi m/n$ and $n$ is odd.

As an example of an odd $n$ case, Fig. 3.3 shows the contours of $\tilde{\psi}$ for $\Theta = 2\pi/3$, which will be used extensively in later investigation. While this asymptotic
flow possesses $2n = 6$ symmetry lines, for non-zero $\tau$ only the symmetry line $y = \tan(-\Theta/2)x$ is preserved, shown in dashed orange. Note that due to reinjection of fluid across the dipoles each streamline forms a closed curve that is broken into three segments, contained in either the grey or white region. Two of these are highlighted in dashed green and dashed purple, which are the two streamlines with the minimum return time $t_{ret}(\tilde{\psi})$, i.e. the time it takes a particle to return to its initial position. To uncover the importance of these streamlines, the averaged streamfunction $\tilde{\psi}$ is used together with the distance $\theta$ along each streamline starting from the intersection point between the streamline and the symmetry plane (shown in dashed orange) as a 1-action coordinate system that describes the flow. In this coordinate system the velocity field is

$$\frac{d\tilde{\psi}}{dt} = 0, \quad \frac{d\theta}{dt} = \Omega(\tilde{\psi}, \theta), \quad (3.12)$$

for some function $\Omega$. The coordinate $\theta$ can be suitably rescaled such that its range is $[0, 1)$ and $\Omega(\tilde{\psi}, \theta)$ does not depend on $\theta$. Thus the advection of a particle for a time $t$ is described by

$$\tilde{\psi}' = \tilde{\psi},$$
$$\theta' = \theta + t \Omega(\tilde{\psi}) \mod 1 \quad (3.13)$$

where $1/\Omega(\tilde{\psi})$ is equal to the return time of the streamline $t_{ret}(\tilde{\psi})$. From eq. (2.7) the twist of this 1-action map is given by

$$\tau(\tilde{\psi}) = \frac{d}{d\tilde{\psi}} t \Omega(\tilde{\psi}) = \frac{d\Omega}{d\tilde{\psi}}. \quad (3.14)$$

Therefore the twist is zero when $\Omega(\tilde{\psi})$, or equivalently the return time $t_{ret} = 1/\Omega(\tilde{\psi})$, reaches a local maximum or minimum. This occurs on the green and purple dashed streamlines of Fig. 3.3, and causes a series of reconnection bifurcations for small but non-zero values of the reorientation period $\tau$, as will be shown in Chapter 5.

### 3.2 The 3DRPM flow

As a model for transport and mixing in 3D fluid flows a periodically reoriented 3D dipole flow is considered, forming the 3D Reoriented Potential Mixing (3DRPM) flow. It is a natural three-dimensional extension of the 2DRPM flow, and many of the results in the previous section have a direct analogue for the 3D flow. Like the 2DRPM flow it is an incompressible potential flow, meaning it approximates fluid transport in homogeneous porous media, while having the obvious advantage over the 2D flow that it is more physically relevant.
3.2. THE 3DRPM FLOW

Figure 3.3: Streamlines of the 2DRPM flow in the limit as $\tau \to 0$ for $\Theta = 2\pi/3$.

With reinjection at each dipole pair, the streamlines form closed curves connected at the dipoles, each of which is contained in either the grey or white region. The two streamlines with the minimum return time are shown in dashed green and dashed purple, and the symmetry line $y = \tan(-\Theta/2)x$ is shown in dashed orange.

3.2.1 Steady dipole flow

Like the 2DRPM flow, a steady dipole flow forms the basis for the time-dependent re-oriented flow. It is driven by a source/sink pair located at $z^\pm = (0, 0, \pm 1)$ (Fig. 3.4). While this dipole flow in two-dimensions possesses a separating streamline coinciding with the unit circle, the free-space 3D dipole flow does not have a stream-surface coinciding with the unit sphere. To ensure that the flow domain is bounded and invariant under dipole rotation, the flow needs to be confined to the unit sphere $S$, and a free-slip boundary condition is used. This flow is axisymmetric about the $z$-axis, admitting an axisymmetric Stokes streamfunction $\Psi$, such that $\boldsymbol{v} = \nabla \times (\Psi/\rho)\hat{e}_\theta$ where $(\rho, \theta, z)$ denote cylindrical coordinates.

Combining incompressibility with the boundary conditions yields the equations governing the flow potential $\Phi$, where $\boldsymbol{v} = \nabla \Phi$,

$$\nabla^2 \Phi = 0, \quad \text{and} \quad \mathbf{n} \cdot \nabla \Phi \big|_{\partial S} = \delta(z - 1) - \delta(z + 1), \quad (3.15)$$

where $\mathbf{n}$ is the outward normal to the boundary $\partial S$ and $\delta$ is the Dirac delta function.

These equations are solved using the method of images [DS12] to find an analytic expression for the flow potential $\Phi$ in cylindrical polar coordinates $(\rho, \theta, z)$

$$\Phi(\rho, \theta, z) = \frac{1}{4\pi} \left( \frac{2}{d^-} - \frac{2}{d^+} + \log \left( \frac{d^+ - z + 1}{d^- + z + 1} \right) \right), \quad (3.16)$$
where \( d^± = \sqrt{\rho^2 + (z ± 1)^2} \) are the distances from the poles \( z^± \). From this potential, expressions can be found for the velocity field \( \mathbf{v} = \nabla \Phi \) and the axisymmetric Stokes streamfunction \( \Psi \) (satisfying \( \mathbf{v} = (\nabla \times \Psi \hat{e}_\theta)/\rho \)):

\[
\Psi(\rho, \theta, z) = \frac{1 - \rho^2 - z^2}{4\pi} \left( \frac{1}{d^-} + \frac{1}{d^+} \right).
\]

Contours of \( \Phi \) are shown in Fig. 3.4 together with the velocity field \( \mathbf{v} \). Both the streamfunction \( \Psi \) and azimuthal angle \( \theta \) are invariants of the steady flow, and fluid particles follow streamlines given by intersections of these two isosurfaces. These streamlines are illustrated in Fig. 3.4b as solid lines on the surfaces.

As in the case of the 2DRPM flow, a closed flow is created by enforcing a reinjection protocol at the source/sink. It is specified that particles that reach the sink are immediately reinjected at the source along the same streamline. This reinjection choice has the advantage of preserving Lagrangian structures during the reinjection process, although it is an arbitrary choice and other valid reinjection protocols exist (see Lester et al.\cite{Lester2009} for examples of several choices).

The solution of the advection equation 2.2 is denoted \( \hat{Y}_t \), describing streamlines as functions of time from an initial condition \( \mathbf{X} \). The map \( \hat{Y}_t \) satisfies

\[
\hat{Y}_0(\mathbf{X}) = \mathbf{X}, \quad \text{and} \quad \frac{d}{dt} \hat{Y}_t(\mathbf{X}) = \mathbf{v} \left( \hat{Y}_t(\mathbf{X}) \right)
\]

Since the velocity \( \mathbf{v} \) is incompressible it follows from Theorem 1 that the advection map \( \hat{Y}_t \) is volume-preserving for each value of \( t \).
3.2. THE 3DRPM FLOW

Passive particles in the steady dipole flow are confined to streamlines of constant azimuth $\theta$ and Stokes streamfunction $\Psi$, and therefore the flow cannot become chaotic. To create the crossings of streamlines required for chaotic motion a time-dependent flow is created by periodically reorienting the dipole. This allows fluid stretching to persist given appropriate flow parameters. Here only the simplest reorientation protocol is considered, involving rotation of the dipole about the $y$-axis, providing the closest resemblance to the 2DRPM flow. The dipole is switched on for a time period $\tau$, then switched off, instantaneously rotated by $\Theta$ about the $y$-axis, and switched back on. The reorientation period $\tau$ is non-dimensionalised such that $\tau = 1$ corresponds to the emptying time of the sphere under the steady dipole flow, i.e. the time it takes for all fluid in the sphere to pass through the sink. In this thesis the rotation angle $\Theta = 2\pi/3$ is primarily used, and the dipole positions for this case are shown in Fig. 3.5 by the blue (sink) and red (source) points. Many of the results for $\Theta = 2\pi/3$ readily generalise to reorientation angles of the form $2\pi m/n$ for $n$ odd due to the similarities in the flow in the limit as $\tau \to 0$. However, for $n$ even or when $\Theta/\pi$ is irrational, fundamentally different phenomena are expected as there is no net flow in the limit as $\tau \to 0$. Consideration of many reorientation angles is beyond the scope of this study, and provides an avenue for future work.

By the same reasoning as for the 2D flow, at low $Re$ the velocity field in the

Figure 3.5: The 3DRPM flow. (a) Reorientation protocol for $\Theta = 2\pi/3$. Dipole pairs are labelled according to the number of reorientations of the base flow modulo 3. (b) A typical particle trajectory for the protocol $(\tau, \Theta) = (0.3, 2\pi/3)$. 
time-dependent flow is given by the piecewise-steady velocity
\[ \hat{v}(x, t) = v \left( R^\theta_{\left\lfloor \frac{t}{\tau} \right\rfloor \Theta} \right) \]
where \( R^\theta_y \) is the rotation matrix corresponding to rotation through the angle \( \beta \) about the \( y \)-axis.

Again, particles are tracked in the rotating dipole frame so that the flow has a finite periodicity for all \( \Theta \), even when \( \Theta/\pi \) is irrational (see Appendix A for more details). Rather than rotating the dipole at the end of each reorientation period \( \tau \), particles are counter-rotated about the \( y \)-axis. Each step of the advection-reorientation cycle can therefore be expressed as
\[ Y_{\tau}^{-\Theta}(x) = R^y_{-\Theta} \hat{Y}_{\tau}(x). \]

This map is the main object of study, and has identical Lagrangian dynamics to the 3DRPM flow in the Eulerian (laboratory) frame.

### 3.2.3 Symmetries

Flow symmetries play an equally important role for 3D flows as 2D, creating topological restrictions for particle transport and Lagrangian structures.

The steady dipole flow possesses two basic symmetries: axisymmetry about the \( z \)-axis and a reflection reversal symmetry in the \( xy \)-plane. Algebraically these can be written respectively as
\[ \hat{Y}_t = R^\gamma_x \hat{Y}_t R^\gamma_x, \]
\[ \hat{Y}_t = S_{xy} \hat{Y}_t S_{xy}^{-1}, \]
where \( S_{xy} \) is reflection in the \( xy \)-plane. These symmetries yield three symmetries for the map \( Y_{\tau}^\Theta \). First, as a special case of the axisymmetry property (3.21), the dipole flow is symmetric in the \( xz \)-plane, i.e.
\[ \hat{Y}_t = S_{xz} \hat{Y}_t S_{xz}^{-1}. \]

As a result \( Y_{\tau}^\Theta \) satisfies
\[ Y_{\tau}^\Theta = R^\Theta_x \hat{Y}_{\tau} = R^\Theta_y S_{xz} \hat{Y}_{\tau} S_{xz}^{-1} = S_{xz} R^\Theta_x \hat{Y}_{\tau} S_{xz}^{-1} = S_{xz} Y_{\tau}^\Theta S_{xz}^{-1} \]
and is therefore also symmetric in the \( xz \)-plane. The \( xz \)-plane \( P_{xz} \) is an invariant surface of the map \( Y_{\tau}^\Theta \), i.e. \( Y_{\tau}^\Theta(P_{xz}) = P_{xz} \), therefore this symmetry guarantees that the dynamics in the \( y^+ \) and \( y^- \) hemispheres mirror each other. As the \( xz \)-plane acts
as an impenetrable barrier, dividing $S$ in two, particle transport only needs to be considered in one (the $y^+$) hemisphere.

Similarly, as another case of the axisymmetry property (3.21) the steady dipole flow is symmetric about the $yz$-plane

$$\hat{Y}_t = S_{yz}\hat{Y}_t S_{yz}.$$  \hfill (3.25)

This translates to the map $Y^\Theta_\tau$ as

$$Y^\Theta_\tau = R^y_\Theta \hat{Y}_\tau = R^y_\Theta S_{yz} \hat{Y}_\tau S_{yz} = S_{yz} R^y_{-\Theta} \hat{Y}_\tau S_{yz} = S_{yz} Y^{-\Theta}_{-\tau} S_{yz}$$ \hfill (3.26)

since $R^y_\Theta S_{yz} = S_{yz} R^y_{-\Theta}$. This is the 3D analogue of the symmetry eq. (3.9) for the 2DRPM flow, having the effect that changing $\Theta$ to $-\Theta$ results in a reflection through the $yz$-plane, but does not alter transport dynamics.

The map $Y^\Theta_\tau$ also possesses a reflection reversal symmetry, inherited from the reflection reversal symmetry of the dipole flow (3.22) as follows,

$$Y^\Theta_\tau = R^y_\Theta \hat{Y}_\tau = R^y_\Theta S_{xy} \hat{Y}_\tau S_{xy}$$ \hfill (3.27)

$$= R^y_\Theta S_{xy} (Y^{\Theta}_{-\tau})^{-1} R^y_{-\Theta} S_{xy} = S_1 (Y^{\Theta}_{-\tau})^{-1} S_1$$

where $S_1 = R^y_\Theta S_{xy}$. This is the 3D analogue of the symmetry eq. (3.10) which produced the symmetry line in the 2DRPM flow. Likewise, direct computation shows that $S_1$ is the map that reflects a point through the plane $z = \tan(-\Theta/2)x$, and this plane forms a symmetry plane about which Lagrangian topology must also evolve symmetrically. As will be demonstrated in Chapter 6, this symmetry has a significant impact on the coherent structures associated with the flow’s periodic points.

### 3.2.4 The limit as $\tau \to 0$

In the limit as the reorientation period $\tau$ approaches zero, the 3DRPM flow exhibits similar behaviour to the 2DRPM flow. The 3DRPM flow becomes steady, and equivalent to having all dipoles in all reoriented positions operating simultaneously. Again the velocity field $\hat{\nu}$ and potential $\hat{\Phi}$ are given by the average of the velocity fields and potentials for each of the reoriented dipole positions, as shown in Fig. 3.6 which shows the flow in the $xz$-plane. However, the average of the axisymmetric streamfunction $\Psi$ in its rotated positions does not provide a streamfunction for the flow in the limit as $\tau \to 0$, since it is defined based on the axisymmetry about the $z$-axis, and the reoriented dipoles do not share the same axis of axisymmetry.

As for the 2DRPM flow, there is only a net flow when the reorientation angle $\Theta = 2\pi m/n$ for $n$ odd, otherwise the dipoles in opposite positions average to zero. For
the odd cases, even though there is no expression for the streamfunction, particles follow one-dimensional streamlines that do not intersect. As for the 2DRPM flow there are two streamlines that have a minimum return time, both located in the $xz$-plane, that are twistless tori.

In cases of odd rotation at small but non-zero $\tau$, particles closely follow the streamlines of the asymptotic flow $\tilde{v}$, creating approximately one-dimensional transport, this is shown in Fig. 7.1(a-d) and will be discussed in more detail in Chapter 7.

### 3.2.5 Adiabatic invariants

Due to the 3DRPM flow’s similarity to the 2DRPM, and the fact that the $xz$-plane and outer sphere are invariant surfaces, it might be expected that particle motion in general would be confined to a set of 2D surfaces. This would be the case if there was an invariant of motion, since particles would then be confined to the isosurfaces of the invariant. However, the 3DRPM flow does not admit an invariant, and particles that are not trapped in KAM-tubes always travel three-dimensionally. However, the rates of transport in each of the three dimensions can be of different order. This is highlighted in Fig. 3.7, where it is seen that after 2,000 iterations of the map $Y_{\tau,\Theta}$ for $(\tau, \Theta) = (0.328, 2\pi/3)$, each particle travels rapidly and chaotically, but they are all loosely confined to surfaces of revolution (about the $y$-axis). Therefore there are two directions of fast transport, parallel to the surfaces of revolution, and one direction of slow transport, transverse to the surfaces of revolution.
Understanding the mechanisms that drive transverse particle transport is critical to understanding transport in general in the 3DRPM flow. As discussed in the literature review, there are several mechanisms that have been discovered that create transverse transport in 3D fluid flows. The question is whether the transverse transport that is exhibited by the 3DRPM flow is caused by one of the known mechanisms or something entirely different. This is the subject of Chapter 7, where it is shown that discontinuous deformations produced by the dipole reorientation create a new mechanism, similar to RID.

In order to analyse and quantify transverse transport, the surfaces of revolution that particles loosely adhere to have been found. This amounts to finding a function $f(y, \sqrt{x^2 + z^2})$ that is approximately conserved by the flow. The advection map $Y^\Theta_\tau$ is composed of a steady dipole advection step $\hat{Y}_\tau$ and a rotation step $R^\Theta_\tau$. Therefore, in looking for invariants of the combined motion it is natural to look at the invariants of each of its components. For the steady dipole advection the invariants
of motion are the streamfunction $\Psi$ and the azimuthal angle $\theta$. Whereas for the rotation map any function of the form $f(y, \sqrt{x^2 + z^2})$ is invariant. Therefore the streamfunction $\Psi(y, \sqrt{x^2 + z^2})$ is a suitable approximate invariant of $Y^\Theta$ since it will be exactly conserved in the $yz$-plane. Thus each surface of revolution is formed by rotating the streamline $L_{y^*}$ that passes through the point $(0, y^*, 0)$ about the $y$-axis, as shown in Fig. 3.8(a,b). The union of all these surfaces of revolution forms the entire hemisphere, and they only intersect on the circle $x^2 + z^2 = 1$ where they all coalesce. The value $y^*$ at which the $y$-axis pierces each surface of revolution is used as the parameter to label these surfaces, and each point in the domain lies on a unique surface with ‘shell number’

$$G_R(x, y, z) = \rho_0 \left( \Psi \left( y, \sqrt{x^2 + z^2} \right) \right), \quad (3.28)$$

Figure 3.8: Construction of the adiabatic invariant $G_R$. (a) The streamline that passes through the point $(0, y^*, 0)$ that is rotated about the $y$-axis to form the surface of revolution, $G_R = y^*$, shown in (b). (c) Three iso-surfaces of $G_R$, with the curves that are rotated to form them. Blue: $G_R = 0$ is the $xz$-plane. Red: $G_R = 1$ is the spherical boundary. Green: $G_R = 0.5$. 
where $\rho_0(\psi)$ satisfies $\Psi(\rho,0) = \psi$ with solution

$$\rho_0(\psi) = \sqrt{2\pi^2 \psi^2 - 2\pi \sqrt{\pi^2 \psi^4 + 2\psi^2} + 1}. \quad (3.29)$$

With this definition, the $xz$-plane corresponds to $G_R = 0$ and the outer hemisphere corresponds to $G_R = 1$.

While the 3DRPM flow does not admit a true invariant, the iso-surfaces of $G_R$ (Fig. 3.8(c)) closely approximate the surfaces that particles loosely adhere to, as seen in Fig. 3.9 where the contours of $G_R$ have been added to the projections Fig. 3.7(b-d). Therefore $G_R$ forms an adiabatic invariant, i.e. it is not exactly conserved by the flow, but it is approximately conserved. By construction $G_R$ is exact along the streamlines $L_{y^*}$ that are used to create it. Therefore any other choice of rotationally symmetric invariant can only be as accurate as $G_R$, i.e. if another function $f(\sqrt{x^2+z^2},y)$ were used, it may be more accurate in some locations, but would no longer be exact along the streamlines $L_{y^*}$. The difference in the adiabatic invariant $\Delta G_R$ after a single iteration of the map $Y_\Theta^\tau$ is shown in Fig. 3.10 for $\tau = 4.096 \times 10^{-2}$ and $\tau = 0.3277$, for particles starting on three iso-surfaces of $G_R$, each projected onto the $xz$-plane. This can be thought of as the ‘error’ in the definition of the adiabatic invariant, and it is seen that this difference is small in most of the domain, with a maximum magnitude in regions close to the circle $x^2 + z^2 = 1$ that either start or finish near the dipole. As particles are advected throughout the domain, they accumulate transport transverse to the iso-surfaces of $G_R$, given by the accumulation of the differences $\Delta G_R$ after each iteration of $Y_\Theta^\tau$. While particles may experience a large deviation in $G_R$ after a single iteration, this may simply indicate an ‘error’ in the definition of $G_R$, and it is therefore necessary to search for deviations in $G_R$ that persist over some period of time.

This topic is explored in more depth in Chapter 7, where the function $G_R$ is used to detect mechanisms that control the transition from approximately 2D transport at low values of the reorientation period $\tau$ to fully 3D transport at high $\tau$. 

Figure 3.9: The projections of Poincaré sections from Fig. 3.7(b-d) shown with the contours of the adiabatic invariant $G_R$, $n$ is the number of flow periods.
Figure 3.10: Difference in the adiabatic invariant $\Delta G_R$ after 1 iteration under the map $Y^{\Theta}_\tau$ for $\tau = 4.096 \times 10^{-2}$ (left) and $\tau = 0.3277$ (right). As $G_R$ is by definition invariant under $R^\Theta_\tau$, these figures do not depend on $\Theta$. For each figure particles are evenly distributed over the corresponding iso-surface of $G_R$ (labelled), then iterated, and the initial particle location (projected onto the $xz$-plane) is coloured according to the difference in the adiabatic invariant $G_R$. 
Chapter 4

Methodology

In this chapter the tools and techniques that form the basis for the computational and analytical study of the 2D and 3D RPM flows are introduced. First, the methods used to track particles in the 2D and 3D RPM flows are outlined. Then a description of Poincaré sections, their applications, and an algorithm to compute their fractal dimension as a measure of transport dimensionality. This is followed by a discussion on periodic points, their implications for transport, and methods for locating them and their associated structures. Then algorithms to compute Lyapunov exponents and the so-called ‘mix-norm’, a multiscale measure for mixing, and some examples of its uses. Finally, a zoning method used to analyse transport transitions via adiabatic invariants is introduced.

4.1 Particle tracking

Tracking individual passive particles is critical to all of the analysis tools used in this thesis, so it is essential to have robust and accurate methods for each flow. The 2DRPM flow admits a pseudo-analytic solution to the advection equation (2.2), which is described in §4.1.1. However, the 3DRPM flow does not, and a numerical solution of the advection equation is required. An explicitly volume-preserving integration scheme has been implemented for the 3DRPM flow, ensuring that attractors are not artificially created in the conservative system. This scheme is described in §4.1.2.

The pseudo-analytic method for the 2DRPM flow and the numerical method for the 3DRPM flow are described below.
4.1.1 2DRPM flow

While a pseudo-analytic solution for the advection equation is described in [LMT+09], the method used here differs slightly. This new method is also described briefly in the appendix of Smith et al. [SRLM16] (in § 5 of this thesis), but more detail is provided here.

Finding the trajectory of a particle requires solving the advection equation (2.2) either numerically or analytically. Since the 2DRPM flow admits an analytic expression for the velocity field $v$, this makes computation significantly easier. While an analytic solution to equation (2.2) is impossible for the 2DRPM flow, a pseudo-analytic method is used to track particles in a similar manner to Lester et al. [LMT+09]. Whereas Lester et al. used coordinates $(\theta, \psi)$ to describe and solve the advection equation, where $\theta$ is the polar angle which becomes parallel to the streamfunction $\psi$ along $\theta = \pm \pi/2$, here $(\phi, \psi)$ coordinates are used because the streamfunction is an invariant of the flow, and the flow potential $\phi$ is by definition orthogonal to the streamfunction ($\nabla \phi \cdot \nabla \psi = 0$).

In order to define the advection equation and hence solve it, it is necessary to convert between Cartesian or polar coordinates and the new frame $(\phi, \psi)$. The functions $\phi$ and $\psi$ have already been found as functions of polar coordinates, eq. (3.2), (3.3), so it remains to invert these functions, finding $r(\phi, \psi)$ and $\theta(\phi, \psi)$. This is achieved by first solving for each of $r$ and $\theta$ in the functions $\phi$ and $\psi$, i.e.

$$r(\theta, \phi) = \frac{(e^{2\phi} + 1)^2 \sin^2(\theta) - (e^{2\phi} - 1)^2 - (e^{2\phi} + 1) \sin(\theta)}{e^{2\phi} - 1}$$  \hspace{1cm} (4.1)

$$\theta(r, \phi) = \arcsin \left( \frac{(r + 1) (1 - e^{2\phi})}{2r (e^{2\phi} + 1)} \right)$$ \hspace{1cm} (4.2)

$$r(\theta, \psi) = \cot(\psi) \left( \sqrt{\cos^2(\theta) + \tan^2(\psi) - \cos(\theta)} \right)$$ \hspace{1cm} (4.3)

$$\theta(r, \psi) = \arccos \left( -\frac{(r - 1) \tan(\psi)}{2r} \right).$$ \hspace{1cm} (4.4)

then $r(\phi, \psi)$ can be found by solving $r(\theta(r, \phi), \psi) = r$, which returns

$$r(\phi, \psi) = \sqrt{1 - \frac{2 \cos(\psi)}{\cos(\psi) + \cosh(\phi)}}.$$ \hspace{1cm} (4.5)

Finally, $\theta(\phi, \psi) = \theta(r(\phi, \psi), \psi)$, which yields

$$\theta(\phi, \psi) = -\frac{|\phi|}{\phi} \cos^{-1} \left( \frac{\sin(\psi)}{\sqrt{\cosh^2(\phi) - \cos^2(\psi)}} \right).$$ \hspace{1cm} (4.6)
In summary, conversion between Cartesian coordinates and \((\phi, \psi)\) coordinates is performed via polar coordinates
\[(x, y) \leftrightarrow (r, \theta) \leftrightarrow (\phi, \psi)\]
\[
r(\phi, \psi) = \sqrt{1 - \frac{2\cos(\psi)}{\cos(\psi) + \cosh(\phi)}}
\]
\[
\theta(\phi, \psi) = \frac{|\phi|}{\phi} \cos^{-1}\left(\frac{\sin(\psi)}{\sqrt{\cosh^2(\phi) - \cos^2(\psi)}}\right)
\]
\[
\phi(r, \theta) = \frac{1}{2} \log \left(\frac{r^2 - 2r \sin(\theta) + 1}{r^2 + 2r \sin(\theta) + 1}\right)
\]
\[
\psi(r, \theta) = \tan^{-1}\left(\frac{2r \cos(\theta)}{1 - r^2}\right).
\]

In these new coordinates the advection equation is given by
\[
\frac{d\phi}{dt} = \left(\cos(\psi) + \cosh(\phi)\right)^2, \quad \frac{d\psi}{dt} = 0.
\]

The system has therefore been reduced to one dimension, though this set of differential equations is still insoluble analytically. On the other hand, the equation
\[
\frac{dt}{d\phi} = \frac{1}{d\phi/dt}
\]
has the analytic solution
\[
t_{\text{adv}}(\phi, \psi) = \csc^2(\psi) \left[-2 \cot(\psi) \tan^{-1}\left(\frac{\psi}{2} \tanh\left(\frac{\phi}{2}\right)\right)\right.
\]
\[
+ \frac{\sin \frac{\psi}{2} + \sinh \frac{\phi}{2}}{\sin \psi} \left(\text{sech}\left(\frac{\phi - i\psi}{2}\right) + \text{sech}\left(\frac{\phi + i\psi}{2}\right)\right)\right]
\]

which gives the advection time from the x-axis \((\phi = 0)\) to the point \((\phi, \psi)\) along the streamline \(\psi^*\). The contours of \(t_{\text{adv}}\) are shown in Fig. 4.1 in (a) \((\phi, \psi)\) and (b) Cartesian coordinates. The residence time of each streamline can then be computed as\textsuperscript{†}
\[
t_{\text{res}}(\psi) = 2 \lim_{\phi \to \infty} t_{\text{adv}}(\phi, \psi)
\]
\[
= -2(\psi \cot(\psi) - 1) \csc^2(\psi),
\]
and reaches a minimum of 2/3 on the streamline \(\psi = 0\) corresponding to the line connecting the source and sink, and a maximum of 2 on the streamlines \(\psi = \pm \pi/2\)

\textsuperscript{†}Note that this function \(t_{\text{adv}}\) has a removable singularity at \(\psi = 0\), therefore in the region \(|\psi| < 10^{-5}\) the first four terms in the Taylor series expansion about \(\psi = 0\) of the form \(a_0(\phi) + a_1(\phi)\psi + \cdots + a_4(\phi)\psi^4\) are used, which ensures accuracy to within \(10^{-20}\).

\textsuperscript{†}This function also has a removable singularity at \(\psi = 0\), and again in the region \(|\psi| < 10^{-5}\) the first four terms of the Taylor series expansion \(\sum_0^\infty b_i\psi^i\) are used.
Figure 4.1: Contours of the advection time $t_{adv}$ in the different coordinate systems. (a) $t_{adv}(\phi, \psi)$. The horizontal axis extends from $-\infty$ to $+\infty$, representing the dipoles, and the contours asymptote towards constant values in these limits. (b) $t_{adv}(x, y)$ in the Cartesian frame.

corresponding to the outer circle, as shown in Fig. 4.2. Knowing these advection and residence time functions, the advection of a particle for the time period $T$ can be expressed as a map $(\phi, \psi) \rightarrow (\phi', \psi)$, where the new value of the potential function satisfies

$$t_{source}(\phi', \psi) = t_{source}(\phi, \psi) + T \mod t_{res}(\psi) \quad (4.12)$$

where $t_{source}(\phi, \psi)$ is the time it takes a particle at the source to reach the point $(\phi, \psi)$ (Fig. 4.3), i.e. eq. (4.12) says the advected point is $T$ units of time further from the source. This time from the source can be expressed in terms of $t_{adv}$ and $t_{res}$ as

$$t_{source}(\phi, \psi) = t_{adv}(\phi, \psi) + \frac{t_{res}(\psi)}{2} \quad (4.13)$$

which is substituted into eq. (4.12) to give

$$t_{adv}(\phi', \psi) = t_{adv}(\phi, \psi) + T \mod t_{res}(\psi) \quad (4.14)$$

However, the function $t_{adv}$ is not invertible, so there is no analytic solution for $\phi'$. Instead, Newton’s root finding method is used to solve eq. (4.12) to machine precision accuracy. The new coordinates are then converted back to Cartesian coordinates via equation (4.7).
4.1. PARTICLE TRACKING

Figure 4.2: The residence time $t_{\text{res}}(\psi)$ of streamlines. The residence time has a minimum of $2/3$ along the streamline $\psi = 0$ and a maximum of $2$ along the streamlines $\psi = \pm \pi/2$.

Figure 4.3: Schematic diagram showing the advection time $t_{\text{adv}}(\phi, \psi)$ from the $x$-axis to a point $(\phi, \psi)$, the residence time $t_{\text{res}}(\psi)$ of a streamline, and the times it takes particles to reach the source $(t_{\text{source}}(\phi, \psi))$ and sink $(t_{\text{sink}}(\phi, \psi))$.

Validation

Since the particle tracking method is pseudo-analytic, and the only numerical step is the inversion of eq. (4.12), the advection of particles is very accurate and very fast. The only tuning parameter is the tolerance used for Newton’s root finding method, which is set to machine precision. The accuracy and robustness of the method are clearly demonstrated in Chapter 6 where Poincaré sections with small scale details are analysed with no computational anomalies detected.
4.1.2 3DRPM flow

While the steady dipole flows in 2D and 3D are qualitatively similar, the quadratic equations used in the coordinate transformation eq. (4.7) become quintic equations for the 3D system (see Appendix B for details), for which there is no general solution using radicals, by the Abel–Ruffini Theorem. Therefore, a numerical integration scheme is used to solve the advection equation. When using the embedded third and fourth order explicit Runge-Kutta method it was found that over large integration times some initially chaotic trajectories would spiral in towards isolated points, indicating the presence of artificial attractors. Therefore, an explicitly volume preserving integration scheme has been implemented using the method of Finn and Chacón [FC05] that preserves Lagrangian coherent structures.

A volume-preserving numerical integration scheme

Following the method outlined in §2.7.4, a volume-preserving integration scheme can be achieved by decomposing the advection equation (scaled by the Jacobian of the curvilinear coordinate transformation) into three 2D area-preserving systems, and using a symplectic integration method. This is simplified for the steady dipole flow since the velocity in the azimuthal direction is zero ($v_\theta = 0$).

For cylindrical coordinates ($\rho, \theta, z$) the Jacobian is $\rho$, and eq. (2.47) becomes

\[
\frac{d\rho}{dt} = \frac{v^1}{\rho}, \quad \frac{d\theta}{dt} = \frac{v^2}{\rho} = 0, \quad \frac{dz}{dt} = \frac{v^3}{\rho}.
\]

(4.15)

In other words, $v^j = \rho v_i(x(\rho, \theta, z), y(\rho, \theta, z), z(\rho, \theta, z))$ where $\mathbf{v} = (v_1, v_2, v_3)$ is the velocity field for the steady dipole flow. Introducing the variable $\lambda$ such that $dt/d\lambda = J = \rho$, these equations become

\[
\frac{d\rho}{d\lambda} = v^1, \quad \frac{d\theta}{d\lambda} = 0, \quad \frac{dz}{d\lambda} = v^3.
\]

(4.16)

which describes a 2D area-preserving system. As shown in §2.7.4, integrating this system with a symplectic method ensures that volume is explicitly preserved. Theorem 4 from §2.7.3 provides a sufficient condition for a Runge–Kutta method to be symplectic, and it follows that all of the Gauss–Legendre Runge–Kutta schemes are symplectic. The 4th order Gauss–Legendre scheme is used here, with Butcher tableau given by eq. (2.41). This provides two additional orders of precision compared to the second order Gauss–Legendre scheme (also known as Crank–Nicolson scheme), with only one extra implicit equation to solve. The implicit equations are solved numerically using the Picard iteration method to within a tolerance of $10^{-15}$. 
A limitation of the Gauss–Legendre methods is that they do not have the embedding capabilities that some explicit Runge–Kutta schemes do\textsuperscript{*}. It is therefore more difficult to accelerate the integration process and control the method’s precision using a variable step size. A way around this is to estimate the local error using the ‘Double Step’ method, that is, integrating using half the current step size and using Richardson extrapolation to create a more accurate approximation. The step-size is then doubled if the magnitude of the difference between the single-step and double-step approximations is less than the minimum desired tolerance (chosen to be $5 \times 10^{-15}$), or halved if the difference is greater than the maximum desired tolerance (chosen to be $10^{-13}$) and the integration step is repeated. This maintains the difference between the two approximations, which is approximately the integration error, always less than $10^{-13}$. The drawback of the ‘Double Step’ method is that it involves three integration steps for every time-step.

Addressing singularities

There are two singularities in the dynamical system described by eq. (4.16). First, the magnitude of the velocity approaches $\infty$ as the source and sink are approached, meaning the integration step-size approaches zero. Also, when integrating from $t = t_0$ to $t_1$, the integration steps are actually in the new variable $\lambda$, integrating $dt/d\lambda$ until the time $t_1$ is reached. Since $dt/d\lambda = \rho$, there is another singularity along the line $\rho = 0$, where the integration step-size approaches infinity.

Each of these singularities are treated separately. First, within a distance $\epsilon$ of the dipole the flow is approximated by an isolated monopole flow, which has an analytic solution. An isolated monopole in 3D has velocity field

$$\frac{dr}{dt} = \frac{Q}{4\pi r^2}, \quad \frac{d\theta}{dt} = \frac{d\phi}{dt} = 0$$

(4.17)

where $(r, \theta, \phi)$ denote spherical coordinates centred at the monopole, and $Q$ denotes the signed strength of the monopole (positive for a source and negative for a sink). Here $Q$ is chosen such that the velocity along the line $\rho = 0$ is the same for the dipole flow and the monopole flow where they meet on the boundary of the divided regions. Eq. (4.17) has the analytic solution

$$r(t) = \left( \frac{3Qt}{4\pi} + r(0)^2 \right)^{\frac{2}{3}},$$

(4.18)

\textsuperscript{*}For example there exist 4th and 5th order Runge–Kutta methods such that the 5th order method shares all the equations of the 4th order method with one extra equation. The 4th order method is said to be ‘embedded’ in the 5th order method. This means that with one extra function evaluation the error in the 4th order method can be approximated using the 5th order method, and the integration step-size can be adjusted accordingly.
Figure 4.4: Schematic diagram of the method used to advect particles that are near the dipole. A particle initially located at the point \((\rho_0, z_0)\) is advected along the streamline of the monopole flow to the point \((\rho^*, z^*)\), and then moved back onto its original streamline to the point \((\hat{\rho}, z^*)\). The green point in the grey region shows why the monopole flow approximation cannot be used as particles can be ejected from the domain.

and the time it takes to get from \(r = 0\) to \(r = r_0\) is

\[
t(r_0) = \frac{4\pi r_0^3}{3Q}.
\]  

There are two concerns about this method, first the streamfunction \(\Psi\) is not conserved when the particle is advected under the monopole flow since the streamlines are not curved. Also, the lack of streamline curvature means that particles in the grey region of Fig. 4.4 can be ejected from the domain, as demonstrated by the trajectory of the green particle. To remedy these issues, particles are forced to stay on the same streamline of the dipole flow. This is achieved by first advecting a particle at the point \((\rho_0, z_0)\) under the monopole approximation to the point \((\rho^*, z^*)\), and then shifting the particle horizontally to the point \((\hat{\rho}, z^*)\) which satisfies \(\Psi(\hat{\rho}, z^*) = \Psi(\rho_0, z_0)\). The value \(\hat{\rho}\) is found by numerically solving \(\Psi(\hat{\rho}, z^*) = \Psi(\rho_0, z_0)\) using Newton’s root finding algorithm with a tolerance of \(5 \times 10^{-14}\). This changes the effective velocity within the region near the poles, but does not have a significant impact on the overall transport dynamics when \(\epsilon\) is chosen sufficiently small (\(\epsilon = 10^{-2}\)).

The singularity along the line \(\rho = 0\) is only present due to the introduction of the variable \(\lambda\). Therefore a cut-off streamline is chosen, \(\psi_c = \max(\Psi) - 10^{-3} = \frac{1}{2\pi} - 10^{-3}\), such that all particles within the region \(\Psi > \psi_c\) (close to the line \(\rho = 0\)) are advected using an embedded 4th and 5th order Runge–Kutta method to integrate the original advection equation (not the one scaled by the Jacobian) which does not have the singularity. This makes integration not strictly volume-preserving in this region, but particles behave as expected in a conservative system.
Validation

To measure the accuracy of the numerical particle tracking scheme, two tests are performed on a grid of equally spaced points ($\Delta \rho = \Delta z = 8 \times 10^{-3}$) in the $\rho z$-plane (the azimuthal angle $\theta$ can be ignored because it is exactly preserved throughout the numerical method). First, according to the reflection-reversal symmetry eq. (3.22),

$$x = \hat{\mathbf{Y}}^{-1}(x) = (S_{xy}\hat{Y} \tau S_{xy})(x)$$ (4.20)

for all points in the domain, and therefore the magnitude of the difference

$$E_1 = |(S_{xy}\hat{Y} \tau S_{xy})(x) - x|$$ (4.21)

is a measure in the error of the particle advection. This error has been calculated across the grid of starting positions for the representative value $\tau = 0.1$, and Fig. 4.5(a) shows that $E_1$ is very small across the entire domain, with a maximum of $5 \times 10^{-10}$, a mean of $10^{-12}$, and a median of $10^{-15}$. As a second test, the error in the streamfunction

$$E_2 = |\Psi(\hat{\mathbf{Y}} \tau (x)) - \Psi(x)|$$ (4.22)

after a single iteration ($\tau = 0.1$) is calculated across the same grid of points, again showing very small errors across the entire domain (Fig. 4.5(b)). The maximum error is $10^{-13}$, and both the mean and median are equal to the machine precision, $10^{-16}$. As expected, both errors $E_1, E_2$ are largest in the regions that are affected by the singularities, between the $z$-axis and the dashed curve, and between the sink and the thick black curve, and this adds further weight to the effectiveness of the volume-preserving integration scheme away from these singularities.

Considering the growth of the streamfunction error

$$E_2(n) = |\Psi(\hat{\mathbf{Y}}^{\tau n}(x)) - \Psi(x)|$$ (4.23)

as a function of time for various initial particle locations, Fig. 4.6 shows that the error grows linearly or sub-linearly, and at a slow rate, with approximately a factor of $10^2$ increase over $10^4$ iterations for the (purple) particle located within the region between the $z$-axis and the dashed curve where the Runge–Kutta method is used.

Therefore, the numerical integration scheme that is used to track particles in the steady dipole flow is highly accurate. This is further demonstrated throughout this thesis by the high resolution of fractal structures at very small scales, and in particular the fact that particles do not cross impenetrable barriers to transport such as invariant tori even over very long tracking times, see Fig. 7.1(a,b) for example.
Figure 4.5: Validation of the numerical method used to track particles in the steady dipole flow with $\tau = 0.1$. Between the $z$-axis and the dashed curve ($\Psi = \psi_c$) the Runge–Kutta method is used to avoid the singularity at $\rho = 0$, and between the dashed curve and the spherical boundary the volume-preserving Gauss–Legendre method is used. The points between the pole at $(\rho, z) = (0, -1)$ and the solid black curve are those such that $t_{sink} < \tau$, i.e. those that pass through the sink during the advection time $\tau$, and are subject to the method used to address the singularity at the dipole shown in Fig. 4.4. (a) The magnitude of the difference $|S_{xy} \hat{Y}_\tau S_{xy} \hat{Y}_\tau(x) - x|$, tested on a grid of points with separation $\Delta z = \Delta \rho = 8 \times 10^{-3}$, measuring the error in the reflection-reversal symmetry eq. (3.22). (b) The magnitude of the difference $|\Psi(\hat{Y}_\tau(x)) - \Psi(x)|$, tested on the same grid, measuring the error in streamline conservation.
4.2 Poincaré sections

Poincaré sections are a commonly used tool for the qualitative analysis of mixing and transport in dynamical systems. They are created by sectioning the system in one of its dimensions, which reduces the dimensionality of the problem. For time-periodic systems, such as the RPM flows, Poincaré sections are typically created by sectioning in time. This amounts to sampling the positions of a number of particles at the end of each flow period. By plotting all the sampled positions after a large number of flow periods (typically in the order of thousands) transport structures of the underlying flow are revealed. For instance, non-mixing regions appear as ‘island’ (or tubular in 3D) formations known as KAM-tori, and mixing regions appear as a topologically distinct ‘chaotic sea’ that consists of a seemingly random scatter of points. These structures are depicted in Fig. 4.7 which shows a typical Poincaré section for the 2DRPM flow. Also shown is the symmetry line \( y = \tan(-\Theta/2)x \) (dashed orange) about which all the Lagrangian structures must be symmetric according to eq. (3.10); and two pairs of alternating elliptic (blue) and hyperbolic (red) periodic point chains that appear inside a KAM-torus as predicted by the Poincaré–Birkhoff Theorem.

For the RPM maps, the iterations of the periodic advection maps \( M = Y^\Theta, Y^\Theta = Y^\Theta \) produce the Poincaré sections. Therefore for a set \( S \) of initial particle positions, the Poincaré section is formed by plotting all iterates \( \{M^i(x) : x \in S, i < N\} \) of the advection maps.
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Figure 4.7: Poincaré section for the 2DRPM flow with \( \tau = 0.2 \) and \( \Theta = 2\pi/3 \). The symmetry line \( y = \tan(-\Theta/2)x \) is shown in dashed orange, and two alternating chains of elliptic (blue) and hyperbolic (red) periodic points are shown inside a KAM-torus, one is period-4 and the other is period-7.

4.2.1 Fractal dimension

To quantify the transition from approximately 1D transport at low \( \tau \) to 3D transport at high \( \tau \) that is observed in the 3DRPM flow, the fractal dimension of Poincaré sections is computed to determine the dimensionality of particle transport. Each Poincaré section consists of a set of isolated points within the 3D domain, and with a sufficiently large number of iterations they should approximately fill out a 1D curve, 2D surface or 3D volume.

The computation of the correlation fractal dimension \( D_2 \) has been performed numerically via a similar algorithm used by Traina et al. [TTWF00]. The principle of the algorithm is to divide the domain into a regular grid of boxes, each with side length \( r \), and count the number of points in the dataset that lie in each box, known as the occupancy \( C_r \). The sum of squared occupancies

\[
S(r) = \sum_{i,j,k} C_r(i,j,k)^2
\]

has a power law relationship with the side length \( r \), such that

\[
S(r) = r^{D_2},
\]

where \( D_2 \) is the correlation fractal dimension. By computing \( S(r) \) for a range of side lengths \( r \), \( D_2 \) is determined as the slope of the linear portion of the \( \log S(r) \) vs. \( \log r \) plot.

*Except in the unlikely event that the particle is chosen at a periodic point, in which case it traces out a zero dimensional finite set of points.
vs log $r$ graph. The spherical domain of the 3DRPM flow is contained within the cube with side lengths 2, therefore the set of side lengths $r$ used is \( \{2^{2p} : p = 1, 2, \ldots P\} \), corresponding to successive subdivisions of the cube into smaller cubes. The description of the algorithm is

**Compute fractal dimension $D_2$ of a dataset $A$**

**input:** dataset $A$ ($N$ points with $d$ dimensions)

**output:** fractal dimension $D_2$

**Begin**

For each point in the dataset

For each side length $r = 2^{2p}$, $p = 1, 2, \ldots P$

Find which grid cell the point falls in, and increment its occupancy

For each side length $r = 2^{2p}$, $p = 1, 2, \ldots P$

Compute the sum of squared occupancies $S(r)$

Plot log $S(r)$ vs log $r$

Return the slope of the linear part of the plot as the fractal dimension $D_2$ of the dataset $A$.

**End**

This algorithm is very efficient since the dataset is only passed through once. For a small number of refinement levels $P$ and a small number of dimensions $d$ it is possible to pre-allocate the lists of cell occupancies, however this results in $\sum_{p=1}^{P} 2^{pd} = \frac{2^d 2^{Pd} - 1}{2^d - 1}$ entries, many of which will be zero. This approach is not feasible for larger numbers of refinement levels and dimensions due to memory constraints. Instead, a linked list in the form of a ‘quad-tree’ (2D) or ‘oct-tree’ (3D) is used, as demonstrated by Fig. 3 in [TTWF00]. For each point the tree is updated by descending through the refinement levels and incrementing the occupancies of the cell that it lies in at each level of refinement. If the point lies in a cell that has not yet been occupied, then the set of subcells at the next level of refinement is added to the start of the linked list at that level. This means that only occupied cells will be allocated memory, and there is no need to sort the linked lists at each level when a new cell is allocated. This method is $O(NdP)$ [TTWF00] where $N$ is the number of points in the dataset. Examples of the results of this algorithm for datasets with known fractal dimension (line, plane and Sierpinski triangle) are shown in Fig. 6 in [TTWF00], demonstrating that in all cases the algorithm is accurate to within 1%. The accuracy will increase if more data points are used since it will create a better representation of the objects at finer resolutions, this is particularly true for fractal objects such as the Sierpinski triangle.
4.3 Periodic point analysis

Periodic points play a central role in the organization of fluid transport in both 2D and 3D periodic flows, determining mixing and non-mixing regions. A period-$n$ point of a map $\Lambda : X \subset \mathbb{R}^d \to \mathbb{R}^d$ satisfies $\Lambda^n(x) = x$, and the local stability near the periodic point is determined by the eigenvalues $\lambda_1, \ldots, \lambda_d$ of the Jacobian or deformation tensor

$$DA = \left( \frac{\partial \Lambda_i}{\partial x_j} \right)$$

(4.26)

evaluated at the periodic point [Ott89]. This is because the linearisation of the system $x_{n+1} = \Lambda(x_n)$ about a periodic point $x^*$ is

$$x_{n+1} = x^* + A(x_n - x^*)$$

(4.27)

where $A$ is the deformation tensor $DA$ evaluated at $x^*$. This has general solution

$$x_n = x^* + \sum_{i=1}^d a_i \lambda_i^n v_i,$$

(4.28)

where $v_i$ is the corresponding eigenvector of $A$ to the eigenvalue $\lambda_i$, and $a = P^{-1}(x_0 - x^*)$ where $P$ is the matrix with columns $v_i$ used in the diagonalisation $A = PDP^{-1}$. Hence any contraction, expansion and rotation is determined by the eigenvalues $\lambda_i$. For a $d$-dimensional volume-preserving map, the product of the eigenvalues, $\prod_i \lambda_i$ is equal to 1. This constrains the possible types of local transport that occurs in the neighbourhood of periodic points, with different possibilities for 2D and 3D systems.

4.3.1 2D systems

In 2D area-preserving systems there are two eigenvalues $\lambda_1 = 1/\lambda_2$ of the deformation tensor. Therefore there are three possibilities for the local stability of periodic points

1. $\lambda_1 = \exp(i\alpha), \lambda_2 = \bar{\lambda}_1$. In this case there is local rotation of fluid but no stretching. These points are called elliptic, and have associated non-mixing regions termed KAM-tori which are the ‘island’ regions in Poincaré sections, as shown in Fig. 4.7.

2. $\lambda_1 = 1/\lambda_2 \neq \pm 1$ and are both real. In this case there is contraction and expansion of nearby fluid, and the periodic point is called hyperbolic. The eigenvector corresponding to the eigenvalue less than 1 is the direction of contraction, and the other eigenvector is the direction of expansion.
3. $\lambda_1 = \lambda_2 = \pm 1$. In this case there is only shearing of fluid and the point is called *degenerate* or *parabolic*. These points are on the cusp of the stable/unstable classification and occur when changes in system parameters leads to a bifurcation in local stability.

Periodic points can also be classified using the so-called ‘Poincaré index’ or ‘fixed point index’ [KH96], which is a topological quantity that relates fixed points to the topological genus of the flow domain according to the Poincaré–Hopf Theorem. The index $\Sigma_C$ for a simple closed curve $C$ in the flow domain is equal to the number of counter-clockwise rotations of the velocity vector in one counter-clockwise traverse of the curve. The index $\Sigma_{x_0}$ of a periodic point $x_0$ is then equal to the Poincaré index of any simple closed curve that encloses the periodic point, and no other periodic points. Under this measure, elliptic points have index $+1$ and hyperbolic points have index $-1$. For simple closed curves that contain more than one periodic point, the index of the curve is equal to the sum of the indices of the periodic points in its interior. Therefore the index $\Sigma_C$ is invariant under continuous deformation of a flow, unless a periodic point crosses the curve $C$. The index therefore constrains the number and type of periodic points created or annihilated during bifurcations.

Also associated with hyperbolic points are two structures known as the stable and unstable manifolds, defined as

$$W^s(x_0) = \left\{ x : \lim_{n \to \infty} \Lambda^n(x) = x_0 \right\}$$

$$W^u(x_0) = \left\{ x : \lim_{n \to -\infty} (\Lambda^{-1})^n(x) = x_0 \right\},$$

i.e. the stable manifold is the set of points whose forwards iterations converge to the periodic point $x_0$ and the unstable manifold are those that converge under iterations of the inverse map. As each manifold is an invariant of motion, i.e. $\Lambda(W^s,u) = W^s,u$, they act as barriers to fluid transport, and their structure, in particular the nature of any intersections, has a significant impact on fluid transport. The stable manifold of a hyperbolic point can intersect the unstable manifold of the same point, known as a *homoclinic connection*, or the unstable manifold of a different hyperbolic point, known as a *heteroclinic connection*. Note that two stable manifolds can never intersect, and likewise for unstable manifolds, because the map $\Lambda$ is invertible. The key factor is not whether intersections are homoclinic or heteroclinic, but whether they are tangent or transverse. Tangent intersections occur when the stable and unstable manifolds exactly coincide, either creating a separatrix connecting two periodic points, or an enclosed loop that confines the fluid within, as demonstrated in Fig. 4.8(a). When an enclosed loop is formed there is always at least one elliptic periodic point in the enclosed region, since the enclosing manifold curve has a
fixed point index equal to +1. On the other hand, when the manifolds intersect transversely, they must intersect infinitely many times, producing a complex tangle between the two curves, as demonstrated in Fig. 4.8(b). These transverse manifold connections are the signature of chaos, producing the stretching and folding motions required to create an exponential increase in the length of material curves, as shown in Fig. 4.8(c).

### 4.3.2 3D systems

Many of the structures and properties of periodic points in 2D area-preserving systems have analogues in 3D volume-preserving systems. This is especially true when periodic points occur as a smooth curve called a periodic line, as particle transport in the neighbourhood of the line is approximately 2D. Since periodic points in the 3DRPM flow generically appear as periodic lines, these are the focus of attention in this section, for a more general exposition of periodic point classification in 3D see [CPC90, Ott89]. In Chapter 6 the periodic lines and associated structures will be studied in greater detail, focusing on the bifurcations that occur at degenerate points and the impact that they have on the organisation of transport.

For a volume-preserving map, the product of the eigenvalues, $\lambda_1\lambda_2\lambda_3$ is equal to 1. If one of the eigenvalues, say $\lambda_3$, is equal to 1, then in a neighbourhood of the
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Figure 4.9: The 2D unstable manifold $W^{u}_{2D}$ for one of the period-3 lines for $\Theta = 2\pi/3$ and $\tau = 1.1\tau_0$, where $\tau_0$ is defined and discussed in Chapter 6. The manifold consists of the disjoint union of 1D manifolds for points along the hyperbolic segment of the periodic line, coloured according to the $y$-coordinate, $y = 0$ (dark red) to maximum (white).

periodic point there is no transport in the direction of the corresponding eigenvector $v_3$, called the null direction. Therefore in an infinitesimally small region around a periodic point with a null direction the map $x' = \Lambda(x)$ can be written as

$$
\begin{align*}
\xi_1' &= f_1(\xi_1, \xi_2; \xi_3), \\
\xi_2' &= f_2(\xi_1, \xi_2; \xi_3), \\
\xi_3' &= \xi_3,
\end{align*}
$$

(4.30)

where $\xi_i$ corresponds to the coordinate in the direction of the eigenvector $v_i$. The result is a 2D system contained in the plane spanned by the two transverse directions $v_{1,2}$. In this case the periodic point forms part of a continuous curve of periodic points, with the line continuing in the null direction [MMS+02]. At each point on the periodic line the null direction provides a local invariant $\xi_3$ according to eq. (4.30). Conversely if a local invariant exists in a region containing a periodic point then there is no transport transverse to the local invariant surfaces, providing a null direction. While it is sufficient, it is not necessary for a system to admit a global invariant for periodic lines to exist, as is demonstrated by the 3DRPM flow.

As in 2D systems, the constraint that the product of the eigenvalues must be equal to 1 limits the possible types of periodic point. When one eigenvalue, say $\lambda_3$, is equal to 1, then $\lambda_1 \lambda_2 = 1$ and the three types of 2D periodic points (elliptic, hyperbolic, degenerate) apply in 3D as well. The structures associated with each
type of 2D periodic point naturally extend to 3D systems with periodic lines as they can be thought of as a nested set of locally 2D systems according to eq. 4.30. KAM-tori become KAM-tubes and the 1D manifolds of the nested 2D systems combine to create 2D manifold surfaces

\[ W_{2D}^{s,u} = \bigsqcup_{x_0 \in S} W^{s,u}(x_0) \] (4.31)

where \(\sqcup\) is the disjoint union and \(S\) is a hyperbolic segment of a periodic line. An example of this for the 3DRPM flow is shown in Fig. 4.9 where each curve (white to dark red) is the 1D unstable manifold for a single point \(W^u(x_0)\) on the hyperbolic segment of a period-3 line, the union of which form the 2D unstable manifold surface. Similar to 1D manifolds in 2D systems, the manifolds \(W_{2D}^{s,u}\) are invariant, and form barriers to fluid transport as they are co-dimension 1. As in 2D systems the nature of manifold intersections plays a significant role in the overall transport dynamics, with tangent intersections creating separated volumes, and transverse intersections creating the stretching and folding required for chaos. However, since the 2D manifolds are formed from the 1D manifolds of individual points along the periodic line, it is possible that a single 2D manifold will have a combination of transverse, tangent, homoclinic and heteroclinic connections. This is the case in Fig. 4.9, where it is seen that for greater \(y\)-values (closer to white) the 1D curves loop back to their initial position, forming tangent homoclinic connections, however at a critical value of \(y\) the 1D manifolds develop a wavy pattern that indicates the presence of transverse connections and chaos.

4.3.3 Computational method to find and classify periodic points in the 3DRPM flow

A numerical approach is used to find and classify periodic points in the 3DRPM flow, focusing on period-1 and period-3 points since they have a dominant influence on the resulting Lagrangian dynamics when \(\Theta = 2\pi/3\). For rotation angles of the form \(2\pi m/n\) with \(n\) odd, the period-1 and period-\(n\) points will have the most influence\(^1\), while for even \(n\) or reorientation angles \(\Theta\) that are incommensurate with \(\pi\) (i.e. \(\Theta/\pi\) is irrational), fundamentally different phenomena occur due to the difference in the nature of the degenerate periodic points along the \(y\)-axis in the limit as \(\tau \to 0\).

\(^*\)As for 2D systems stable manifolds cannot intersect other stable manifolds, and likewise for unstable manifolds, so the 1D manifolds that comprise a 2D manifold cannot intersect and must be disjoint.

\(^1\)Note that the period-1 and period-\(n\) points in the rotating dipole frame are all period-1 points in the laboratory frame.
reflection reversal symmetry eq. (3.27) means all periodic points must be distributed symmetrically about the symmetry plane \( z = \tan(-\Theta/2)x \). Furthermore, as the map \( Y_\Theta^\tau \) is the composition of a map \( \hat{Y}_\tau \) that preserves the azimuth \( \theta = \arctan(y/x) \), and a rotation \( R_{-\Theta}^y \), it follows that period-1 points satisfy \( x = (Y_\Theta^\tau)^{-1}(x) = (\hat{Y}_\tau)^{-1}R_{-\Theta}^y(x) \), and the azimuthal angle of \( R_{-\Theta}^y(x) \) must equal the azimuthal angle of \( x = (x, y, z) \).

This can be expressed as

\[
\arctan \left( \frac{y}{x \cos \Theta - z \sin \Theta} \right) = \arctan \left( \frac{y}{x} \right),
\]

and implies that either \( z = \tan(-\Theta/2)x \) (i.e. the point is on the symmetry plane) or \( y = 0 \) and the point is on the \( xz \)-plane. Since the \( xz \)-plane is invariant and contains all the dipole locations, it is qualitatively similar to the 2D RPM flow, for which it can be shown that period-1 points must lie on the symmetry plane by essentially the same argument as above except using the streamfunction \( \Psi \) instead of the azimuthal angle \( \theta \) [LMT+09]. This also applies to the 3D RPM flow, as the streamfunction \( \Psi \) is conserved by the steady dipole advection \( \hat{Y}_\tau \), and so a period-1 point must satisfy \( \Psi(R_{-\Theta}^y(x)) = \Psi(x) \). Therefore, all period-1 points must lie on the symmetry plane \( z = \tan(-\Theta/2)x \). It is observed that all periodic points in the 3D RPM flow with odd period occur as smooth curves, each intersecting the \( xz \)-plane, i.e. no isolated odd periodic points have been found. Therefore, the initial search for periodic points is further restricted to the line given by the intersection of the symmetry plane and the \( xz \)-plane, which significantly reduces the search space. Solutions to \( (Y_\Theta^\tau)^N(x) = x \) are found by sampling a number of points along the line of intersection of the symmetry plane and \( xz \)-plane and measuring the difference \( |(Y_\Theta^\tau)^N(x) - x| \) that needs to be minimised. Resolution is increased around local minima until the desired resolution is reached \( |(Y_\Theta^\tau)^N(x) - x| < 10^{-6} \).

Once all the solutions to \( (Y_\Theta^\tau)^N(x) = x \) have been found, the deformation tensor for each is computed numerically using a 2nd order central difference scheme to approximate the partial derivatives

\[
\frac{\partial (Y_\Theta^\tau)^N}{\partial x_j} \approx \frac{1}{2h} \left( (Y_\Theta^\tau)^N(x + he_j) - (Y_\Theta^\tau)^N(x - he_j) \right),
\]

where \( e_j \) is the unit vector in the direction \( x_j \) and \( h \ll 1 \). From the deformation tensor the null direction is found as the eigenvector corresponding to the eigenvalue equal to 1. This null direction is then used as a first approximation to find the periodic point a fixed distance \( \delta = 0.001 \) away along the periodic line. The deformation tensor also determines the stability of the periodic point, and the eigenvalues and eigenvectors are recorded. This process is repeated until the periodic line terminates, either reaching the outer boundary of the domain, or looping back around
Figure 4.10: Periodic lines in the 3DRPM flow. a Period-1 lines shown in the symmetry plane for $(\Theta, \tau) = (2\pi/3, 1.3)$. Elliptic and hyperbolic segments are coloured blue and red respectively. Bifurcation points are illustrated as open squares (period-doubling), open circles (period-tripling) and closed circles (saddle–centre). b The period-1 and period-3 lines for $(\Theta, \tau) = (2\pi/3, 1.1\tau_0)$, $\tau_0$ is the value of $\tau$ such that the period-1 lines intersect the $y$-axis at the origin at integer multiples of $\tau_0$. The significance of this value is explored in greater detail in Chapter 6.

to the $xz$-plane so that the periodic line forms a closed loop when considering both hemispheres.

The typical nature of period-1 lines in the 3DRPM flow is shown in Fig. 4.10. Only the points in the $y^+$ hemisphere are shown, since those in the $y^-$ hemisphere can be obtained by reflection through the $xz$-plane. At degenerate points there are three types of bifurcation that occur in the 3DRPM flow: period-tripling bifurcations (open circles), saddle–centre bifurcations (closed circles), and period-doubling bifurcations (squares), the consequences of which are explored in Chapter 6.

**Stable and unstable manifolds**

The stable and unstable manifolds associated with hyperbolic points are found using a fairly simple technique. For the unstable manifold, a number of particles are placed along the eigenvector corresponding to expansion, close to the periodic point, as shown in Fig. 4.11(a). The particles are then advected for some number of flow periods, tracing out the manifold. By definition the particles will spread exponentially, with exponent given by the logarithm of the corresponding eigenvalue. Good resolution of the manifold can be achieved by starting with a very large number of particles, but this is inefficient and particle separation will eventually become large. To avoid this, a scheme has been implemented that adaptively inserts new points
when a tolerance $\delta$ for the particle separation distance is exceeded. If after $k$ flow periods the distance between neighbouring particles exceeds $\delta$, as in Fig. 4.11(c), then particles are inserted between those points at the previous flow period $n = (k - 1)$, demonstrated by the cyan points in Fig. 4.11(c,d). These new particles can be inserted using any interpolation method. Here cubic interpolation is used, though there is no qualitative difference when linear interpolation is used instead. Examples of the manifolds produced using this method are shown in Fig. 6.9. This method can be tuned by adjusting the length of the initial line of particles (smaller is better), the tolerance in the distance between particles along the manifold, and the interpolation method used to insert particles when the tolerance is exceeded.

The stable manifold is essentially the same, except particles are advected backwards in time starting from the eigenvector corresponding to contraction.
Figure 4.11: Schematic diagram of the method used to compute stable and unstable manifolds. (a) The initial set of points (green) lying on the eigenvector with eigenvalue greater than 1. (b) The computed manifold (green points) on the actual unstable manifold (black) after \( k - 1 \) flow periods. The separation of all neighbouring points is less than the threshold \( \delta \). (c) After \( k \) flow periods the separation of one pair of neighbouring particles is greater than \( \delta \), so new particles (pink) are inserted at the previous step, (d), so that the separation of all particles is less than \( \delta \) after \( k \) periods, as in (e).
4.4 Lyapunov exponents

Lyapunov exponents are used to quantify the exponential divergence of nearby particles that characterises chaotic advection. For a filament $dX$ located at $X$ with initial orientation $M_i$, the rate of divergence is measured by the Lyapunov exponent

$$\sigma(X, M_i) = \lim_{t \to \infty} \frac{1}{t} \lim_{dX \to 0} \ln \left( \frac{|dX(t)|}{|dX|} \right), \quad (4.34)$$

where $dX(t)$ denotes the deformation of the filament $dX$ after time $t$ [Ott89]. For $d$-dimensional volume-preserving flows there are $d$ Lyapunov exponents $\sigma_1, \ldots, \sigma_d$, whose sum is zero. In ergodic regions the Lyapunov exponents are independent of the starting position, as in the limit as $t \to \infty$ the orbit of a particle in an ergodic region will densely and evenly cover the entire region.

A similar formulation applies to discrete maps $\Lambda$. The Lyapunov exponent for the filament $dX$ located at $X$ with initial orientation $M_i$ is

$$\sigma(X, M_i) = \lim_{N \to \infty} \frac{1}{N} \lim_{dX \to 0} \ln \left( \frac{|\Lambda^N(dX)|}{|dX|} \right). \quad (4.35)$$

For periodic flows such as the 2D and 3D RPM flows this definition is used to find the Lyapunov exponents, using the maps $\Upsilon_{\tau}, \Upsilon_{\theta}^\tau$. For 2D systems such as the 2DRPM flow, there are two Lyapunov exponents $\sigma_1 = -\sigma_2 > 0$, and for a given initial condition, almost all* initial orientations $M_i$ will converge to the positive exponent $\sigma_1$. Therefore, in an ergodic region it is only necessary to consider the evolution of a single filament $dX$, initially located at $X$ with orientation $M_i$, to find the Lyapunov exponents of the region as a whole.

To compute Lyapunov exponents numerically a variant of the Benettin algorithm [BGGS80] is used, an initial particle location $x_0$ is chosen in the ergodic region, and a second point $z_0$ is chosen, close to the first (here $10^{-6}$ separation is used). These two points define the position $x_0$ and orientation $z_0 - x_0$ of the filament $dX$, and by iterating them the values $|\Lambda^N(dX)|/|dX|$ can be found. Now, it is assumed that the magnitudes $|dx_N| = |\Lambda^N(dX)| = |z_N - x_N|$ and $|dX|$ are both small, as the Lyapunov exponent is defined in the limit as $dX \to 0$. However, in chaotic systems the separation of the two initial particles will grow exponentially. Therefore, a threshold $\epsilon$ is set such that when the separation of the two particles $|dx_N| > \epsilon$, the filament $dx_N$ is re-normalised to $\tilde{dx}_N$ with magnitude $\delta|dx_N|$, where $0 < \delta < 1$ is chosen sufficiently small. Then the equation

$$\frac{|dx_N|}{|dX|} = \frac{1}{\delta} \frac{|\tilde{dx}_N|}{|dX|} \quad (4.36)$$

can be substituted into eq. (4.35) to find the Lyapunov exponent.

*In the measure theoretic sense, i.e. all except in a set of measure zero.
4.5 The mix-norm: a multiscale measure for mixing

While the Lyapunov exponent is a good measure for mixing in systems with smooth deformations, where mixing is created by stretching and folding, it is not able to capture the effects of discontinuous cutting and shuffling actions, that occur in both the 2D and 3D RPM flows. To counter this, Mathew et al. [MMP05] have introduced the mix-norm, that is able to measure the quality and rate of mixing even when the Lyapunov exponent is zero, and no stretching is involved.

4.5.1 Formulation

For a concentration field $c(x)$ with mean zero defined on the $n$-torus $\mathbb{T}^n = \mathbb{R}^n/\mathbb{Z}^n$, a point $p \in \mathbb{T}^n$ and a length-scale $s$, the average of $c$ over the ball $B(p, s) = \{x : |x - p| < s/2\}$ is

$$d(c, p, s) = \frac{1}{\text{vol}(B(p, s))} \int_{x \in B(p, s)} c(x) \mu(dx)$$

(4.37)

where $\mu$ denotes the Lebesgue measure, i.e. standard integration in $\mathbb{R}^n$. Before defining the mix-norm, the intermediate function $\phi(c, s)$ is defined as the $L^2$-norm of the function $d(c, p, s)$ over all points $p \in \mathbb{T}^n$, i.e.

$$\phi(c, s) = \left( \int_{p \in \mathbb{T}^n} d^2(c, p, s) \mu(dp) \right)^{1/2}.$$  

(4.38)

This function is a measure of how well mixed the concentration field $c$ is at the length-scale $s$. A concentration field that is very well mixed at a given length-scale $s$ will have average $d(c, p, s)$ close to zero for all points within the domain, and therefore $\phi(c, s)$ will be small as well. Finally, the mix-norm $\Phi(c)$ is defined as the $L^2$-norm of $\phi(c, s)$ over length-scales in the range 0 to 1, i.e.

$$\Phi(c) = \left( \int_{s=0}^1 \phi^2(c, s) \mu(ds) \right)^{1/2}$$

(4.39)

which is a combined measure of how well mixed $c$ is over all length-scales. Note that this definition given by Mathew et al. [MMP05] can be readily generalised to other topologies, with the only change necessary being the range of length scales $s$ in eq. (4.39).

4.5.2 Numerical computation

To compute the mix-norm of an initial concentration field $c_0(x)$, and its iterates under an invertible map $\Lambda : \mathbb{T}^n \rightarrow \mathbb{T}^n$, the concentration field is sampled after each
iteration on a regular grid, and then the integrals (4.37–4.39) are approximated
using Riemann sums. Note that this is different to the method outlined in [MMP05]
which uses a Fourier transform of the sampled concentration field. This is because
here the primary interest is computing the mix-norm in cases where discontinuous
deformations are involved. Therefore, the concentration fields will not be smooth,
and this can create significant errors in Fourier transforms. Additionally, the method
used here has the advantage that it can be used for more complex geometries than
the \( n \)-dimensional torus.

The concentration after \( N \) iterations of the map \( \Lambda \) at a point \( x \) is
\[
c_N(x) = c_0 \left( \Lambda^{-N}(x) \right).
\] (4.40)

This is used to find the concentration on a regular grid of points in \( \mathbb{T}^n \). Note that
for the remainder of this section it is assumed that the domain is 2D, i.e. \( n = 2 \),
though the methods can be easily extended to other dimensions. The integral (4.37)
can be approximated as
\[
d(c_N, p, s) \approx \frac{1}{\pi (s/2)^2} \sum_{x_{i,j} \in B(p,s)} c_N(x_{i,j}) \Delta x \Delta y,
\] (4.41)
where the grid points \( x_{i,j} \) are separated by \( \Delta x \) and \( \Delta y \) in the \( x \) and \( y \) directions
respectively. Next, the function \( \phi^2(c_N, s) \) can be approximated as
\[
\phi^2(c_N, s) \approx \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_y-1} d^2(c_N, x_{i,j}, s) \Delta x \Delta y,
\] (4.42)
where \( N_x = 1/\Delta x \) and \( N_y = 1/\Delta y \) are the number of points in the \( x \) and \( y \) directions
respectively. Lastly, the square of the mix-norm \( \Phi^2(c_N) \) can be approximated by
sampling \( \phi^2(c_N, s) \) over a suitable range of \( s \) values, \( \{s_k\} \), and computing the
integral numerically. This last integral over \( s \) can be performed using methods such
as the trapezoidal rule, Simpson’s rule etc. There are two methods used here to
approximate the integral of \( \phi^2(c_N, s) \), depending on the shape of the function. At
small numbers of iterations \( N \), \( \phi^2(c_N, s) \) is generally well approximated by cubic in-
terpolations, so the cubic interpolation function is found and integrated. However,
at higher numbers of iterations, when the concentration field is typically well-mixed,
the function \( \phi^2(c_N, s) \) has a steep descent from the \( s = 0 \) value, as seen in Fig. 4.15,
4.16, 4.18, and cubic interpolation is not satisfactory in these cases. In these cases
the first four \( s \) values \( s = 0, s_1, s_2, s_3 \) are used to find a fit of the form \( ae^{bs} + c \). This
is then integrated from \( s = 0 \) to \( s_1 \), and a cubic interpolation is used to approximate
the integral from \( s_1 \) onwards as before.
To obtain a high accuracy computation of the mix-norm, a high resolution sampling grid is required, increasing the computation time. There are a number of ways to reduce the computation time for a given resolution. First, letting $A_k$ denote the gridpoints $x_{i,j}$ that are contained in the ball $B(\mathbf{0},s_k)$, then the average of $c_N$ over the ball $B(x_{i,j},s_k)$ centred at one of the gridpoints is approximated as

$$d(c_N,x_{i,j},s_k) \approx \frac{\Delta x \Delta y}{\pi (s_k/2)^2} \sum_{(n,m) \in A_k} c_N(x_{i+n,j+m}) = \frac{4 \Delta x \Delta y}{\pi s_k^2} \sigma_{i,j,k},$$  \hspace{1cm} (4.43)$$

i.e. $A_k$ is shifted to the gridpoint $x_{i,j}$. Substituting eq. (4.43) into eq. (4.42) yields

$$\phi^2(c_N,s_k) \approx \Delta x \Delta y \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_y-1} \left( \frac{4 \Delta x \Delta y}{\pi s_k^2} \sigma_{i,j,k} \right)^2$$

$$= \frac{16 \Delta x^3 \Delta y^3}{\pi^2 s_k^4} \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_y-1} \sigma_{i,j,k}^2$$ \hspace{1cm} (4.44)$$

so the problem reduces to finding the values $\sigma_{i,j,k}$. Now, the set $A_{k-1}$ is contained within the set $A_k$, so

$$\sigma_{i,j,k} = \sum_{(n,m) \in A_k} c_N(x_{i+n,j+m}) = \sigma_{i,j,k-1} + \sum_{(n,m) \in A_k \setminus A_{k-1}} c_N(x_{i+n,j+m}).$$ \hspace{1cm} (4.45)$$

This recurrence relation saves computational time by not having to repeat the same sums that have previously been computed. The method implemented here uses this recurrence relation to step through $k$ values, and the computations over $i$ and $j$ are distributed to parallel CPUs.

4.5.3 Examples

To see how the mix-norm behaves, three prototypical examples are considered. In the Baker’s map and the Standard Map mixing is achieved by the repeated stretching and folding of fluid, whereas in an Interval Exchange Transformation (IET) mixing is created by cutting and shuffling of fluid, like shuffling a deck of cards $^*$. For each map, the same initial concentration field $c_0(x,y) = \cos(2\pi y)$ (shown in Fig. 4.12) is used, and the mix-norm is calculated for 10 iterations (Fig. 4.13).

The Baker’s map

The Baker’s map is analogous to a baker stretching out dough to double its original length, then cutting the dough in two and stacking the two pieces together. This

$^*$Note that a similar comparison between the Baker’s map and IET’s is carried out in [CLO11].
4.5. THE MIX-NORM: A MULTISCALE MEASURE FOR MIXING

Figure 4.12: The initial concentration field \( c_0(x, y) = \cos(2\pi y) \) that is iterated under the Standard map, Baker’s map and an Interval Exchange Transformation (IET) to demonstrate properties of the mix-norm.

is a highly efficient mixing method and many fluid mixers have been designed that attempt to replicate this process [GAPM03, SHH04, LMT13]. The map is given by

\[
\Lambda_{BM}(x, y) = \left( 2x - \lfloor 2x \rfloor, \frac{1}{2} (y + \lfloor 2x \rfloor) \right)
\]  

(4.46)

where \( \lfloor a \rfloor \) denotes the largest integer less than \( a \) (the floor function). A schematic of this map is shown in Fig. 4.14, consisting of stretching of fluid followed by cutting and stacking. The Baker’s map is invertible, with inverse

\[
\Lambda_{BM}^{-1}(x, y) = \left( x + \frac{\lfloor 2y \rfloor}{2}, 2y - \lfloor 2y \rfloor \right).
\]  

(4.47)

While the cutting and stacking motion introduces a discontinuous deformation, this only occurs on a set of measure zero, everywhere else the fluid experiences horizontal stretching by a factor of 2 and vertical contraction by a factor of \( 1/2 \). Therefore the Lyapunov exponent is \( \ln 2 \).

The concentration fields \( c_N \) (Fig. 4.15) rapidly become mixed under the Baker’s map, and after 4 iterations the function \( \phi(c_N, s) \) is close to zero for all length-scales greater than 0.3. For the Baker’s map the mix-norm \( \Phi(c_N) \) decreases exponentially, as shown by the linear trend in Fig. 4.13 which uses a logarithmic scale on the vertical axis. Performing a linear regression, the exponent is \(-0.3436\), which is close in magnitude to half the Lyapunov exponent \( (\ln 2)/2 \approx 0.3466 \). This exponential decay of the mix-norm with exponent equal to half the Lyapunov exponent is expected for systems where the deformation is uniform throughout the domain [MMP05].
The Standard Map

The Standard Map is used as the main example by Mathew et al. [MMP05] to study the mix-norm. Unlike the Baker’s map it is smooth and the deformation tensor is defined everywhere. The map is given by

\[ \Lambda_{SM}(x, y) = (x + y + \epsilon \sin(2\pi x), y + \epsilon \sin(2\pi x)) \mod 1, \]

with perturbation parameter \( \epsilon \) controlling the transport dynamics. At \( \epsilon = 0.4 \) the map has both chaotic and non-mixing regions, as evidenced by the sequence of concentration fields shown in Fig. 4.16. Even though the Lyapunov exponent is positive in the chaotic region, the mix-norm does not decay exponentially (Fig. 4.13) due to the presence of the non-mixing regions.
4.5. THE MIX-NORM: A MULTISCALE MEASURE FOR MIXING

Figure 4.15: (a) Iterations $c_N$ of the initial concentration field $c_0(x, y) = \cos(2\pi y)$ under the Baker’s map eq. (4.46) for $N = 1, 2, 3, 4$ iterations. (b) The corresponding functions $\phi(c_N, s)$, measuring the degree of mixing at each length scale $s$. 
Figure 4.16: (a) Iterations $c_N$ of the initial concentration field $c_0(x, y) = \cos(2\pi y)$ under the Standard map eq. (4.48) with $\epsilon = 0.4$ for $N = 1, 2, 4, 8$ iterations. (b) The corresponding functions $\phi(c_N, s)$, measuring the degree of mixing at each length scale $s$. 
Interval Exchange Transformation

Interval Exchange Transformations (IETs) provide examples of systems where mixing can be achieved without stretching. They consist of cutting the domain into a set of rectangles that span the length of the domain, and then shuffling the rectangles according to a fixed permutation \( \Pi \), as demonstrated in Fig. 4.17. Following Krotter et al. [KCOL12] a specific type of IET is implemented that is guaranteed to produce mixing. The height of the domain is divided into \( N \) disjoint segments \( \mathcal{S} = \{ \mathcal{I}_1, \ldots, \mathcal{I}_N \} \), such that the lengths \( |\mathcal{I}_i| \) differ by a fixed ratio \( |\mathcal{I}_i|/|\mathcal{I}_{i-1}| = r \geq 1 \). Since the sum of the lengths \( |\mathcal{I}_i| \) must sum to 1, the length \( l \) of the interval \( \mathcal{I}_1 \) satisfies

\[
\sum_{i=1}^{N} r^{i-1}l = 1 \tag{4.49}
\]

which implies that

\[
l = \frac{r - 1}{r^N - 1}. \tag{4.50}
\]

Therefore \( r \) and \( N \) determine the intervals that form the rectangles that will be shuffled.

As an example, \( r = 1 + \pi/30 \), \( N = 5 \), and \( \Pi(12345) = 25413 \) are used since they satisfy the Keane minimality condition [Via06, KCOL12], meaning the resulting IET will be weakly mixing. The action of this map on the initial concentration field Fig. 4.12 is shown in Fig. 4.18, the first iteration has mixing comparable to the Baker’s Map and Standard Map, but after that the mixing is much slower. In contrast to the Baker’s Map and Standard Map, this IET does not stretch fluid, and has Lyapunov exponent equal to zero. However, it is still able to mix fluid sub-exponentially, as is quantified by the sub-exponential decay rate of the mix-norm in Fig. 4.13. While the mix-norm for this IET is greater than that of the Standard Map after 10 iterations, the mix-norm of the Standard Map will asymptote due to the presence of non-mixing regions whereas the mix-norm for the IET will continue to decay towards zero. Therefore there will be some number of iterations after which the IET has a lower mix-norm than the Standard Map.

![Figure 4.17: Schematic diagram of the IET with \( r = 1.5 \), \( N = 4 \) and \( \Pi = 3142 \).](image)
Figure 4.18: (a) Iterations $c_N$ of the initial concentration field $c_0(x, y) = \cos(2\pi y)$ under the Interval Exchange Transformation shown in Fig. 4.17 for $N = 1, 2, 4, 8$ iterations. (b) The corresponding functions $\phi(c_N, s)$, measuring the degree of mixing at each length scale $s$. 
4.6 Change detection in time series by a zoning method

An important tool in the study of the transition to 3D transport in the 3DRPM flow is the adiabatic invariant $G_R$ (introduced in §3.2.5), as transport transverse to the iso-surfaces of $G_R$ represents fully 3D transport. Therefore, a method to detect changes in $G_R$ as time evolves is needed. This is complicated by the inexact nature of the adiabatic invariant $G_R$, meaning that the time series $\{g_i = G_R(x_i)\}_{i=1}^N$ corresponding to the particle trajectory $x_i = Y^\Theta(x_{i-1})$ is noisy, as illustrated by Fig. 4.19. In this time series it is noted that the particle tends to oscillate around a value of $G_R$ before jumping to a new value of $G_R$. This ‘shell jumping’ is typical of the particle transport throughout the entire domain and across a broad range of $\tau$ values.

Detection of the jumps is performed using the data zoning method introduced by Hawkins [Haw72, HM73], which divides a sequential dataset into segments such that the piecewise constant approximation is optimised. Essentially, for a dataset $x_1, \ldots, x_N$ and a zoning into $k$ segments, the homogeneity of each segment can be measured by the sum of squared deviations of the segment’s points from the segment’s mean, for example for the segment $x_i, \ldots, x_j$ ($i < j$) this sum is

$$r(i, j) = \sum_{k=i}^{j} (x_k - \bar{x}_{i,j})^2,$$

where $\bar{x}_{i,j}$ is the average of the data $x_i, \ldots, x_j$. Then for the $k$ segments $\{x_1, \ldots, x_{n_1}\}$, $\{x_{n_1+1}, \ldots, x_{n_2}\}$, up to $\{x_{n_{k-1}+1}, \ldots, x_N\}$, the total quality of the zoning can be measured by

$$W(Z) = r(1, n_1) + r(n_1 + 1, n_2) + \cdots + r(n_{k-1} + 1, N),$$

Figure 4.19: A time series of the adiabatic invariant $G_R$ corresponding to 1,000 iterations of a particle in the 3DRPM flow with $(\Theta, \tau) = (2\pi/3, 0.1159)$. 

![Image](image-url)
where $Z = \{n_1, \ldots, n_{k-1}\}$ denotes the set of zone boundaries. The zoning $Z$ is an optimal $k$-zoning if $W$ is minimized, which is found by considering the values

$$F_j(m) = \min_{Z \in Z_j^m} W(Z),$$

(4.53)

where $Z_j^m$ is the set of possible $j$-zonings of the first $m$ points $x_1, \ldots, x_m$, i.e. $F_j(m)$ is the value of $W$ corresponding to the optimal zoning of the first $m$ points. For a single zone there is no segmentation, so $F_1(m) = r(1, m)$ for $m = 1, \ldots, N$. Also, if $\{n_1, \ldots, n_{j-1}\}$ is an optimal zoning of the first $m$ points, then the zoning $\{n_1, \ldots, n_{j-2}\}$ must be an optimal zoning of the first $n_{j-1}$ points, which gives the recurrence relation

$$F_j(m) = \min_{1 \leq n \leq m} [F_{j-1}(n) + r(n+1, m)].$$

(4.54)

Therefore, for the optimal $k$-zoning of the original data, the value of $W$ is $F_k(N)$, and the boundaries of the optimal zones can be found from a ‘traceback’. When computing $F_k(N)$, the value of $n$ that minimised $F_{k-1}(n) + r(n+1, N)$ gives $n_{k-1}$, and the value of $n$ that minimised $F_{k-2}(n) + r(n+1, n_{k-1})$ gives $n_{k-2}$. Repeating this process gives the entire set of zone boundaries. Therefore, the process of the algorithm is to form a table of the values $F_j(m)$ for $m = 1, \ldots, N$ and $j = 1, \ldots, k$ while also noting which values of $n$ are used in the equation (4.54). An example of the zoning method applied to the time series Fig. 4.19 is shown in Fig. 4.20.
4.6.1 Issues and solutions

While effective, this method has limitations. First, it is not possible to know a priori how many zones should be used for a given dataset, this therefore has to be adjusted manually. Also, the computation time is proportional to $kN^2$, so for large datasets the computation takes a very long time. This is overcome using two methods. First, the dataset can be broken up into smaller datasets, which reduces the computation time and still detects jumps in the time series. However, this also means that if the zones of the subsets are recombined the resulting zoning will not be optimal. The computation time can also be reduced by sampling the data at fixed intervals, i.e. forming a new dataset with every $i^{th}$ point of the original dataset and then performing the zoning. This is effective if the original data varies slowly and is qualitatively the same after sampling, as in Fig. 4.21 where the blue time series is a sample of the original black time series taking every $5^{th}$ point. In this case the number of iterations is reduced from 5,000 to 1,000 without affecting the jumps in the original time series.

Another issue occurs when regions of the data have high amplitude oscillations, such as in Fig. 4.22. These regions correspond to quasi-periodic orbits. In this case

![Zoning of a $G_R$ time series with 5,000 iterations of a particle for $(\Theta, \tau) = (2\pi/3, 0.04096)$. The original data is shown in black, and is sampled every 5 iterations (blue). The blue time series is zoned, with piecewise approximation shown in orange.](image-url)
the zoning method creates zone boundaries within quasi-periodic regions, as shown in Fig. 4.22(a), which do not appear to correspond to changes in the time series. This is overcome by considering the frequency spectrum obtained via a Fourier transform in a small region of time close to each zone. The width of this region is determined by finding the 3 closest local maxima to the zone location $m_1 < m_2 < m_3$, so for a periodic signal $m_3 - m_1$ will correspond to approximately 2 periods, and $3/2(m_3 - m_1)$ corresponds to approximately 3 periods. The width $N = 2n + 1$ of the region around the zone is then chosen as $n = \lceil 3/4(m_3 - m_1) \rceil$, where $\lceil x \rceil$ denotes the ceiling of $x$, i.e. the smallest integer greater than $x$. With this choice of width, corresponding to approximately 3 periods, it is expected that in a periodic region the transformed sequence

$$X_k = \sum_{j=0}^{N-1} x_j e^{-2\pi ikj/N} \quad (4.55)$$

will have a peak at $|X_3|$. To determine the existence of periodicity in each region around the zone boundaries, Fisher’s test can be used [Fis29]. This is performed by normalising the transformed sequence $\{X_k\}_{k=0}^{N-1}$ as

$$Y_k = \frac{|X_k|^2}{\sum_{j=1}^{n} |X_j|^2}, \quad \text{for } k = 1, \ldots, n, \quad (4.56)$$

and if $S = \max Y_k$ exceeds the critical value $g_F(n, \alpha)$ (see [Fis29, Sie80, Ant95]), then a periodicity exists with significance $p < \alpha$. However, an issue with this is that the jumps in the time series near ‘good’ zone boundaries appear in the Fourier spectra as peaks at $X_1$, as expected for a step function. This has two effects, first, it reduces the relative peak $Y_k$ at higher frequencies (as they all sum to 1). Second, Fisher’s test will determine that a large number of zones contain periodicity though they may only contain a step. Therefore, a zone boundary is determined to be in a region of periodicity and not a true ‘jump’, if $S_3 = \max_{k=3} Y_k > \lambda g_F(n, \alpha)$ and $Y_1 < \lambda g_F(n, \alpha)$. Here $0 < \lambda \leq 1$ is chosen to adjust for the possibility of both a jump and a periodicity, or the possibility of multiple periodicities as per Siegel’s test [Sie80]. Several values of $\lambda$ were tested, balancing the preservation of jumps and the removal of zone boundaries in quasi-periodic regions, and $\lambda = 0.4$ was found to produce consistently good results, as demonstrated in Fig. 4.22(b) compared to Fig. 4.22(a).
4.6. CHANGE DETECTION IN TIME SERIES BY A ZONING METHOD

Figure 4.22: Two zonings of a time series of the adiabatic invariant $G_R$ for 1,000 iterations of a particle with $(\Theta, \tau) = (2\pi/3, 0.1159)$. (a) The original zoning based on 40 zone boundaries (vertical grey lines) and piece-wise approximation by the median (orange). (b) Modified zoning performed by removing zones in periodic regions, as determined by the local Fourier spectrum.
Chapter 5

Mixing of Discontinuously Deforming Media

In this chapter the effect of cutting and shuffling (CS) created by the opening and closing of valves combined with free-slip boundaries is discussed, in particular the significant role it plays in the organisation of transport at low values of $\tau$ in the 2DRPM flow. Cutting and shuffling is an unexpected consequence of the dipole re-orientation. In essence, a finite fluid region that is only partially advected through the dipole is cut in two when the dipole is switched off and reoriented. The two separated fluid parcels can then move independently and in general need not re-connect. This cutting produces discontinuous deformations in the system even though the base flow (steady 2D or 3D dipole flow) is smooth.

While non-physical free-slip boundaries are necessary to produce this cutting mechanism when the injection/extraction points are on the boundary of the domain, a similar cutting mechanism occurs in systems with no-slip boundaries where fluid is extracted and reinjected from multiple points inside the domain, such as the Pulsed Source Sink (PSS) flow [JA88], and other flows with switching between multiple injection and extraction points [Col04, CSFS06, BGCR10, BO07, HSW07]. Jones and Aref [JA88] recognised that the PSS flow produced cutting of fluid, but did not examine the impact of cutting on coherent structures. The other studies fail to note the existence of cutting, which is likely due to fluid motion being dominated by classical stretching and folding (SF) actions. In the RPM flows this is also the case at larger values of $\tau$, where the effect of CS is less than SF. However, at small values of $\tau$ CS significantly affects the transport structures within the flow, ‘destroying’ many of the structures that would be expected in a smooth flow, and breaking otherwise impenetrable transport barriers such as the stable and unstable manifolds. These topics are explored in greater detail in [SRLM16], embedded in §5.1 of this chapter.
Following the paper a number of related topics are discussed:

1. The bifurcations observed at low values of $\tau$ are recognised as reconnection bifurcations associated with twistless tori, though ‘half’ of the bifurcation is destroyed by the cutting at the dipole.

2. The simple Cut-Shear-Shear (CSS) map introduced in the paper is extended to include non-perpendicular cuts and shears, which reflects the behaviour observed in the interior of the 2DRPM flow domain.

3. Using the mix-norm introduced by Mathew et al. [MMP05] the mixing rates of linear systems are compared to the same systems with a discontinuous cutting deformation added, showing that cutting can either enhance or impede mixing.

4. The discontinuous deformations in the 2DRPM flow also produce a region of high stretching that can be advected into the bulk flow*. By computing the Lyapunov exponents of individual particle trajectories the stretching produced as a consequence of the discontinuous deformation versus the stretching created by classical transport structures such as hyperbolic periodic points is decoupled and compared.

### 5.1 Publication: Mixing of discontinuously de-
forming media


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*Note that this does not refer to the discontinuous deformation itself, which could be thought of as an infinite stretch, but another mechanism that produces large but finite stretching as a consequence of the discontinuous deformation.*
Monash University

Declaration for Thesis Chapter 5
Declaration by candidate

In the case of the publication in Chapter 5, the nature and extent of my contribution to the work was the following:

<table>
<thead>
<tr>
<th>Nature of contribution</th>
<th>Extent of contribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Writing, editing, performing simulations, and data analysis.</td>
<td>85%</td>
</tr>
</tbody>
</table>

The following co-authors contributed to the work:

<table>
<thead>
<tr>
<th>Name</th>
<th>Nature of contribution</th>
<th>Extent of contribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Prof. Murray Rudman</td>
<td>Project supervision and conception, manuscript revision.</td>
<td>N/A</td>
</tr>
<tr>
<td>Dr. Daniel R. Lester</td>
<td>Project supervision and conception, manuscript revision.</td>
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<td>Prof. Guy Metcalfe</td>
<td>Project supervision and conception, manuscript revision.</td>
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</tbody>
</table>

The undersigned hereby certify that the above declaration correctly reflects the nature and extent of the candidate’s and co-authors’ contributions to this work.

Candidate’s Signature:

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Date: 19/04/2016
Mixing of discontinuously deforming media

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Mixing of materials is fundamental to many natural phenomena and engineering applications. The presence of discontinuous deformations—such as shear banding or wall slip—creates new mechanisms for mixing and transport beyond those predicted by classical dynamical systems theory. Here, we show how a novel mixing mechanism combining stretching with cutting and shuffling yields exponential mixing rates, quantified by a positive Lyapunov exponent, an impossibility for systems with cutting and shuffling alone or bounded systems with stretching alone, and demonstrate it in a fluid flow. While dynamical systems theory provides a framework for understanding mixing in smoothly deforming media, a theory of discontinuous mixing is yet to be fully developed. New methods are needed to systematize, explain, and extrapolate measurements on systems with discontinuous deformations. Here, we investigate “webs” of Lagrangian discontinuities and show that they provide a template for the overall transport dynamics. Considering slip deformations as the asymptotic limit of increasingly localised smooth shear, we also demonstrate exactly how some of the new structures introduced by discontinuous deformations are analogous to structures in smoothly deforming systems. © 2016 AIP Publishing LLC.

I. INTRODUCTION

Dynamical systems theory is the natural language of particle transport and mixing in fluid flows. Since its introduction over three decades ago, the signatures of chaos have been found in biological flows,1–7 geo- and astro-physical flows,8–11 and industrial and microfluidic flows.12–16 This approach1—termed chaotic advection—has uncovered the fundamental mechanisms which control fluid mixing and transport in natural and engineered systems.

While chaotic advection largely applies to smoothly deforming materials, there also exist large classes of materials that deform discontinuously, including granular matter, colloidal suspensions, plastics, polymers, and alloys.17,18 These materials can exhibit highly localized, discontinuous deformations such as shear banding19 and industrial and microfluidic flows.20,21 This approach1—termed chaotic advection—has uncovered the fundamental mechanisms which control fluid mixing and transport in natural and engineered systems.

Understanding the transport and mixing dynamics of these materials is critical to engineering applications such as the development of effective processing methods for granular matter, and understanding natural phenomena such as identifying the deformations which give rise to observed geological formations.

Moreover, Lagrangian discontinuities may also arise in smoothly deforming materials under certain conditions. For

When highly localized discontinuous deformations are added to an otherwise smoothly deforming medium, additional topological freedom for particle transport is created, such as “jumping” between streamlines.22 We show which structures associated with smooth dynamical systems are preserved in the presence of discontinuous deformation, which are destroyed, and the reason for each. The freedom created by discontinuous deformations enables the creation of new types of transport structures. In particular, we uncover a novel mixing mechanism that can only arise under combined stretching, cutting, and shuffling, and demonstrate this in a model fluid flow where the opening and closing of valves combined with a slip boundary condition induces fluid cutting. The mechanism is fundamentally different to both classical smoothly deforming bounded systems and systems with only cutting and shuffling as it exhibits exponential mixing rates in the absence of folding. We introduce the “webs” of Lagrangian discontinuities as a method for studying systems with both continuous and discontinuous deformations that is able to provide a template for the overall transport dynamics, including classical structures found in smoothly deforming systems and new structures that are introduced by discontinuous deformations. We show that these new structures are analogous to structures in smoothly deforming systems by considering a cut as the asymptotic limit of increasingly localized shears.
example, in fluid flows with valves and free-slip boundaries, the opening and closing of valves cuts fluid filaments, and the free-slip boundaries allow the cut to be advected into the fluid bulk. Essentially fluid is able to undergo a discontinuous slip deformation analogous to shear-banding. Valves are common to a vast array of applications, including piping networks, vascular networks, multifunctional microfluidic analysis chips, river networks with locks, and the heart (Fig. 1d). Hence, Lagrangian discontinuities arise in a wide range of flows, not just discontinuously deforming materials, and it is important to understand the mixing and transport properties of such flows.

The essence of mixing in materials that deform smoothly is stretching and folding, but discontinuous deformation introduces fluid cutting. This seemingly small change has profound consequences for mixing and transport. Cutting introduces an extra degree of topological freedom, hence the cutting action of discontinuities admits new transport and mixing mechanisms, and indeed ergodic mixing is possible in such systems by cutting and re-arranging material elements alone. While stretching and folding (SF) and cutting and shuffling (CS) can each lead to complete mixing in the sense of the unbounded increase in the interfacial area between marked parts of the continuum, the key difference is that CS does not involve material deformation; the rate of mixing, quantified by the Lyapunov exponent, in SF systems can be exponential, but in CS systems mixing can only be algebraic. In the terms of ergodic theory, CS can only achieve “weak mixing” but not the “strong mixing” characteristic of SF systems.

Discontinuous deformations cannot be represented as a smooth invertible transformation (diffeomorphism), a building block of classical dynamical systems theory. The stability of periodic points, associated manifolds and interactions captures the global dynamics for smooth systems; however, this is not the case for systems with discontinuous deformation due to the added topological freedom. We must therefore extend the scope to include other tools. We introduce the “webs” of Lagrangian discontinuities as a complete tool for studying systems with Lagrangian discontinuities. The “web of preimages” is made up of all points where material will eventually experience a discontinuous deformation, and the “web of images” comprises points where the discontinuous deformations are advected into the fluid bulk. They provide additional information to periodic point analysis, creating a template for the overall structure of the system.

In practice, materials that exhibit slip or shear-banding may deform visco-elastically prior to failure, resulting in a mix of CS and SF, and in general, a mix of CS and SF arises in all but highly idealized systems. The interactions from even vanishingly weak SF and CS are non-trivial. Mixing in these combined CS and SF systems has been considered, but the focus is typically on SF dominated systems where strong mixing occurs. While the coherent structures in CS-only systems can be understood using piecewise-isometries, there has been no previous work on understanding the new structures that can be created in systems with both CS and SF. To illustrate these concepts, we consider a model fluid flow in a parameter range where fluid deformation is dominated by CS, but weak stretching can also occur. We show that these combined dynamics produce mixing dynamics that are fundamentally different to those found in SF dominated systems or in CS-only systems. While our model flow exhibits exponential increase in interfacial area normally associated with SF systems, folding is not present. Instead, crossing of invariant curves is achieved via “streamline jumping” produced by the Lagrangian discontinuity, similarly to what occurs in CS-only systems. Using a simple map comprising composite shear and cutting motions, we demonstrate the essential physics which govern mixing of discontinuously deforming media. The generality of this map (consisting of only shearing of material and slip surfaces) means it is universal to the broad class of systems with Lagrangian discontinuities.
To probe the connection between smooth and discontinuous deformations more deeply, we consider a discontinuous slip surface as the asymptotic limit of increasingly localised shear. The new structures that are introduced by the discontinuous deformation appear as classical coherent structures when the cut is smoothed, but are destroyed in the singular limit towards a cut. These new structures therefore provide the analogues for discontinuous deformations of the classical coherent structures.

II. A SMOOTH FLOW WITH LAGRANGIAN DISCONTINUITIES

To illustrate how valves and slip boundaries are able to create discontinuous deformations of fluid that resemble slip surfaces and shear banding of materials, we consider a periodically reoriented dipole flow, the Reoriented Potential Mixing (RPM) flow.\(^{11,13,23}\) We choose RPM flow parameters such that CS dominates but some weak fluid stretching is also present. The flow is a 2D incompressible potential (Darcy) flow that approximates flow in porous media, where singularities of the dipole flow mimic valveved wellbores used in groundwater applications. The model has been studied both numerically\(^{11}\) and experimentally\(^{13}\) in the context of chaos and mixing in groundwater flow.\(^{23}\) This prototypical model introduces a mix of CS and SF dynamics based on parameters of the flow, and so is well-suited to studying the mixing dynamics from CS-dominated to SF-dominated flows. We highlight the difference between the transport behaviour in the RPM flow compared to classical dynamical systems and CS-only systems.

The RPM flow is driven by a periodically reoriented dipole flow (Fig. 2) within the unit circle, the boundary of which is a separating streamline for the unconfined flow, and hence corresponds to a free-slip boundary. After each time period \(\tau\) (non-dimensionalized by the emptying time of the domain), the dipole is instantaneously rotated by the angle \(\Theta\) to a new position and switched on again. In the limit of vanishing fluid inertia, the RPM flow can be considered piecewise steady. Hence, the parameters \(\tau, \Theta\) control the kinematics of mixing and transport in this flow. Previous studies\(^{11}\) have shown the strength of chaos and hence SF increases with increasing \(\tau\), and so we expect CS to dominate for small \(\tau\), and for large \(\tau\) the classical dynamics to dominate.

The motion of fluid particles within the flow is described by the advection equation

\[
\frac{dx}{dt} = v(x, t),
\]

where \(x\) is the position of the particle and the velocity \(v\) is controlled by \(\Theta, \tau\). We denote the position of a particle initially located at the point \(x\) after time \(T\) by \(Y_T(x)\). This advection map is area-preserving since the velocity \(v\) is incompressible. In this study, we consider the RPM flow in closed mode, such that particles are re-injected from the sink to the source along the same streamline. Example trajectories are shown in Fig. 2(b) together with the sequence of dipole orientations (see Appendix A for details on the particle tracking method).

The steady dipole flow is a 2D incompressible flow, and therefore, a one degree-of-freedom Hamiltonian system. While the tools and techniques of Hamiltonian chaos are directly applicable to mixing in 2D incompressible flows, reorientation of the dipole by switching valves combined with the slip boundary condition introduces a Lagrangian discontinuity that is advected into the bulk flow, with consequences for transport that we explore.

A. CS-dominated transport structures

To illustrate the difference between CS and SF dominated flows, we visualize Lagrangian dynamics via a Poincaré section; which for temporally periodic flow is a stroboscopic map that captures particle positions over many periods of the flow. Non-mixing regions in the Poincaré section appear as distinct “islands” (termed KAM-tori) visible in Fig. 3(a), whereas mixing regions appear as a topologically distinct “chaotic sea.” Coherent structures for classical Hamiltonian systems are largely organized by the local stability of periodic points, with low-period points playing a dominant role. Elliptic points involve local rotation only and so are locally stable, producing the non-mixing KAM-tori. Conversely, hyperbolic points are locally unstable, with a direction of contraction and a direction of expansion, and generate the chaotic sea. These features are illustrated in the Poincaré section in Fig. 3(a) for the RPM flow with \((\Theta, \tau) = (2\pi/3, 0.2)\) and are symmetric about the line \(y = \tan(-\Theta/2)x\) shown in dashed orange. The Poincaré–Birkhoff theorem states that in a Hamiltonian system the KAM-tori around an elliptic point will eventually breakup as an alternating chain of elliptic and hyperbolic points, as shown in Fig. 3(a) by the red (hyperbolic) and blue (elliptic) points. At such large values of \(\tau\), the RPM flow is dominated by SF and the organization of structures is essentially the same as a classical Hamiltonian system.

At low values of \(\tau\), the Lagrangian discontinuities play a greater role, resulting in structures that are fundamentally different to those encountered in a classical Hamiltonian system. This is seen in Fig. 3(c) which shows detail of the Poincaré section for \((\Theta, \tau) = (2\pi/3, 5.012 \times 10^{-4})\). We primarily focus on this fixed dipole rotation angle \(\Theta = 2\pi/3\) and fixed switching time \(\tau = 5.012 \times 10^{-4}\), denoted \(\tau^*\). The resulting structures violate the Poincaré–Birkhoff theorem...
because chains of elliptic points now exist that have no hyperbolic points between them. At such small values of $s$, the flow becomes less chaotic over large length scales, and particles closely follow streamlines of the steady flow $v_0$ (Fig. 3(b)) which arises in the limit $s \to 0$, consisting of an average of $v(x, t)$ over all dipole orientations. For small values of $s$, particle trajectories are perturbed slightly from the streamlines of $v_0$, leading to the small-scale structures illustrated in Fig. 3(c). This subset is representative of the small-scale behaviour across the entire domain.

It is convenient to define the streamline return time $t_{\text{return}}$ of the steady flow $v_0$ as the time it takes a particle on a given streamline to return to its initial position. The two streamlines with minimum return time are shown in dashed green and cyan, with the streamline return time, such that for integers $p, q$, if $t_{\text{return}} = p/q$ then the period of the island chain is $q$. As the Poincaré–Birkhoff theorem does not apply to flows with Lagrangian discontinuities, these KAM-tori manifest in the RPM flow as a dense tiling of islands without hyperbolic points between them. The absence of hyperbolic points is explained via a symmetry argument: as coherent structures are part of the same chain. (d) and (e) Sketches of the discontinuity produced in the velocity field by (d) co-rotating elliptic islands and (e) hyperbolic points with no elliptic orbit at the centre, such as occurs in the RPM flow.

FIG. 3. Poincaré sections for the RPM flow. (a) $(\Theta, \tau) = (2\pi/3, 0.2)$, the symmetry line $y = \tan(-\Theta/2)x$ is shown in dashed orange. Chains of elliptic and hyperbolic points are illustrated by blue and red points, respectively. (b) Streamlines of the asymptotic $(\tau \to 0)$ flow $v_0$ (black), each of which is contained in either the gray or white sectors. The two streamlines with the minimum return time are shown in dashed green and cyan, with the symmetry line again shown in dashed orange. The location of the window used for (c) is shown in pink (not to scale). (c) A small section of the Poincaré section for the RPM flow with $(\Theta, \tau) = (2\pi/3, \tau^*)$, with $\tau^*$ defined in the text. The orbit of each particle has a fixed color, showing which structures are part of the same chain. (d) and (e) Sketches of the discontinuity produced in the velocity field by (d) co-rotating elliptic islands and (e) hyperbolic points with no elliptic orbit at the centre.
positions must be hyperbolic points, as in Fig. 4(c). However, we will see in Sec. II B that the dipoles are the source of the discontinuous deformations, and any Lagrangian coherent structure that is advected onto the dipole will be destroyed, and hence destroy the entire chain of hyperbolic points. This lack of hyperbolic points allows a denser tiling of islands, a smaller chaotic set, and much slower transport between the islands. With such a dense tiling of islands, large jumps in the velocity are produced at the boundaries of neighbouring islands. As predicted by the Poincaré–Birkhoff theorem, the point between the elliptic islands in this smoothed approximation is a hyperbolic periodic point, and vice versa. In the limit of a Lagrangian discontinuity, these hyperbolic and elliptic points are destroyed by the discontinuity, and hence are denoted as “pseudo-hyperbolic points” and “pseudo-elliptic points,” respectively.

**B. Valves and wall slip acting as a slip surface**

Lagrangian discontinuities significantly influence the transport dynamics of incompressible flows. We examine how the opening and closing of valves combined with slip boundary conditions creates Lagrangian discontinuities. Fig. 5 shows how this manifests in the RPM flow (Multimedia view). Fluid cutting is achieved by closure of the valve, and once closed the slip boundaries allow the disjoint fluid elements to move independently, as occurs via the operation of the reoriented dipoles. If the disjoint fluid does not reconnect to the valve immediately before it is reopened, this discontinuity can be advected through the valve and into the bulk fluid. For flows such as the RPM with non-uniform velocities on the boundary, the “cut” appears as a slip deformation. This Lagrangian discontinuity occurs along the curve separating fluid that passes through the valve from the rest of the domain, the dot-dashed curve in Fig. 5 that is approximately semicircular. It can be found by solving $t_{valve}(x) = \tau$, where $t_{valve}$ is the time it takes a particle to reach the valve.

Under no-slip boundary conditions, fluid would remain attached to the valve and cutting could not occur. Fluid close to the valve would experience a highly localized shear that can be approximated as a cut when the boundary layer is thin. This idea is discussed in more detail in Sec. V.

**C. The webs of Lagrangian discontinuities**

We now introduce the “webs” of Lagrangian discontinuities, which provide a template for the overall transport dynamics of a system with discontinuous deformations. We demonstrate how the web alone provides information on the nature of the cutting mechanism, the location and stability of periodic points, and pseudo-periodic points.

Lagrangian discontinuities occur at locations where fluid will be cut into disconnected pieces, either via shear banding or slip or via cutting from opening and closing fluid boundaries. In the case of the RPM flow, this occurs at points that are advected onto the valve at the time when the dipole reorients, i.e., the dot-dashed curve in Fig. 5. We can extend this notion by considering locations where fluid will eventually experience discontinuous deformation, not just in the next flow period, but in any subsequent flow period. This corresponds to finding points that will be cut after some number of flow periods, which we achieve by taking successive preimages of the original Lagrangian discontinuity $D^t_0$, the
dotted-dashed curve in Fig. 5, under the map $Y_s$. The result is an infinite web of preimages $D_s = \{D_s^n = Y_{s/C_0}^n, n > 0\}$, some of which are shown in Fig. 6(a) for the RPM flow. Fluid that straddles the $N$-th preimage $D_s^n$ will remain connected until the $N$-th iteration when it will be cut into disconnected pieces.

The web of preimages identifies points that will experience discontinuous deformation at some future time. We can also consider points where these discontinuous deformations will propagate throughout the domain, i.e., points where successive iterations under the inverse map $Y_{s^-1}$ leads to discontinuous deformation at the dipole. In this case, the initial discontinuity consists of points that are advected onto the sink under the inverse flow, which begins with the dipole in its final orientation (position 3 in Fig. 2) and polarity reversed. This coincides with the set $D_t^1$ reflected through the symmetry line $y = \tan(-\Theta/2)x$, and we denote it $D_t^1$. Taking successive images of $D_t^1$ under the map $Y_t$, yields the web of images $D_t = \{D_t^n = Y_t^n(D_t^1), n > 0\}$, some of which are shown in Fig. 6(b). A cutting of fluid that occurs on the $m$-th iteration will appear along the $N$-th image.
after $N + m$ iterations. The web of images can also be found as the web of preimages of the reverse flow $Y^{-1} / C_0$, and vice versa. Furthermore, due to the RPM flow’s reflection-reversal symmetry about the line $y = \tan(-\Theta/2)x$, the web of images is the reflection of the web of preimages through the symmetry line.

Analysing the webs in Figs. 6(a) and 6(b), it can be seen that when a higher order preimage (i.e., further away in time, denoted by colours closer to purple) meets a lower order preimage (closer to orange), the higher order curve is cut by the lower order curve. For the web of preimages the upper portion is shifted to the right, and for the web of images it is shifted to the left. This means that cutting of fluid in the flow results in a shift of the upper portion to the left (direction is reversed for the preimages since it is using the inverse flow) where the higher order preimage acts as the slip surface. This prediction based on the webs can be verified by the inset in the last figure of Fig. 5. Furthermore, it is easy to distinguish classical non-mixing KAM islands in the webs, within which there must exist elliptic periodic points. Hyperbolic periodic points can also be distinguished as points where the webs converge inwards, the web of preimages converges along direction of expansion (unstable manifold $W^s$), whereas the web of images converges along direction of contraction (stable manifold $W^u$).
the direction of contraction (stable manifold $W^s$), two examples of this convergence are illustrated by arrows, and this is made clearer by the blown up figure in Fig. 6(b). Elliptic and hyperbolic points could also be found using standard periodic point analysis, however, the pseudo-elliptic and pseudo-hyperbolic points occur where the signs are opposite.

![Classification of pseudo-periodic points based on the cutting of higher order (dashed) images/preimages by a lower order image/preimage (solid) in the webs of Lagrangian discontinuities. The vertical axis is the signed distance between the end-points of the cut image/preimage, i.e., the displacement of the upper curve relative to the lower curve. Pseudo-hyperbolic points occur where the gradient of the images/preimages has the same sign as the cut, and pseudo-elliptic points occur where the signs are opposite.](image)

![The CSS map. (a)–(f) The deformations that comprise the CSS map: (a) no deformation, (b) horizontal shear $S_h$, $\gamma_1 = 0.2$, (c) and (d) positive and negative horizontal cut $C$, $a = \pm 0.2$, (e) and (f) negative and positive vertical shear $S_v$, $\gamma_2 = \pm 0.2$. (g)–(j) Combined deformation and associated Poincaré section for different combinations of the basic deformations. Period-1 points are shown as triangles (elliptic) or circles (hyperbolic), and only exist in (g) and (h).](image)

This type of analysis can be applied to general systems with discontinuous deformations, not only fluid flows. The web of Lagrangian discontinuities creates a template for the overall transport dynamics and provides additional information compared to the standard periodic point analysis.

In Sec. III, we discover the underlying mechanisms that generate the webs and the implications for transport and mixing in general systems with Lagrangian discontinuities.

### III. BASIC MECHANISMS OF DISCONTINUOUS MIXING

To elucidate the transport mechanisms associated with cutting and shuffling and stretching and folding motions in materials with Lagrangian discontinuities, we consider a simple map which captures the key features present in real systems. In many systems, complex mixing dynamics can be idealized as a sequence of shears. If discontinuities are present, then cutting of material can also occur. We introduce a simple map, the Cut-Shear-Shear (CSS) map, such that the net deformation $\Lambda$ consists of a sequence of horizontal cutting (Figs. 8(c) and 8(d)), horizontal shearing (Fig. 8(b)) and vertical shearing (Figs. 8(e) and 8(f))

$$C(x, y) = (x + a \text{sgn}(y), y), \quad S_h(x, y) = (x + \gamma_1 y, y), \quad S_v(x, y) = (x, y + \gamma_2 x), \quad \Lambda(x, y) = S_h S_v C(x, y),$$

subject to periodic boundary conditions at $y = \pm 2a/\gamma_1$. The map $C$ mimics the action of a slip-line as naturally occurs in shear-bandng materials, or via a Lagrangian discontinuity which arises from the boundary motion as in the RPM flow. The parameters $a$, $\gamma_1$, and $\gamma_2$ quantify the magnitude and direction of cutting, horizontal shear, and vertical shear, respectively; we will see that varying these parameters can fundamentally change the system. While a large set of simple maps may be constructed from compositions of elementary deformations (cutting, shear, rotation), the CSS map...
captures the essential features of the dynamics observed in the RPM flow and we will only consider this map here. An exhaustive exploration of these dynamics is required to develop a complete theory of discontinuous mixing, but this is beyond the scope of this study.

For the CSS map, there are four topologically distinct combinations for the Lagrangian dynamics. These depend on the signs of \(a_1, a_2, b_1, b_2\) and are shown in Figs. 8(g)–8(j). For \(a_2 < 0\) the cut and horizontal shear act in opposite directions, and the Poincaré sections (Figs. 8(g) and 8(h)) reflect the qualitative behaviour of the RPM flow on each side of the minimum return streamline. Conversely, for \(a_2 > 0\) (Figs. 8(i) and 8(j)), the cut and horizontal shear act in the same direction. There is therefore no “balancing” of the two deformations and hence no period-1 points. With a positive vertical shear, the behaviour in Fig. 8(i) at the origin is qualitatively similar to a classical hyperbolic point. The two shears create contraction in one direction and stretching in another. However, the presence of the discontinuities along the x-axis and at the periodic boundaries perturbs the motion and “kicks” particles between streamlines, creating widespread chaos. Reversing the vertical shear, the Poincaré section Fig. 8(i) has similarities to Fig. 8(g). Both have a dense fractal tiling of KAM tori. However, there are no period-1 points in this case, and the largest KAM tori are much smaller than the period-1 KAM islands in Fig. 8(g). For the remainder of the paper, we focus on the cases with \(a_2 < 0\) (Figs. 8(g) and 8(h)) to connect the CSS map to the transport and mixing processes of the RPM flow.

In Fig. 8(h), the map has two hyperbolic points (circles) which create a pseudo-elliptic island between them, similar to those which occur on the right side of Fig. 3(c). To analyse mixing in these regions, we performed a dye trace simulation (Fig. 10(a) (Multimedia view), leading to a well-mixed state within 50 iterations of the CSS map. Similar to stretching and folding alone, the combination of CS and stretching leads to exponential separation of nearby particles, which can be found as \(\log(\max(|x|_2)) \approx \log(51 + \sqrt{101}) \approx 6.0\) using Equation (86).

To elucidate the mechanisms which drive chaotic motion and leaking of particles, we consider the curves

\[
\frac{x^2}{\gamma_1} - \frac{\left( \frac{y + a_2}{\gamma_2} \right)^2}{\gamma_1} + s \left( \frac{y + a_2}{\gamma_1} \right) = c, \quad c \in \mathbb{R}
\]

that are invariant under the CSS map, shown as blue and red in Fig. 10(b). The system can be thought of as two affine linear systems “glued” together along the x-axis, such that the composite CSS map can be expressed as

\[
A(x, y) = \begin{pmatrix} \frac{1}{\gamma_2} & \gamma_1 & \frac{x}{y} & a \sgn(y) \frac{1}{\gamma_2} \\ \gamma_2 & 1 + \gamma_1 \gamma_2 & 1 + \gamma_1 \gamma_2 & 0 \end{pmatrix}.
\]

A particle above the x-axis will follow the blue invariant curves, and below it will follow the red. The key is that when crossing the x-axis, e.g., from red to blue, it will not follow the blue invariant curve until the start of the next iteration, allowing it to jump onto a range of blue curves (any of those before the line \(y = \gamma_2 x\) which is shown in dashed black). This “streamline jumping” is directly due to the discontinuity along the x-axis and causes the widespread chaos. Successive jumps outward can result in particles escaping the pseudo-elliptic island, and likewise particles from outside are able to jump in.

Fig. 8(g) shows that by simply reversing the direction of the vertical shear, the two period-1 points become elliptic (triangles) and a dense fractal tiling of non-mixing islands is created. This is qualitatively similar to the dynamics observed in the RPM flow on the left side of Fig. 3(c). While there is no mixing within the islands, Fig. 11(b) shows that a particle initially located at the origin will eventually trace out the entire region between them, forming the chaotic set. In this case, the combination of the two shears results in a rotation and hence the distance between initially close particles will not grow until the cut separates them, as shown in

FIG. 9. The separation of nearby particles in the CSS map. Particles were initially located at \((0, 0)\) and \((10^{-4}, 0)\). (a) Using the same parameters as in Fig. 8(g). The large jump in separation distance is caused by the two particles being cut in opposite directions, which occurs when their \(y\)-coordinates have opposite signs. (b) Using the same parameters as in Fig. 8(h), the exponent agrees with the Lyapunov exponent associated with the hyperbolic points, which can be found as \(\log(\max(|x|_2)) \approx \log(51 + \sqrt{101}) \approx 6.0\) using Equation (86).
Fig. 9(a). This case is therefore a CS-only system, consisting of only elliptic rotation and cutting, and hence is associated to a piecewise isometry. The complex structures for the webs of the CSS map are anticipated by the theory of piecewise isometries. They are multifractal and can be very difficult to resolve numerically at small length scales. The structure of the web depends only on the rotation angle generated by the elliptic points. Similar webs appear in other contexts, including the outer billiards map, overflow in digital filters, and kicked Hamiltonians, all of which are driven by elliptic rotations and discontinuous deformation, much the same as the CSS map in this case.

Repeating the process of finding successive preimages of Lagrangian discontinuities resolves the webs of Lagrangian discontinuities (Fig. 11(a)). As in the RPM flow, the webs form a template for the system, revealing the nature of the cutting mechanism, the periodic points, and the pseudo-periodic points. It can also be seen that the web Fig. 11(a) coincides with the chaotic set Fig. 11(b).

The dynamics of the CSS map clearly demonstrates how Lagrangian discontinuities create two new types of transport mechanism that are not possible in classical SF systems. The first is via pseudo-elliptic islands, where the Lagrangian discontinuity enables jumping between invariant curves and mixing in a leaky region via a process of stretching, cutting, and shuffling. Exponential separation of nearby particles, and hence strong mixing, is achieved due to the presence of stretching. This leads to more rapid mixing than can be achieved in a CS-only system. The second mechanism is in the measure-zero set amongst the densely packed elliptic regions given by the webs of preimages and images. In this set particles travel ergodically, experiencing a combination of rotation and cutting deformations. Such a dense tiling of elliptic points without any hyperbolic points is impossible in

![Image of pseudo-elliptic islands](https://dx.doi.org/10.1063/1.4941851.2)

**Fig. 10.** Pseudo-elliptic islands in the CSS map with the same parameters as Fig. 8(h). The pair of period-1 hyperbolic points are shown as black/red stars. (a) Dye trace simulation. An initially circular blob of fluid particles (half red, half blue) is iterated under the CSS map \( K \). (b) Invariant curves for the CSS map (red, blue) and particle trajectories (black, green arrows). The dashed black line \( y = \frac{1}{3} x \) defines the region where particles may jump onto new invariant curves. (Multimedia view)
classical Hamiltonian systems, but is characteristic of other CS-only systems (piecewise isometries) that are driven by rotation and cutting. We have demonstrated that these transport behaviours can occur in real systems even when the base system is conservative, and can play a fundamental role in the overall dynamics of transport and mixing.

IV. THE IMPACT OF NON-LINEAR DEFORMATIONS

A. The non-linear CSS map

The CSS map only considers linear shear, but in most applications, stress is non-uniform, resulting in varying shear rates even in Newtonian materials, with the potential for much stronger variation if yield stress or shear rate dependence is present. In fluids, they arise in flows that have non-uniform velocity profiles, which occur in the RPM flow based on the non-linear return time distribution of the asymptotic flow $v_0$. We extend the CSS map by replacing the linear vertical shear $S_v$ with the non-linear vertical shear $S_{nl}$ (Fig. 12(a))

$$S_{nl}(x, y) = (x, y + f(x)), \quad A_2(x, y) = S_{nl}S_v(x, y). \quad (7)$$

In Fig. 12, $f(x) = 0.05x^2 - 0.2$ (dashed) is quadratic such that the shear is negative for $x < 0$ and positive for $x > 0$. Locally, the non-linear CSS map behaves similarly to the linear CSS map but includes regions of positive and negative vertical shear. We do not show it here, but by approximating the non-linear function $f(x)$ with a piecewise linear function, the linear CSS map can make a piecewise approximation to the non-linear CSS map to arbitrary accuracy. Thus the Poincaré section for the non-linear map (Fig. 12(b)) has both the novel pseudo-elliptic islands and the dense tiling of non-mixing islands from Figs.8(g) and 8(h). Using this quadratic function $f(x)$, the Poincaré section for the non-linear model (Fig. 12(b)) captures the key features of the RPM flow (Fig. 3(c)). We are therefore able to understand the mechanisms driving the transport in the RPM flow at a fundamental level, and because any function $f(x)$ can be approximated by sequences of the up- or down-going vertical shears, these basic transport structures will appear for every non-linear shear profile.
B. Segregated mixing

The quadratic CSS map shows that it is possible to combine the mixing capabilities of pseudo-elliptic points with non-mixing regions using non-linear vertical shears. By using more complex functions \( f(x) \) in Equation (7), it is possible to engineer systems that have multiple mixing and non-mixing regions. Pseudo-elliptic islands are created anywhere that the function \( f(x) \) has \( x \)-intercepts with a positive gradient, and dense non-mixing islands are created when the \( x \)-intercepts have negative gradient. It is therefore simple to design systems that combine mixing and non-mixing regions by controlling the location and gradients of \( x \)-intercepts of \( f \).

An example is shown in Fig. 13, where segregated mixing is achieved using the piecewise linear function \( f(x) \) shown in Fig. 13(b). Mixing regions are created on the left and right via pseudo-elliptic points, and in the center, there is a thin non-mixing region. The fact that the non-mixing islands form a dense tiling means that they form vertical barriers to transport with very slow leakage across them, separating the two mixing regions. The segregated mixing is clearly illustrated by the dye trace in Fig. 13(c) (Multimedia view), within 25 iterations the left and right sides are well mixed, but there is little intermixing between the left and the right.

V. TRANSITION FROM SF TO CS

The Lagrangian discontinuity in the CSS map is caused by the cutting map \( C \). By approximating the cut with a smooth sequence of progressively sharper deformations, we can analyse the transition of smooth systems with mixing controlled by SF towards a system with Lagrangian discontinuities and CS. We replace the map \( C \) in the CSS map with the smoothed map

\[
C_b(x, y) = (x + a g_b(y), y), \quad \text{where} \quad \tag{8}
\]

\[
g_b(y) = \begin{cases} 
A \tanh \left( b \left( y + \frac{a}{|y|} \right) \right) - 2, & y < -\frac{a}{|y|} \\
A \tanh(b y), & |y| \leq \frac{a}{|y|} \\
A \tanh \left( b \left( y - \frac{a}{|y|} \right) \right) + 2, & y > \frac{a}{|y|}
\end{cases} \quad \tag{9}
\]

\[
A = \coth \left( \frac{a}{|y|} \right) \quad \tag{10}
\]

As shown in Fig. 14, the \( C^1 \)-continuous functions \( g_b(y) \) converge pointwise to \( \text{sgn}(y) a \) as \( b \to \infty \). Therefore, the maps \( C_b \) converge pointwise to the cutting map \( C \), and the associated smoothed CSS map \( \Lambda_b = S_b C_b \) only has Lagrangian discontinuities in the limit \( b \to \infty \).

Comparing the dye trace simulations in Figure 15 for a fixed number of iterations \( n = 6 \), the only difference between the CSS map \( (b \to \infty) \) and the smoothed map \( \Lambda_b \) with large but finite \( b \) is that material that is cut by the CSS map

\[
\text{FIG. 13. Segregation of mixing regions using a piecewise-linear vertical shear. (a) The Poincaré section generated using the piecewise linear function shown in (b) as } f(x) \text{ in Equation (7). Hyperbolic and elliptic period-1 points are shown as circles and triangles, respectively. (c) A dye trace simulation with four initially separated colours of dye. Dye is shown after 0, 1, 25 iterations, respectively. (Multimedia view) [URL: http://dx.doi.org/10.1063/1.4941851.3].}
\]
remains connected by thin striations. The striations occur along lines that coincide with the images of the Lagrangian discontinuity \( f^l \) and become infinitely thin as \( b \to \infty \). This is expected since this web consists of the points that experience discontinuous deformation. Therefore, transport structures for the smooth and discontinuous maps will converge everywhere except the web of post-images of the Lagrangian discontinuity, \( D^+ \), a set of measure zero.

In order to analyse the transition as \( b \to \infty \), we consider the Poincaré sections and period-1 points. Fig. 16 demonstrates the convergence of the Poincaré sections for the smooth systems towards the discontinuous limits Figs. 8(a) and 8(b).

Unlike the CSS map, in each case at low values of \( b \) the chains of periodic points alternate between elliptic (triangles) and hyperbolic (circles), as anticipated by the Poincaré–Birkhoff theorem. Focusing on the period-1 points for \( \gamma_2 = -0.2 \) (top row of Fig. 16), as for the CSS map there are the two elliptic points at \( (0, \pm 1) \). In contrast to the CSS map that has pseudo-hyperbolic points at the origin and on the periodic boundary at \( (0, -|a/\gamma_1|) \), the smoothed maps \( A_b \) have genuine hyperbolic points. Hence mixing in the chaotic sea between KAM islands is generated by SF rather than CS. As \( b \to \infty \), the magnitude of the shear about the origin increases, and the eigenvalues \( \lambda_1 = 1/\lambda_2 \) approach \( \infty \) and 0 (Appendix B 3), meaning infinite expansion and contraction. The corresponding eigenvectors

![Figure 14](image_url)

**FIG. 14.** The smooth functions \( g(x) \) used to approximate the discontinuous function \( \text{sgn}(x) \). Inset is the deformation of a square by the smoothed cut \( C_b \) with \( b = 10 \).

![Figure 15](image_url)

**FIG. 15.** The effect of the smoothing parameter \( b \) on a dye trace simulation with the same parameters as Fig. 8(b). (a) The initial configuration of the dye is a red disk enclosed within a blue annulus. The hyperbolic period-1 points at \( (0, \pm 1) \) are shown as black stars. (b) The location of the dye after 6 iterations of the CSS map \( K \). The dashed rectangle is the domain used for (c), (d), and (e). (c) Increasing the smoothing parameter \( b \), converging towards the discontinuous limit. (d) The dye trace for the CSS map with the web of images of the Lagrangian discontinuity, \( D^+ \). Further from red is more distant in time. This web coincides with the location of the striations at high values of \( b \). (e) The dye trace for the CSS map shown with the unstable manifold (black) associated with the hyperbolic point at the origin for the smoothed map \( A_b \) with \( b = 200 \). As \( b \) approaches infinity the unstable manifold converges to the same web of post-images of the Lagrangian discontinuity in (d). Likewise the stable manifold converges to the web of pre-images of the Lagrangian discontinuity.
give the directions of expansion and contraction, in the limit $b \to \infty$ they approach $(1, \gamma_2)$ and $(1, 0)$ which correspond to the first image and preimage in the webs of Lagrangian discontinuities, and the only two lines that are tangent to both of the period-1 elliptic islands for the CSS map.

Conversely, when the vertical shear is reversed (bottom row of Fig. 16) there are two period-1 hyperbolic points at $(0, \pm 1)$ for the CSS map, but there are two more period-1 points, at the origin and on the periodic boundary at $(0, -|a/\gamma_1|)$. These two new period-1 points share the same characteristics for each set of flow parameters. For low values of the smoothing parameter $b$, they are elliptic and the corresponding KAM islands are bounded by the parallel heteroclinic connections of unstable manifolds associated with the hyperbolic points. As $b$ increases, the heteroclinic connections become transverse, creating a chaotic sea around the KAM islands, gradually engulfing them. The KAM islands become increasingly thin, to the point where they undergo period-doubling bifurcations, each creating a period-1 hyperbolic point and two period-2 elliptic points. For the case shown with $(a, \gamma_1, \gamma_2) = (-0.2, 0.2, 0.2)$, this bifurcation occurs around $b \approx 101$ (Appendix B 3). As in the $\gamma_2 = -0.2$ case, the eigenvalues approach $\infty$ and 0, with eigenvectors converging to $(1, \gamma_2)$ and $(1, 0)$, and associated stable and unstable manifolds converging to the webs of Lagrangian discontinuities $D'$, $D''$, respectively (Figures 15(d) and 15(e)). These webs can therefore be considered as the analogues of the stable and unstable manifolds for systems with discontinuous deformations.

A fundamental difference between the stable and unstable manifolds (Fig. 17) for the CSS map compared to the smoothed map $\Lambda_b$ is that the Lagrangian discontinuity cuts both manifolds into disconnected pieces. Material lines such as the stable and unstable manifolds form impenetrable barriers to transport, but cutting them creates "gaps," allowing material to pass through freely. For sufficiently large $b$, almost all individual particles follow the same trajectories using the smoothed and discontinuous maps, however, finite area material parcels have greater freedom in the presence of Lagrangian discontinuities. In the limit $b \to \infty$, the material barriers disappear, and material parcels are able to cross the destroyed barriers, whereas for finite $b$ high levels of stretching are required to ensure that barriers are not crossed.
flows have no-slip boundaries, so fluid would always remain connected across valves. Instead of being cut, fluid will experience highly localised shear depending on the thickness of the boundary layer. We therefore expect that with no-slip boundary conditions in the RPM flow, the structures seen in Fig. 3(c) would be replaced by their smoothed analogue as in Fig. 16, where the thickness of the boundary layer acts as the smoothing parameter \( b \).

VI. CONCLUSIONS

Cutting by Lagrangian discontinuities drastically alters how mixing and transport can arise in materials and systems that have slip planes, shear bands or valves and wall slip. Cutting opens up a wider range of possibilities for the long-time organization of material by increasing the topological freedom of Lagrangian transport. Using a simple map consisting of cutting and shearing motions, we have found a novel mixing mechanism that arises in general systems that combine stretching and CS, which we call a pseudo-elliptic island. Within these islands strong mixing occurs, an impossibility for CS-only systems and SF systems without folding. The map can also produce fractal tilings of classical non-mixing islands with a greater density of islands than is possible in a classical SF system, resulting in slower transport and weak mixing. We have only considered a few of the possibilities for maps composed of simple shear, cut and rotation deformations. Further study of the full array of possibilities could reveal fundamentally different structures that may appear in physical systems.

Our map demonstrates qualitatively similar mixing and transport as that seen in a realistic example flow for relevant ranges of the control parameters. We have shown that even with a smooth incompressible base flow, the opening and closing of valves combined with a slip boundary condition creates Lagrangian discontinuities, leading to transport behaviour that cannot be found in classical Hamiltonian systems. Slip walls are necessary if the opening and closing of valves occurs on the boundary, but Lagrangian discontinuities will also arise in flows with no-slip boundary conditions if the fluid is injected into and extracted from points in the domain away from boundaries.

The standard methods used for studying SF systems—periodic point analysis, dye trace simulations—are still relevant in systems with Lagrangian discontinuities, but new methods are needed to fully understand them. We have introduced the webs of Lagrangian discontinuities as a more comprehensive tool. These webs determine the location and stability of periodic points, the nature of the cutting mechanism, and the locations of new structures such as pseudo-periodic points.

While we have used 2D examples, extension of this analysis to fully 3D systems will be challenging. A third dimension creates even more topological possibilities for coherent structures, for instance, the web of Lagrangian discontinuities is made from 1D curves in 2D systems but in 3D there will be a web of interlaced 2D surfaces. The introduction of a Lagrangian discontinuity is anticipated to create...
fundamentally different structures to those observed in 2D systems.

Future study should focus on developing a complete framework for 2D transport in the presence of Lagrangian discontinuities, studying the full range of interactions between CS and SF.

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APPENDIX A: PARTICLE TRACKING IN THE RPM FLOW

Tracking individual particles within the RPM flow is essential for the production of Poincaré simulations. Finding the path of a particle requires solving the advection equation (1) either numerically or analytically. For the RPM flow, the velocity field \( \mathbf{v} \) can be found analytically, making computation significantly easier. While an analytic solution to Equation (1) is impossible for the RPM flow, a pseudo-analytic method is used to track particles in a similar manner to Lester et al.11 The main difference being the use of the potential function \( \Phi \) and streamfunction \( \Psi \) as orthogonal coordinates, instead of using the polar angles \( \theta \) and \( \Psi \) as coordinates which are parallel along the \( y \)-axis. Using the streamfunction as a coordinate is beneficial since it is a constant of motion, and the potential function is a canonical choice since it must be orthogonal to the streamfunction. Conversion between Cartesian coordinates and \((\phi, \psi)\) coordinates is performed via polar coordinates

\[
(x, y) \rightarrow (r, \theta) \rightarrow (\phi, \psi)
\]

\[
r(\phi, \psi) = \sqrt{1 - \frac{2 \cos(\psi)}{\cos(\phi) + \cosh(\phi)}}
\]

\[
\theta(\phi, \psi) = -\frac{\phi}{\psi} \cos^{-1} \left( \frac{\sin(\psi)}{\sqrt{\cosh^2(\phi) - \cos^2(\psi)}} \right)
\]

\[
\phi(r, \theta) = \frac{1}{2} \log \left( \frac{r^2 - 2 \sin(\theta) + 1}{r^2 + 2 \sin(\theta) + 1} \right)
\]

\[
\psi(r, \theta) = \tan^{-1} \left( \frac{\sqrt{2 \cos(\theta)}}{1 - r^2} \right)
\]

The advection equation in these new coordinates is given by

\[
\frac{d\phi}{dt} = \left( \cos(\Psi) + \cosh(\Phi) \right)^2, \quad \frac{d\Psi}{dt} = 0.
\]

We have therefore reduced the system to one dimension, though this differential equation is still insoluble. On the other hand, the equation

\[
\frac{dt}{d\Phi} = \frac{1}{d\Phi/dt}
\]

has the analytic solution

\[
\tau_{\text{adv}}(\phi, \psi) = \csc^2(\psi) \left[ -2 \cot(\phi) \tan^{-1} \left( \tan \frac{\phi}{2} \tanh \frac{\psi}{2} \right) + \sin \frac{\phi}{2} + \sinh \frac{\phi}{2} \left( \frac{\sinh \frac{\psi}{2}}{\sin \frac{\psi}{2}} \right) + \frac{1}{2} \left( \frac{\phi + i \psi}{2} \right) \right]
\]

\[
\text{mod} \left( \frac{t_{\text{adv}}(\phi, \psi)}{2} \right) = \frac{t_{\text{adv}}(\phi, \psi)}{2} + T \mod t_{\text{adv}}(\psi).
\]

The advection of a particle for the time period \( T \) can be expressed as a map \((\phi, \psi) \rightarrow (\phi', \psi')\), where the new value of the potential function satisfies

\[
t_{\text{adv}}(\phi', \psi') + \frac{t_{\text{adv}}(\phi, \psi)}{2} = \frac{t_{\text{adv}}(\phi, \psi)}{2} + T \mod t_{\text{adv}}(\psi).
\]

However, the function \( t_{\text{adv}} \) is not invertible, so there is no analytic solution for \( \phi' \). We use Newton’s root finding method to solve Equation (A6) to machine precision accuracy. The new coordinates are then converted to Cartesian coordinates via Equation (A1).

APPENDIX B: PERIODIC POINT ANALYSIS

Periodic points and their stability play a pivotal role in the organisation of particle transport, and lower order (smaller period) points play a greater role than higher order points. We therefore focus on finding the period-1 points of maps \( f(x) \), which satisfy \( f(x) = x \). The local stability of period-1 points is determined by the eigenvalues of the deformation tensor \( F = (\partial f/\partial x)_x \). For area-preserving maps, the eigenvalues must satisfy \( \lambda_1 \lambda_2 = 1 \). If the eigenvalues are real, then \( \lambda_1 = 1/\lambda_2 \), leading to a direction of contraction and a direction of expansion. In this case, the periodic point is called hyperbolic. The only other possibility for an area-preserving map is that the eigenvalues form a complex conjugate pair \( \lambda_1 \lambda_2 = \cos \theta \pm i \sin \theta \), in which case there is a rotation about the periodic point, and the point is called elliptic.

1. The CSS map

To find and classify the period-1 points of the CSS map, we write the map explicitly as

\[
\Lambda(x, y) = (x', y')
\]

\[
x' = x + y_1 y + a \cdot \text{sgn}(y)
\]

\[
y' = \left( y_2 x' + y + \frac{2}{|y'|} \mod \frac{4}{|y'|} \right) - \frac{2}{|y'|}.
\]

\[
\tau_{\text{adv}}(\phi, \psi) = \csc^2(\psi) \left[ -2 \cot(\phi) \tan^{-1} \left( \tan \frac{\phi}{2} \tanh \frac{\psi}{2} \right) + \sin \frac{\phi}{2} + \sinh \frac{\phi}{2} \left( \frac{\sinh \frac{\psi}{2}}{\sin \frac{\psi}{2}} \right) + \frac{1}{2} \left( \frac{\phi + i \psi}{2} \right) \right]
\]

\[
\text{mod} \left( \frac{t_{\text{adv}}(\phi, \psi)}{2} \right) = \frac{t_{\text{adv}}(\phi, \psi)}{2} + T \mod t_{\text{adv}}(\psi).
\]
where $\gamma' = \gamma/a$. This includes the periodic boundaries at $y = \pm2/\gamma'$. Period-1 points must therefore satisfy the pair of equations

$$x + \gamma y + a \cdot \text{sgn}(y) = x,$$

$$\left(\frac{\gamma_2}{\gamma_1}x + y + \frac{2}{\gamma_1} \mod \frac{4}{\gamma_1}\right) - \frac{2}{\gamma_1} = y. \quad (B2)$$

The second equation simplifies to

$$\gamma_2 x + y + \frac{2}{\gamma_1} = y + \frac{2}{\gamma_1} + \frac{n}{\gamma_1}, \quad n \in \mathbb{Z} \quad (B3)$$

which implies that

$$x = n \frac{4}{\gamma_1} y, \quad |y| = -\frac{a}{\gamma_1}, \quad n \in \mathbb{Z}. \quad (B4)$$

Therefore, period-1 points only exist when $\gamma' = \gamma/a < 0$, and in these cases occur at the points $(n \frac{4}{\gamma_1} y, -\frac{a}{\gamma_1})$.

For the CSS map, the deformation tensor is

$$F = \begin{pmatrix} 1 & \gamma_1 \\ \gamma_2 & 1 + \gamma_1 \end{pmatrix}, \quad y \neq 0, \pm \frac{2}{\gamma_1} \quad (B5)$$

and is undefined if $y = 0, \pm2/\gamma'$. We have real periodic boundaries created by the cutting transformation and periodic boundary. The eigenvalues of $F$ are

$$\lambda_{1,2} = \frac{1}{2} \left(2 + \gamma_1 \gamma_2 \pm \sqrt{\gamma_1 \gamma_2 (4 + \gamma_1 \gamma_2)}\right). \quad (B6)$$

Assuming that $\gamma_1 > 0$ and $\gamma_2 > -4\gamma'_1$, the eigenvalues are real when $\gamma_2 > 0$ and form a complex conjugate pair when $\gamma_2 < 0$. In terms of stability, this means that the period-1 points are hyperbolic when $\gamma_2 > 0$ and they are elliptic when $\gamma_2 < 0$.

2. The non-linear CSS map

The function $f(x)$ in the quadratic vertical shear $S_a$ can be written as $f(x) = 2x^2 - \beta$. The period-1 points of the non-linear CSS map can be found in a similar manner to those in the linear CSS map. The map can be written explicitly as

$$\Lambda_2(x, y) = (x', y'),$$

$$x' = x + \gamma y + a \cdot \text{sgn}(y),$$

$$y' = \left(2x^2 - \beta + y + \frac{2}{\gamma_1} \mod \frac{4}{\gamma_1}\right) - \frac{2}{\gamma_1}. \quad (B7)$$

Period-1 points satisfy $(x', y') = (x, y)$, which is true when

$$x = \pm \frac{1}{2} \left(\beta + \frac{4}{\gamma_1}\right), \quad |y| = -\frac{a}{\gamma_1}, \quad n \in \mathbb{Z}. \quad (B8)$$

This can only occur when $\frac{1}{2} \left(\beta + \frac{4}{\gamma_1}\right) > 0$ and $\gamma' < 0$. The deformation tensor $F_2$ can be computed at every point except along the lines $y = 0, \pm2/\gamma'$

$$F_2(x, y) = \begin{pmatrix} 1 & \gamma_1 \\ 2x' & 1 + 2x' \end{pmatrix}. \quad (B9)$$

It can be seen that $F_2$ is equivalent to $F$ but with $\gamma'_2$ replaced with $2x'$. Assuming that $\gamma_1 > 0$ and $x > 0$, we can therefore say, that the period-1 points are elliptic when $x < 0$ and hyperbolic when $x > 0$.

3. Smoothed CSS map

Essentially, the same analysis as for the CSS map applies to the smoothed map at the points $(0, \pm1)$. The value of the smoothing parameter $b$ has some effects on the values of the eigenvalues and eigenvectors of the deformation tensor, but the nature of the points remains the same.

For the period-1 points at the origin and on the periodic boundary at $(0, -2[a/\gamma'_1])$, direct computation of the deformation tensor $F_b = (\partial \Lambda'_b/\partial x)$ yields

$$F_b(x, y) = \begin{pmatrix} 1 & \beta \\ \frac{4}{\gamma'_1} & \frac{4}{\gamma'_1} + \gamma_1 \end{pmatrix} \quad (B10)$$

where

$$\beta = ab \coth \left(\frac{b}{\gamma'_1} \right) + \gamma_1 \quad (B11)$$

is the net horizontal shear at the origin from the maps $C_b$ and $S_a$. This deformation tensor is in the same form as Equation (B5), and thus the two eigenvalues are

$$\lambda_{1,2} = \frac{1}{2} \left(2 + \beta \gamma_2 \pm \sqrt{\beta \gamma_2 (4 + \beta \gamma_2)}\right). \quad (B12)$$

As $b \to \infty$, the eigenvalues converge to 0 and $-\infty$, respectively.

The nature of the periodic point is determined by the discriminant

$$\Delta = \beta \gamma_2 (4 + \beta \gamma_2). \quad (B13)$$

for $\Delta > 0$ the period-1 point is hyperbolic, for $\Delta < 0$ it is elliptical and when $\Delta = 0$ it is degenerate. Assuming that $\gamma_1 > 0, \gamma_2 \neq 0$ and $a < 0$, there are a number of cases. The discriminant will be zero when

$$b = 0, \quad \text{or} \quad b = -\frac{4}{\gamma_2}. \quad (B14)$$

Restricting to the case when $\gamma_1 = -a$, then $b = 0$ is equivalent to $b \coth b = 1$, implying that $b = 0$. Therefore, the period-1 point becomes degenerate as the smoothing parameter $b \to 0$. This can also be seen by the fact that as $b \to 0$, $g_b(y) \to y$ so $C_b \to S_{-1}$ and hence $\Lambda_0 \to S_a$.

The other case in Equation (B14), $\beta = -\frac{4}{\gamma_2}$, is equivalent to

$$b \coth \left(\frac{b}{\gamma'_1}\right) = -\frac{1}{a} \left(\frac{4}{\gamma_2} + \gamma_1\right) \quad (B15)$$

which will have a solution provided the right hand side is greater than 1. If a solution exists then the period-1 point will experience either a period-doubling or period-halving
bifurcation. In the main text, the cases used are \((a, c_1, c_2) = (-0.2, 0.2, \pm 0.2)\). For \(c_2 = 0.2\), the right hand side of Equation (B15) is equal to 101, and hence there is a period-doubling bifurcation of the elliptic point at \(b = 101\). On the other hand, for \(c_2 = -0.2\), the right hand side of Equation (B15) is equal to \(-99\) and hence there is no solution. In this case, the point remains hyperbolic for all values of \(b\).

The eigenvectors of the deformation tensor \(F_b\) corresponding to the eigenvalues \(\lambda_{1,2}\) are given by

\[
v_1 = \left(1, \frac{c_2}{1 - \lambda_2}\right) \quad \text{and} \quad v_2 = \left(1, \frac{-c_2}{1 - \lambda_1}\right)
\]

Hence as \(b \to \infty\) the eigenvectors converge to \((1, 0)\) and \((1, 2)\), respectively.

---

5.2 Cutting interacting with twistless tori and reconnection bifurcations

The chains of elliptic and hyperbolic periodic points observed in Fig. 3 in the previous section are created by a sequence of saddle–centre bifurcations that occur along the minimum return streamline of the flow $v_0$ in the limit as $\tau \to 0$. In this section it is shown that these bifurcations are reconnection bifurcations that interact with the Lagrangian discontinuity. These bifurcations occur when $\tau$ becomes resonant with the minimum return time of the flow $v_0$, i.e. when $t_{\text{ret}}^{\min} = \frac{m}{n} \tau$ then period-$n$ elliptic and hyperbolic point chains are created. As $\tau$ increases to $\tau + \Delta \tau$ these chains move away from the minimum return streamline of $v_0$, and move to a streamline with the same resonance, i.e. the streamline(s) $\tilde{\psi}$ of the limiting flow $v_0$ such that $t_{\text{ret}}(\tilde{\psi}) = \frac{m}{n}(\tau + \Delta \tau)$. This results in the chains of elliptic points moving towards the centre of the circle, and the chains of hyperbolic points moving towards the circular boundary. An example of the bifurcation is shown in Fig. 5.1, where a sequence of saddle–centre bifurcations creates a chain of elliptic islands on the left and a chain of hyperbolic points on the right. As discussed in Smith et al. [SRLM16] in §5.1 here, in a Hamiltonian system it would be expected that hyperbolic points would interleaver the elliptic point chain and vice versa for the hyperbolic point chain. However, the Lagrangian discontinuity ‘destroys’ these periodic points.

These bifurcations can be replicated by the non-linear CSS map, as shown in Fig. 5.2, by varying the value $\beta$ used to generate the quadratic vertical shear function $f(x) = \alpha x^2 - \beta$. Since each $x$-intercept of $f(x)$ corresponds to the $x$-coordinate of a pair of period-1 points, for $\beta < 0$ there are no intercepts and therefore no period-1 points. For $\beta = 0$ there is a pair of period-1 points, but the vertical shear $f'(x)$ is zero at these points so there is no deformation of fluid and the points are degenerate. Finally, for $\beta > 0$ there are two pairs of period-1 points, each pair having one elliptic and one hyperbolic point. Therefore, the value $\beta = 0$ corresponds to a pair of saddle–centre bifurcations.

Now, it was shown in §3.1.4 that the minimum return streamline is a twistless torus, and from §2.6 it is expected that reconnection bifurcations should occur along this streamline. At first glance the bifurcations in Fig. 5.1 and Fig. 5.2 do not appear to be reconnection bifurcations (Fig. 2.4), since there is no reconnection of manifolds and the elliptic points are not interleaved with hyperbolic points and vice versa. However, the destroyed periodic points, termed pseudo-periodic points in [SRLM16] (§5.1 here), complete the picture of the reconnection bifurcation, providing the interleaved periodic points whose manifolds can reconnect. To illustrate
Figure 5.1: Poincaré sections demonstrating a reconnection bifurcation in the 2DRPM flow with $\Theta = 2\pi/3$. The green and orange dashed lines are the minimum return streamline of $v_0$ and symmetry line respectively, as in Fig. 3 of [SRLM16]. (a) $\tau = 5.01 \times 10^{-4}$, (b) $\tau = 5.011 \times 10^{-4}$, (c) $\tau = 5.01125 \times 10^{-4}$. 
5.2. CUTTING INTERACTING WITH TWISTLESS TORI

Figure 5.2: The non-linear vertical shears $S_{nl}$ (left) and corresponding Poincaré sections (right) for the non-linear CSS map eq. (7) in [SRLM16] (§5.1) demonstrating a reconnection bifurcation. The quadratic functions $f(x) = \alpha x^2 - \beta$ are shown in blue on each of the shear plots (left), with the $x$-intercepts shown in pink indicating the $x$-coordinates of any period-1 points. (a) $f(x) = 0.05x^2 + 0.1$, (b) $f(x) = 0.05x^2$, (b) $f(x) = 0.05x^2 - 0.2$.

This clearly, the non-linear CSS map $\Lambda_2$ (eq. (7) in [SRLM16]) has been smoothed using the smoothed cut $C_b$ as detailed in §V in [SRLM16]. Considering a variety of smoothing parameters $b$, where the limit $b \to \infty$ corresponds to a discontinuous cut, Fig. 5.3 clearly shows that a reconnection bifurcation occurs for $b = 5$ (high smoothing), with a braiding of two periodic point chains as in Fig. 2.4. Increasing $b$ adds a perturbation the system, leading to the destruction of many of the tori and creating chaotic regions. At $b = 50$ there is a clear resemblance with the bifurcation in the limit as $b \to \infty$ (Fig. 5.2).

Therefore, the bifurcations that produce the chains of elliptic and hyperbolic points can be thought of as reconnection bifurcations, however half of the coherent structures are destroyed by the discontinuous deformation.
Figure 5.3: The equivalent of Fig. 5.2 for the smoothed non-linear CSS map, using the smoothed cut $C_b$, with non-linear vertical shears $S_{nl}$ of the form $f(x) = 0.05x^2 - \beta$. For $b = 5$ the reconnection bifurcation results in a braiding, as in Fig. 2.4, whereas for $b = 20, 50$ the braiding connections become transverse.
5.3 A deeper look at transport dynamics across a range of $\tau$ values

In [SRLM16], in §5.1 here, the transport structures are primarily considered at a fixed low value of $\tau = 5.012 \times 10^{-4}$, and only in the region of Fig. 5.4 denoted by Window 1, centred on the intersection between the symmetry line (dashed orange) and the streamline with the minimum return time (dashed green). This window is particularly interesting since it is where the reconnection bifurcations take place, creating the island chains that move towards the centre of the circle, and the hyperbolic chains that move towards the boundary. In this section two additional scenarios are discussed. First, transport in Window 2 from Fig. 5.4, towards the centre of the circle, and at the same low value of $\tau$ is considered. Next, a larger (but still small) value of $\tau = 10^{-2}$ is studied, and a larger subset is used, Window 3 from Fig. 5.4, since the transport structures are much larger. In each of these cases the transport structures are similar to those originally studied, but with some interesting differences. The mechanisms that generate these difference are explained by extending the CSS map to include non-horizontal cuts and shears.

5.3.1 Transport at low $\tau$ away from the minimum return streamline

Once island chains are created at the minimum return streamline, they move towards the centre of the circle with increasing $\tau$, eventually passing through Window 2 in Fig. 5.4. The Poincaré section in this window at $\tau = 5.012 \times 10^{-4}$ is shown in Fig. 5.5(a). There are two main differences between this Poincaré section compared to that in Window 1 (Fig. 3c in §5.1). First, there is more space between successive islands in a given island chain. In Window 1 the islands appear to kiss, whereas in Window 2 the gap between successive islands is clearly visible, and is approximately half the length of the islands’ semi-major axes. This impacts transport by allowing particles to move more freely amongst the island array, as there is a larger gap for them to move through. In addition, the range of periods of islands in Window 2 seems to be much less than in Window 1, i.e. in Window 2 there are the largest islands that have period $3n + 1$ for $n = 262, \ldots, 275$ (shown in Fig. 5.5(b)), and the smaller islands with approximately double the period of their larger neighbour,
Figure 5.4: The subsets of the domain used to view Poincaré sections (not to scale).

(1) The region centred on the minimum return streamline (dashed green) and symmetry line (dashed orange) used for Fig. 3c in [SRLM16] (§5.1) and Fig. 5.1. (2) A region centred on the symmetry line closer to the centre of the circle, used for Fig. 5.5. (3) A larger region containing both regions 1 and 2, used for Fig. 5.9.

with period $6n + 5$ for $n = 262, \ldots, 275^\ast$. On the other hand, in Window 1 the islands with double, triple, quadruple and quintuple period are still clearly visible. This is due to the horizontal spacing between successive island chains being reduced in Window 2, so the higher order island chains become too small to see. This horizontal compression is predicted since the second derivative of the streamline return time $t_{\text{ret}}(\xi)$ (Fig. 5.6) in the limit as $\tau \to 0$ (Fig. 3.3) is always positive†, where $\xi$ is the distance of the streamline from the origin along the symmetry line $y = \tan(-\Theta/2)x$. This means that for a fixed difference in return time $\delta$ (equal to $3\tau$ for the largest islands with periodicity $3n + 1$) the respective distances between island chains, starting from the minimum return streamline, will decrease. This is illustrated in Fig. 5.6 by the distances $d_1 > d_2 > d_3$.

To capture the mechanisms at play that create these differences in the Poincaré sections, the CSS map introduced in [SRLM16] (§5.1) is extended to include cuts and shears that are not horizontal. This is motivated by the fact that the preimages of the Lagrangian discontinuity in Fig. 5.5(b) are not horizontal like they are in Window 1, but are offset at an approximately constant angle. Therefore, the cut and first shear in the CSS map are offset at a constant angle as well, so that the

---

$\ast$It is not clear why the periods take these forms. The fact that they are $a \mod 3n$ is likely due to the flow reorientation having period-3, as $\Theta = 2\pi/3$, but it is not clear why they are $1 \mod 3$ and $5 \mod 6$ etc.

†The graph is ‘concave up’.
Figure 5.5: (a) Poincaré section for the 2DRPM flow with \((\Theta, \tau) = (2\pi/3, 5.012 \times 10^{-4})\), the same as Fig. 3c in [SRLM16] (§5.1), viewed in the subset Window 2 from Fig. 5.4. (b) The Poincaré section from (a) shown as grey with the web of preimages of the Lagrangian discontinuity shown in colour (closer to red being closer in time, and closer to blue being more distant in time). The periodicities of the periodic points at the centre of each island are also shown.
Figure 5.6: Streamline return time $t_{\text{ret}}$ as a function of distance ($d$) along the symmetry line $y = \tan(-\Theta/2)x$ (dashed orange curve in Fig. 3.3) from the origin. The location of the streamline with the minimum return time is shown as the dashed red line, corresponding to the purple and green streamlines in Fig. 3.3. The black lines show that a constant difference $\delta$ in return time corresponds to decreasing distances $d_1, d_2, d_3$ in streamline separation when starting from the minimum return streamline.

The map becomes

$$\Lambda_3(x, y) = S_{\alpha}R_{\alpha}S_hCR_{-\alpha}(x, y).$$

(5.1)

For $\alpha = \pi/5$ the offset deformations $C^\alpha = R_{\alpha}CR_{-\alpha}$ and $S_{h}^\alpha = R_{\alpha}S_hR_{-\alpha}$ are illustrated in Fig. 5.7. Comparing the corresponding Poincaré section (Fig. 5.8) to the Poincaré section in Window 2 it can be seen that this modified CSS map captures the key features. The gap between the large islands is caused by the Lagrangian discontinuities (white). The islands can never intersect these lines but kiss them tangentially, horizontal lines would allow the islands themselves to kiss, but an offset angle prohibits this and creates a gap between them.

Figure 5.7: The offset cut and shear deformations of that define the map $\Lambda_3$ with $\alpha = \pi/5$. 
5.3. TRANSPORT ACROSS A RANGE OF $\tau$ VALUES

Figure 5.8: Poincaré section corresponding to the CSS map $\Lambda_3$ from eq. (5.1) with the offset cut and horizontal shears as in Fig. 5.7. The cutting lines that are offset by an angle $\pi/5$ from the $x$-axis are shown in white.

5.3.2 Transport at higher (but still small) $\tau$

Now the nature of particle transport at larger values of $\tau$ are considered. As the periodic point chains are created by the resonance of $\tau$ with the return time of the minimum return streamline, the periodicity of these chains reduces as $\tau$ increases. This causes the size of the elliptic islands to increase. Therefore, a larger subset is needed to view the transport structures, and Window 3 shown in Fig. 5.4 is used. The Poincaré section and preimages of the Lagrangian discontinuity in this window at $\tau = 10^{-2}$ (Fig. 5.9) are similar to the low values of $\tau$ except the structures are much larger. One key difference is that there is a finite area chaotic sea between the elliptic islands, rather than the fractal set amongst a dense set of islands. This could be caused by some elliptic points in this region undergoing period-doubling bifurcations, creating hyperbolic points and associated chaotic regions. The presence of a finite area chaotic set significantly improves particle transport amongst the islands, as particles do not have to ‘squeeze’ through very small gaps.

Therefore, by extending the CSS map to include non-perpendicular cuts and shears, the transport structures of the 2DRPM flow at low values of $\tau$ can be completely understood.
Figure 5.9: (a) Poincaré section for the 2DRPM flow with $(\Theta, \tau) = (2\pi/3, 0.01)$ shown in the region Window 3 from Fig. 5.4. (b) The corresponding web of preimages of the Lagrangian discontinuity with the Poincaré section shown faint. Preimages closer in time are coloured closer to red and those more distant in time are coloured orange.

5.3.3 Remnants of discontinuous deformation at high $\tau$

At the larger values of $\tau$, around and above 0.1, the Lagrangian discontinuities still play a role. This is clearly seen in Fig. 5.10, where pseudo-hyperbolic points (P-H) can be identified in the Poincaré sections and webs of Lagrangian discontinuities amongst the chains of elliptic islands. However, at these values of $\tau$ the chains of islands begin to deviate away from the streamlines of the velocity in the limit as $\tau \to 0$, and the island chains occupy less area as $\tau$ increases. At $\tau = 0.374$ and $\tau = 0.666$ (Fig. 5.11) the island chains are still visible, but are contained within the small regions marked by the blue curves, while the majority of the domain is chaotic.

Therefore, structures associated with the discontinuous deformations such as
pseudo-hyperbolic points persist for large values of \( \tau \), but the area in which they are found decreases as \( \tau \) increases. In §5.5 the impact of these discontinuous deformations at large values of \( \tau \) will be further explored using decoupled Lyapunov exponents.

Figure 5.10: Poincaré sections (a,c) and webs of preimages of the Lagrangian discontinuity (b,d) in the 2DRPM flow with \( \Theta = 2\pi/3 \) and (a,b) \( \tau = 0.1 \), (c,d) \( \tau = 0.2 \). On each Poincaré section the original Lagrangian discontinuity is shown as red, and this is mapped backwards in time under \( (\Upsilon^\Theta)^{-1} \) to find the corresponding webs of preimages. Pseudo-hyperbolic points (P-H) are indicated in the Poincaré sections and webs of preimages. Pseudo-elliptic points also occur but are less obvious.
5.4 Cutting can enhance or impede mixing

Using the mix-norm that was introduced in §4.5, the mixing rate of the CSS map can be compared to the linear system that consists of the same shears but with the cut removed. This isolates the influence of the cut on mixing.

For the CSS map the height of the domain is $4|a/\gamma_1|$, and the width is infinite, though the structures are periodic in the $x$-direction with period $4|a/(\gamma_1\gamma_2)|$. Therefore, $|\gamma_1/a| = 1$ and $|\gamma_2| = 1$ are kept fixed, so that the height and periodic width are both equal to 4, and the square domain $[-2, 2) \times [-2, 2)$ completely characterises the transport and mixing properties. Varying the values $|\gamma_1/a|$ and $|\gamma_2|$ does not change the mixing characteristics, only the length scales of the domain. Therefore the two parameters that determine the quality and rate of mixing are $\gamma_1$ and the sign of $\gamma_2$.

The linear map consisting of the horizontal and vertical shears of the CSS map is

$$\Lambda_{SS}(x, y) = (x + \gamma_1 y, \gamma_2 x + (1 + \gamma_1 \gamma_2)y)$$  \hspace{1cm} (5.2)

with deformation tensor

$$D\Lambda_{SS}(x, y) = \begin{pmatrix} 1 & \gamma_1 \\ \gamma_2 & 1 + \gamma_1 \gamma_2 \end{pmatrix}.$$  \hspace{1cm} (5.3)

From the discussion in Appendix B1 in [SRLM16] (§5.1) it follows that the period-1
5.4. CUTTING CAN ENHANCE OR IMPEDE MIXING

point at the origin for the linear map has the same stability as the pair of period-1 points located on the y-axis in the CSS map. For \((\gamma_1, \gamma_2) = (0.04, -1)\) these periodic points are elliptic, and the bottom row of Fig. 5.12 shows that under the linear map \(\Lambda_{SS}\) the concentration field undergoes approximately a half rotation in 16 iterations, and that there is no mixing. On the other hand, with the addition of the cut the concentration field is better mixed after 16 iterations as the different islands have different periodicities. If all these periodicities are commensurate (rational multiples of one another), then the system as a whole will still be periodic, and will eventually un-mix. However, if the periodicities are incommensurate, then the system will never return to its initial configuration and the mixing will persist. The difference between the mixing in the CSS map compared to the linear map \(\Lambda_{SS}\) is reflected in the evolution of the mix-norm (Fig. 5.13). For the linear map \(\Lambda_{SS}\) (green, thick, dashed) the mix-norm initially decays as the ‘bands’ are compressed, but it begins to grow again as the concentration is rotated to an angle close to \(\pi\). On the other hand, for the CSS map (solid green), the mix-norm experiences approximately the same initial decay, but continues to decay when the mix-norm of \(\Lambda_{SS}\) begins to grow.

Performing a similar comparison for the case when \(\gamma_2 = 1\) and the periodic points are hyperbolic (Fig. 5.14), the presence of the discontinuous cut deformation inhibits the rate of mixing. This is because particles are loosely trapped near the pseudo-elliptic points, creating regions of low transmissivity. For both the smooth and discontinuous maps, fluid at every point that is not affected by the cut experiences

\[
N = 1 \quad N = 2 \quad N = 4 \quad N = 8 \quad N = 16
\]

Figure 5.12: A comparison of the iterates of the initial concentration field \(c_0(x, y) = \cos(\pi y)\) under the CSS map with \((a, \gamma_1, \gamma_2) = (-0.04, 0.04, -1)\) (top row) and the linear map \(\Lambda_{SS}\) using the same horizontal and vertical shears (bottom row). The concentration is shown after \(N = 1, 2, 4, 8, 16\) iterations.
The constants $a_1, a_2, a_3$ are chosen such that the linear map and theoretical curves coincide at $N = 5$ when each of the dashed curves decay exponentially.

The same deformation, a stretch in one direction and contraction in another. As a result the Lyapunov exponent of both maps is equal to $\lambda_{\text{max}} = \max(\log(|\lambda_1|, |\lambda_2|))$ where $\lambda_{1,2}$ are the eigenvalues of the deformation tensor (5.3). Therefore, the predicted decay rate of the mix-norm is $-\lambda_{\text{max}}/2$, and this prediction is accurate for the linear map (the decay rates of the mix-norm, thick dashed in Fig. 5.13, match the predicted values, dotted). However, when the cut is included the decay rate of the mix-norm (solid) is sub-exponential.

Therefore, the addition of a discontinuous cutting deformation to an otherwise linear system can significantly affect the mixing dynamics, either enhancing or impeding mixing. When the linear system is purely hyperbolic, i.e. fluid is uniformly stretched in one direction and contracted in another, the mixing rate quantified by
5.4. CUTTING CAN ENHANCE OR IMPEDE MIXING

\[ N = 1 \quad N = 2 \quad N = 4 \quad N = 8 \quad N = 16 \]

\[ \gamma_1 = 0.04 \]

\text{no cut}

\[ \gamma_1 = 0.08 \]

\text{no cut}

\[ \gamma_1 = 0.16 \]

\text{no cut}

Figure 5.14: The same as Fig. 5.12 except with \( \gamma_2 = 1 \), i.e. the vertical shear is in the opposite direction, and various values of \( \gamma_1 \).
the decay of the mix-norm is exponential. However, when the cut is introduced pseudo-elliptic points are created, producing regions where particles are loosely trapped. Mixing is impeded and becomes sub-exponential even though the Lyapunov exponent is positive at every point at which it is defined. On the other hand, when the linear system is purely elliptic, i.e. every point in the domain undergoes a rotation, the mix-norm evolves periodically, meaning there is no mixing. However, when the discontinuous deformation is added the domain becomes tiled by a fractal, dense set of KAM-tori, each of which has multiple frequencies (e.g. in a period-2 island there are the two frequencies given by the periodicity of the island chain – 2 – and the winding number about the centre of the islands which could be rational or irrational). When these frequencies are incommensurate or irrational, the system as a whole is no longer periodic and persistent mixing can occur.

Simple modification of the CSS map could also result in similar interesting behaviour. For instance, removing the periodic boundaries creates a doubly infinite flow domain, allowing the magnitude of the cut, $a$, to be reduced to zero while keeping the magnitude of the two shears, $\gamma_1, \gamma_2$ constant. Under such a map a pair of period-1 points will be created along with their associated pseudo-periodic point at the origin. As $a$ decreases the two period-1 points approach the origin, so in the case of hyperbolic period-1 points the corresponding pseudo-elliptic region will shrink in size but will always exist, impeding the rate of mixing.

5.5 Comparison of competing stretching mechanisms via decoupled Lyapunov exponents

Having seen that discontinuous deformations can significantly affect the mixing and transport dynamics, the smooth stretching and folding deformations are now considered in more detail. The presence of discontinuous deformations created by the source and sink have a significant impact on the smooth deformations as well, creating regions of enhanced stretching. To begin, the study conducted by Jones and Aref [JA88] considering the Pulsed Source Sink (PSS) flow is discussed, as it shows similar characteristics to the RPM flows.

Jones and Aref [JA88] noted that the PSS flow produced ‘intermittent convergence’ of the Lyapunov exponent, i.e. the convergence consisted of a sequence of ‘jumps’ that correlated with the particle being reinjected through the dipole. However, the mechanism that creates this intermittent convergence was not fully uncovered. Reinjection of fluid through the source and sink is not sufficient to create the intermittent convergence, even though fluid is stretched as it approaches the
sink, it is ‘unstretched’ once it exits the source, yielding zero net deformation. The true cause of the intermittent convergence is related to the Lagrangian discontinuity produced by the reinjection. When fluid partially passes through the source/sink, it is cut into disconnected pieces, as shown in Fig. 5.15. Moreover, the fluid that does not pass through the sink is moved away from the sink during the source phase of motion, and the fluid that was connected to the sink before it was switched off remains on the axis connecting the source and sink (the dashed line), which is an invariant of the flow. Therefore, the fluid that becomes attached to the invariant line remains attached forever, producing the tendrils seen in Fig. 5.15(c,d). These tendrils are only possible due to the singularity at the source/sink, and yield enhanced stretching that produces the intermittent convergence of the Lyapunov exponent.

Similar behaviour occurs in the 2DRPM flow due to the Lagrangian discontinuity introduced by reinjection at the dipole and free-slip boundaries. Fluid that partially passes through the dipole has points that are connected to the dipole, on the boundary of the domain, which is a flow invariant like the line connecting the source and sink before. When the dipoles are reoriented, the fluid attached to the boundary remains attached, but is free to move away from the original dipole position. When the dipole returns to its initial position, the two attached points no longer match up with the dipole, although they must still remain attached to the boundary as it is invariant. This creates the thin striations seen in Fig. 5 of [SRLM16] (§5.1) that connect the fluid to the boundary, and fluid inside these striated regions experiences much greater stretching compared to the surrounding fluid. Therefore when computing the Lyapunov exponent associated with the trajectory
Figure 5.16: (a) Intermittent convergence of the Lyapunov exponent (blue) for \((\tau, \Theta) = (0.01, 2\pi/3)\) after 20,000 iterations. The right hand axis (red) is the value of \(s\), which is essentially the inverse of the distance from the Lagrangian discontinuity. (b) The same as (a) except only iterations between \(N = 5,000\) and 10,000 are shown.

of a single initial position and orientation, the convergence undergoes a jump each time the particle enters this region of additional stretching, as demonstrated by the blue curve in Fig. 5.16. To see that these jumps occur when the particle is close to the Lagrangian discontinuity, the location of which is described by the set of points \((\phi, \psi)\) that will be advected onto the sink after the time \(\tau\), i.e. those satisfying

\[
2\tau \mod t_{\text{res}}(\psi) = t_{\text{sink}}(\phi, \psi) = \frac{t_{\text{res}}(\psi)}{2} - t_{\text{adv}}(\phi, \psi)
\]  

(5.4)

and hence the value

\[
s(\phi, \psi) = \left( \frac{t_{\text{res}}(\psi)}{2} - t_{\text{adv}}(\phi, \psi) - (2\tau \mod t_{\text{res}}(\psi)) \right)^{-1}
\]  

(5.5)

is the inverse of the advection time from the Lagrangian discontinuity, and can be thought of as the inverse of the distance from the Lagrangian discontinuity. This is
plotted on the right (red) axis of Fig. 5.16, and it is shown that there is a strong correlation between jumps in the convergence of the Lyapunov exponent and peaks of \( s \).

Therefore there are two competing mechanisms that contribute to the convergence of the Lyapunov exponent: classical stretching and folding associated with structures such as hyperbolic points, and stretching associated with the Lagrangian discontinuity. To find which is the dominant form of stretching and mixing within the 2DRPM flow, the Lyapunov exponent can be decoupled into contributions from each mechanism. To decouple the total Lyapunov exponent \( \sigma_{\text{tot}} \), defined as

\[
\sigma_{\text{tot}} = \lim_{N \to \infty} \frac{1}{N} \lim_{dX \to 0} \ln \left( \frac{|dx_N|}{|dX|} \right) = \lim_{N \to \infty} \frac{1}{N} \lim_{dX \to 0} \sigma_{\text{tot}}^{(N)}(dX),
\]

(5.6)

where \( x_0 = X \) and \( x_{n+1} = Y^\Theta(x_n) \), into a component associated with classical stretching and folding and a component associated with the Lagrangian discontinuity, it is recognised that

\[
\frac{|dx_N|}{|dX|} = \frac{|dx_N|}{|dx_{N-1}|} \frac{|dx_{N-1}|}{|dx_{N-2}|} \cdots \frac{|dx_1|}{|dX|},
\]

(5.7)

and hence

\[
\sigma_{\text{tot}}^{(N)}(dX) = \ln \left( \frac{|dx_N|}{|dX|} \right) = \sum_{i=1}^{N} \ln \left( \frac{|dx_i|}{|dx_{i-1}|} \right).
\]

(5.8)

By dividing the total set of iterations into those that are affected by the Lagrangian discontinuity, \( S_{\text{LD}} \), and those that are not, \( S_{\text{SF}} \), the sum (5.8) can be divided into components

\[
\sigma_{\text{tot}}^{(N)}(dX) = \sum_{i=1}^{N} \ln \left( \frac{|dx_i|}{|dx_{i-1}|} \right) = \sum_{i \in S_{\text{LD}}} \ln \left( \frac{|dx_i|}{|dx_{i-1}|} \right) + \sum_{i \in S_{\text{SF}}} \ln \left( \frac{|dx_i|}{|dx_{i-1}|} \right) = \sigma_{\text{LD}}^{(N)}(dX) + \sigma_{\text{SF}}^{(N)}(dX).
\]

(5.9)

Therefore the total Lyapunov exponent can be decoupled into components

\[
\sigma_{\text{LD}} = \lim_{N \to \infty} \frac{1}{N} \lim_{dX \to 0} \sigma_{\text{LD}}^{(N)}(dX)
\]

\[
\sigma_{\text{SF}} = \lim_{N \to \infty} \frac{1}{N} \lim_{dX \to 0} \sigma_{\text{SF}}^{(N)}(dX)
\]

(5.10)

such that \( \sigma_{\text{tot}} = \sigma_{\text{LD}} + \sigma_{\text{SF}} \).

The set \( S_{\text{LD}} \) is determined by setting a threshold \( \Xi \) for the function \( s(i) \) as each iteration \( i \), so that when \( s(i) > \Xi \) the iterations \( i, \ldots, i + 3^* \) are added to \( S_{\text{LD}} \) as that is when the stretch takes place, as shown in Fig. 5 from [SRLM16] (§5.1). Note that the threshold \( \Xi \) depends on \( \tau \), at smaller \( \tau \) a smaller area is affected by the

\*For \( \Theta = 2\pi m/n \) it will be the iterations \( i, \ldots, i + n \).
Lagrangian discontinuity meaning $\Xi$ must be larger. In the following the threshold $\Xi$ is determined by eye, looking at which values of $s$ the jumps occur at, and this is further tested by performing the decoupling and seeing if the jumps are removed from the exponent $\sigma_{SF}$.

5.5.1 $\tau = 5 \times 10^{-4}$

Considering two initial particle positions for $\tau = 5 \times 10^{-4}$, whose Poincaré sections are shown in Fig. 5.17(a), one in the chaotic set amongst the densely tiled elliptic islands (blue), and the other (red) in the chaotic region between the minimum return streamline (dashed green) amongst the hyperbolic points and pseudo-elliptic points. For the particle located amongst the dense set of KAM-tori (blue), the convergence of the Lyapunov exponents $\sigma_{tot}$ (blue), $\sigma_{LD}$ (orange), and $\sigma_{SF}$ (green) is shown in Fig. 5.18(a) using a threshold of $\Xi = 10^5$ for $s$. In this case the Lagrangian discontinuity provides the greatest contribution to the total Lyapunov exponent, with $\sigma_{LD}/\sigma_{tot} = 0.814$. This is expected as the elliptic islands do not create stretching, and it has been shown in [SRLM16] (§5.1) that there are no hyperbolic points in this region. In contrast, for the red Poincaré section the total Lyapunov exponent is dominated by classical stretching and folding ($\sigma_{LD}/\sigma_{tot} = 0.0239$), as shown in Fig. 5.18(b). This is due to the presence of hyperbolic points and associated manifold connections in this region. Furthermore, the ‘jump’ events are much less frequent in this region (1 jump in 50,000 iterations vs 8 in the other case), so the exponent $\sigma_{LD}$ is close to 0. This difference in jumping frequency could be caused by the fact that the total areas affected by the Lagrangian discontinuity are the same in both cases, but the area of the chaotic set is much smaller for the blue Poincaré section as it is amongst a dense set of KAM-tori. Therefore a particle in the chaotic set amongst the KAM-tori is more likely to be in the set that is affected by the Lagrangian discontinuity.

5.5.2 $\tau = 0.01$

Repeating the process for a larger value of $\tau = 0.01$, again considering two initial particle positions, whose Poincaré sections are shown in Fig. 5.17(b), one in the chaotic set amongst the densely tiled elliptic islands (blue), and the other (red) in the chaotic region between the minimum return streamline (dashed green) amongst the hyperbolic points and pseudo-elliptic points. Similar phenomena are observed compared to $\tau = 5^{-4}$. For the blue Poincaré section, the total Lyapunov exponent is dominated by the Lagrangian discontinuity, $\sigma_{LD}/\sigma_{tot} = 0.656$, as shown in Fig. 5.19(a,b). On the
Figure 5.17: Poincaré sections for the 2DRPM flow with $\Theta = 2\pi/3$ using various initial conditions chosen on the symmetry line $y = \tan(-\Theta/2)$ (dashed orange) and various values of $\tau$. In each plot the streamlines of the flow in the limit as $\tau \to 0$ are shown in grey, and the streamlines with minimum return time are shown in dashed green and pink. The location of the Lagrangian discontinuity is shown as the black/red curve that is approximately semicircular. (a) $\tau = 5 \times 10^{-4}$. Two particles initially at radii 0.76 (blue) and 0.95 (red), chosen on each side of the minimum return streamline, are advected for 50,000 flow periods. (b) $\tau = 0.01$. The two particles are initially at radii 0.8 (blue) and 0.95 (red) and are advected for 20,000 flow periods. (c) $\tau = 0.1$. One particle (black) initially located at $x = y = 0.5$ is advected for 10,000 iterations.
Figure 5.18: Decoupling the total Lyapunov exponent $\sigma_{\text{total}}$ (blue) for the Poincaré sections in Fig. 5.17(a) ((a) blue, (b) red) into components from the Lagrangian discontinuity $\sigma_{\text{LD}}$ (orange) and classical stretching and folding $\sigma_{\text{SF}}$ (green). The function $s$ (dashed black) is plotted against the right vertical axis, and the threshold $\Xi = 10^5$ is used to determine jumps.

At a larger value of $\tau = 0.1$, particles no longer closely follow the streamlines of the flow in the limit as $\tau \to 0$ (grey), as evidenced by the Poincaré section Fig. 5.17(c). In this case approximately two fifths of the total Lyapunov exponent is contributed by the Lagrangian discontinuity ($\sigma_{\text{LD}}/\sigma_{\text{tot}} = 0.380$, Fig. 5.20), meaning classical stretching and folding is dominant, but they each provide a significant contribution.
Figure 5.19: Decoupling the total Lyapunov exponent $\sigma_{\text{total}}$ (blue) for the Poincaré sections in Fig. 5.17(b) ((a,b) blue, (c) red) into components from the Lagrangian discontinuity $\sigma_{\text{LD}}$ (orange) and classical stretching and folding $\sigma_{\text{SF}}$ (green). The function $s$ (dashed black) is plotted against the right vertical axis, and the threshold $\Xi = 4,000$ is used to determine jumps. (b) shows a subset of (a) between iterations 5,000 and 10,000.
Figure 5.20: Decoupling the total Lyapunov exponent $\sigma_{\text{total}}$ (blue) for the Poincaré section Fig. 5.17(c) into components from the Lagrangian discontinuity $\sigma_{\text{LD}}$ (orange) and classical stretching and folding $\sigma_{\text{SF}}$ (green). The value of the function $s$ (dashed black) is plotted against the right vertical axis, and the threshold $\Xi = 200$ is used to detect jumps. (b) shows a subset of (a) between iterations 2,000 and 4,000 where the jumps are more evident.
A summary of all these cases is provided in Table 5.1. It is clear that at all values of \( \tau \) considered the additional stretching created by the Lagrangian discontinuity has a significant effect on the overall transport dynamics, creating enhanced stretching.

<table>
<thead>
<tr>
<th>( \tau )</th>
<th>P-section</th>
<th>( \sigma_{\text{tot}} )</th>
<th>( \sigma_{\text{LD}} )</th>
<th>( \sigma_{\text{SF}} )</th>
<th>( \sigma_{\text{LD}}/\sigma_{\text{tot}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 5 \times 10^{-4} )</td>
<td>blue</td>
<td>( 1.688 \times 10^{-4} )</td>
<td>( 1.373 \times 10^{-4} )</td>
<td>( 3.143 \times 10^{-5} )</td>
<td>( 0.814 )</td>
</tr>
<tr>
<td>( 5 \times 10^{-4} )</td>
<td>red</td>
<td>( 3.782 \times 10^{-4} )</td>
<td>( 9.050 \times 10^{-6} )</td>
<td>( 3.691 \times 10^{-4} )</td>
<td>( 0.0239 )</td>
</tr>
<tr>
<td>0.01</td>
<td>blue</td>
<td>( 5.458 \times 10^{-3} )</td>
<td>( 3.579 \times 10^{-3} )</td>
<td>( 1.880 \times 10^{-3} )</td>
<td>( 0.656 )</td>
</tr>
<tr>
<td>0.01</td>
<td>red</td>
<td>( 8.158 \times 10^{-3} )</td>
<td>( 2.589 \times 10^{-4} )</td>
<td>( 7.899 \times 10^{-3} )</td>
<td>( 0.0317 )</td>
</tr>
<tr>
<td>0.1</td>
<td>black</td>
<td>0.1272</td>
<td>0.04826</td>
<td>0.07889</td>
<td>0.380</td>
</tr>
</tbody>
</table>

Table 5.1: Decoupled Lyapunov exponents for various values of \( \tau \) and initial particle locations for \( \Theta = 2\pi/3 \).

### 5.6 Conclusions

Discontinuous deformations play a significant role in the overall organisation of transport in the 2DRPM flow, and when combined with smooth deformations, complex transport structures are created that are not predicted by the theory for smooth deformations, including ‘pseudo-elliptic’ and ‘pseudo-hyperbolic’ points. These discontinuous deformations occur in a vast array of applications, and generically occur in fluid flows with extraction and reinjection of fluid, such as the 2DRPM flow, resulting in non-Hamiltonian particle transport even though the base flow (the steady dipole flow) is Hamiltonian.

Considering the methodologies usually employed to study smoothly deforming systems applied to systems with discontinuous deformations, periodic point analysis is still useful, however the presence of discontinuous deformations invalidates much of the theory, including the Poincaré–Birkhoff Theorem. This manifests in the 2DRPM flow as chains of elliptic (hyperbolic) periodic points without hyperbolic (elliptic) points alternately interleaving them. By introducing the concept of ‘pseudo-periodic’ points, which occur in the limiting approximation of a cut as a localised shear, the Poincaré–Birkhoff theorem can be recovered, in the sense that pseudo-hyperbolic points interleave chains of elliptic points and pseudo-elliptic points interleave chains of hyperbolic points. These chains of elliptic and pseudo-hyperbolic points are created together with chains of hyperbolic and pseudo-elliptic points in reconnection bifurcations that resonate with a twistless torus. The pseudo-periodic points can be found by constructing the webs of images and preimages of the Lagrangian discon-
tinuity, a concept that has been introduced to provide a comprehensive kinematic template for systems with discontinuous deformations, analogous to the template created by periodic points in smoothly deforming systems.

Furthermore, the rate of mixing in smoothly deforming systems is usually characterised by the Lyapunov exponent, however it has been demonstrated that this is not a good measure for systems with combined CS and SF, as mixing can be achieved even when the Lyapunov exponent is equal to zero almost everywhere*. Conversely, mixing can be impeded in pseudo-elliptic regions even though every point in the domain not affected by the discontinuous deformation experiences uniform contraction and expansion. In these systems with combined CS and SF, a better measure for mixing is the mix-norm introduced by Mathew et al. [MMP05], which is able to capture the impact of the discontinuous deformation in addition to the smooth deformations. Using the mix-norm it is clearly demonstrated that mixing created by the CSS map is either impeded or enhanced compared to the equivalent linear system with the cutting action removed.

In extraction and reinjection systems the discontinuous deformation also impacts transport via tendrils that arise in the fluid cutting mechanism and connect fluid in the interior of the domain to the boundary. Fluid along these tendrils experiences large stretching and contraction, leading to ‘intermittent convergence’ of the Lyapunov exponent. Therefore, there are two mechanisms that contribute to the total stretching and contraction experienced by fluid in extraction/reinjection systems, classical stretching and folding generated by tangles of the stable and unstable manifolds associated with hyperbolic points, and stretching created by the cutting mechanism. The contributions of each of these mechanisms to the total fluid stretching can be determined by decoupling the total Lyapunov exponent $\sigma_{\text{tot}}$ into contributions $\sigma_{\text{SF}}$ (stretching and folding) and $\sigma_{\text{LD}}$ (cutting mechanism) arising from each stretching mechanism. It is observed that the stretching created by the cutting mechanism provides a significant contribution at all values of $\tau$, and is responsible for most of the stretching that occurs at small values of $\tau$ in the regions with a dense tiling of elliptic islands interleaved by pseudo-hyperbolic points. On the other hand, at the same values of $\tau$, the cutting mechanism provides a minor contribution in the region on the other side of the minimum return streamline, that is tiled by hyperbolic and pseudo-elliptic points.

*In the strict measure theoretic sense, i.e. it is non-zero, or not defined, on a set of measure zero.
5.6.1 Future work

Extending these results, future work should focus on:

- **Generalisation to arbitrary reorientation angles** $\Theta$. This study has primarily focused on the reorientation angle $\Theta = 2\pi/3$, and the results are generic to all reorientation angles of the form $2\pi m/n$ with $n$ odd, due to the $n$-fold symmetry of the flow in the limit as $\tau \to 0$. However, for reorientation angles with $n$ even or such that $\Theta/\pi$ is irrational, fundamentally different phenomena are expected, as there is no net flow in the limit as $\tau \to 0$, and therefore no twistless torus. In these cases there is still a Lagrangian discontinuity created by the dipole, however the resultant structures will be different.

- **No-slip boundary conditions applied to the 2DRPM flow.** By changing from free-slip to no-slip boundary conditions, the Lagrangian discontinuity in the 2DRPM is removed, and fluid deformation is smooth. It is expected that the structures observed in the 2DRPM flow with free-slip boundaries created by discontinuous deformations, such as pseudo-periodic points, will have analogues in the no-slip flow similar to those observed in the smoothed CSS map compared to the original discontinuous CSS map (§V in [SRLM16], §5.1). In the case of the 2DRPM flow with no-slip boundaries, the thickness of the boundary layer will play a role similar to the smoothing parameter $b$ in the smoothed CSS map.

- **Discontinuous deformations in 3D.** It has been demonstrated that discontinuous deformations can significantly affect the transport dynamics of 2D systems, and in 3D the effect could be even more profound due to the additional topological freedom. As the 3DRPM flow shares the extraction/reinjection and free-slip boundary properties of its 2D counterpart, it provides a natural system in which to study the impact of discontinuous deformations in 3D. This is considered in Chapter 7, where it is shown that the Lagrangian discontinuity also creates a mechanism for 3D transport, however this only provides a glimpse of the vast possibilities that exist in this area. Extending the simple CSS map to 3D itself opens up a huge number of possibilities for new transport phenomena.
Chapter 6

Local Transport Bifurcations

As discussed in §4.3, periodic points and lines create an organisational template for the transport kinematics of fluid flows. These structures are analysed in this chapter, in particular the degenerate type periodic points that represent bifurcations in local stability. The different types of bifurcations that occur in the 3DRPM flow are uncovered: period-doubling bifurcations, period-tripling bifurcations and saddle–centre bifurcations (Fig. 4.10). The nature of period-doubling and saddle–centre bifurcations is reasonably well understood, but here they are further classified as tangent bifurcations since they must occur at points along periodic lines where the associated eigenvectors become co-planar. These points are subject to topological constraints on their type based on the fixed-point index (or Poincaré index).

Period-tripling bifurcations have been observed in the 3D study [MJM05], however the impact of the bifurcation on transport organisation is not discussed in detail. Here it is shown that these bifurcations play a dominant role in the organisation of transport in the 3DRPM flow, creating confining regions, ‘sticky’ regions, and chaotic regions. Furthermore, twistless tori have been shown to be generic to period-tripling bifurcations in 2D systems [DMS00], and here it is shown that twistless tori occur as a ‘twistless tube’ in the 3DRPM flow. While twistless tubes have been demonstrated for 1-action maps [DM12], this is the first time twistless tubes have been observed in a 2-action region of a 3D system that does not admit an invariant, i.e. a system that is not a nested set of 2D systems. The presence of this twistless tube is expected to produce interesting and non-classical behaviour in its vicinity, including reconnection bifurcations and regions of low transmissivity under perturbation.
6.1 Period-tripling bifurcations

To study the impact of period-tripling bifurcations in the 3DRPM flow, a simple 2D model is first introduced.

6.1.1 2D model

Period-tripling bifurcations have been observed in a number of studies [BM77, DMS00, MJM05] in 2D and 3D systems, but their transport characteristics in 3D systems have not been studied. In 3D systems these bifurcations occur at points on periodic lines where the rotation angle $\alpha$ (from the eigenvalues $\lambda_{1,2} = e^{\pm i\alpha}$) around an elliptic segment as it is traversed reverses direction, and a chain of period-3 lines intersect at the degenerate point. Due to the complexity of the period-tripling bifurcations in the 3DRPM flow, the basic structure is first illustrated with a simple model flow derived from an expansion of the flow about a degenerate point with a Poincaré index of $-2$. This model is a perturbation of the steady 2D six-roll mill flow [BM77], with Hamiltonian

$$F(x, y; \omega) = \frac{x^3}{3} - xy^3 + \omega(x^2 + y^2),$$

(6.1)

which is related to the elliptic umbilic catastrophe [Tho89] and the Henon–Heiles potential [Hén83]. A period-tripling bifurcation occurs when the vorticity $\omega$ is varied as a control parameter, as shown in Fig. 6.1. At $\omega = 0$ there is no vorticity and there is a degenerate fixed point at the origin, with three stable and three unstable directions, yielding a Poincaré index of $-2$. For positive or negative $\omega$, the vorticity creates an elliptic fixed point at the origin, and for the Poincaré index to remain constant three hyperbolic fixed points are created whose heteroclinic manifold connections form the outer barrier for the invariant tori. When transitioning from positive to negative $\omega$, or vice versa, the vorticity changes direction, resulting in a reversal in the orientation of the triangular structure seen in Fig. 6.1. A similar phenomenon occurs if vorticity is added to the streamfunction of a 2$n$-roll mill for odd $n$. Instead of three stable and unstable directions there are $n$, and for $\omega \neq 0$ there will be $n$ hyperbolic points arranged in an $n$-gon around an elliptic point, with a Poincaré index of $1 - n$.

6.1.2 3DRPM flow

Period-tripling bifurcations are present in the 3DRPM flow with rotation angle $\Theta = 2\pi/3$ for all values of $\tau$. They manifest at points on periodic lines where
Figure 6.1: A period-tripling bifurcation in the elliptic-umbilic catastrophe, eq. 6.1, occurs at $\omega = 0$. Three hyperbolic fixed points (red) and one elliptic fixed point (blue) coalesce at the bifurcation point.

The elliptic rotation angle becomes $2\pi/3$, shown in Fig. 6.2(a) as open circles. At these points the map $\hat{Y}_r^\Theta$ experiences a $1/3$ resonance, i.e. particles in the vicinity of the elliptic periodic point will approximately return to their initial position after three iterations. If particles are tracked in the non-rotating (laboratory) frame then the local rotation angle becomes $\epsilon = \alpha - 2\pi/3$. The parameter $\epsilon$ varies along the period-1 line, and becomes 0 at points where $\alpha = 2\pi/3$, indicating the presence of degenerate points. At these $1/3$ resonant degenerate points period-tripling bifurcations are generic [DMS00], with the rotation angle $\epsilon$ playing the role of $\omega$ in eq. (6.1).

As for the model system given by eq. (6.1) there are three hyperbolic lines (period-3 in the rotating dipole frame but period-1 in the non-rotating laboratory frame) that intersect the elliptic period-1 line, resulting in a reversal of triangular invariant tori on each side of the bifurcation point, as shown in Fig. 6.3. These invariant tori join to form pyramidal invariant tubes that connect at the bifurcation point. To provide additional evidence of this behaviour, Fig. 6.2(b) shows that period-3 lines (coloured) intersect the period-1 lines (grey) at every location where the rotation angle is $2\pi/3$ (the open circles). Furthermore, the magnitude of stretching along the hyperbolic sections of the period-3 lines, characterised by
Figure 6.2: (a) The same as Fig. 4.10(a) except hyperbolic points are shown as grey and elliptic points are coloured according to local rotation angle $\alpha$, from 0 (purple) to $\pi$ (red). Points with $\alpha = 2\pi/3$ are marked as open circles and correspond to period-tripling bifurcations. (b) In order to show the intersection of period-1 and period-3 lines in the symmetry plane, the period-1 lines of panel (a) are redrawn in panel (b) as solid grey lines. The coloured lines of panel (b) are period-3 lines. Elliptic segments are coloured blue and hyperbolic segments are coloured according to the local transverse stretching/contraction factor, with purple (red) corresponding to zero (maximum) stretching/contracting.

Figure 6.3: Period-tripling bifurcation in the 3DRPM flow with $\tau = 1.1\tau_0$. Period-1 and period-3 lines meet at a degenerate point on the $y$-axis (red - hyperbolic, blue - elliptic). Green and orange points correspond to Poincaré sections at $y$-levels above and below the bifurcation point $y_0$. 
the magnitude of the logarithm of the transverse eigenvalues $\lambda_{1,2}$ of the Jacobian, becomes zero (purple) at the period-tripling bifurcations. This means that although the period-1 rotation angle is not zero, these bifurcation points can be considered as period-3 degenerate points.

### 6.1.3 Creation and annihilation

Examining the creation and annihilation of period-tripling bifurcation points, integer multiples of a critical value of the reorientation period, $\tau_0 \approx 0.29344$, are considered. This value of $\tau$ corresponds to the return time of a particle initially located at the origin under the steady dipole flow. At the values $\tau = N\tau_0$ the origin is invariant under both the steady dipole advection and rotation that comprise the combined map $Y_\tau^\Theta = R_\Theta \hat{Y}_\tau$, hence the origin is a period-1 point (Fig. 6.4(a)). Moreover, after three iterations of the map $Y_\tau^\Theta$ there is no net local deformation of fluid near the origin, and so this point is a period-3 degenerate point, in particular a period-tripling bifurcation point. In the 3DRPM flow this occurs at any point where a period-1 line intersects the $y$-axis, not just at the origin. For a particle initially located on the $y$-axis to return to its initial position, it must return after the steady dipole advection step, as the rotation cannot move a point that is off the $y$-axis onto the $y$-axis. During the steady dipole advection, fluid at these period-1 points experiences a shear of the form

$$D\hat{Y}_\tau = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & N\gamma_1 & 1 \end{pmatrix} \tag{6.2}$$

where $N$ is the number of times the particle is reinjected during the steady dipole advection, and $\gamma_1$ is the value of the shear experienced during a single reinjection, which depends on the location $y^*$ of the periodic point on the $y$-axis according to Fig. 6.4(b). Therefore, for a reorientation angle $\Theta$, the Jacobian is given by

$$DY_\tau^\Theta = R_\Theta^\Theta D\hat{Y}_\tau \tag{6.3}$$

with eigenvalues $1, \exp(\pm i\Theta)$, and can be diagonalized as $DY_\tau^\Theta = PD P^{-1}$ where $D$ is the diagonal matrix

$$D = \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{i\Theta} & 0 \\ 0 & 0 & e^{-i\Theta} \end{pmatrix} \tag{6.4}.$$  

Hence, for $\Theta = 2\pi m/n$, the Jacobian satisfies $(DY_\tau^\Theta)^n = I$, making it a period-$n$ degenerate point. In particular, for $\Theta = 2\pi/3$, the periodic points on the $y$-axis are period-3 degenerate points, and thus period-tripling bifurcations.
6.1. PERIOD-TRIPLING BIFURCATIONS

Figure 6.4: (a) The values of $\tau$ for which there is a periodic point on the $y$-axis at $(0, y^*, 0)$. $N$ is the number of times the particle is reinjected. (b) The magnitude of the corresponding shear matrix $D\hat{Y}_\tau$ in eq. (6.2).

Tracking the individual period-1 lines with increasing $\tau$, they initially appear as isolated degenerate points resulting from saddle–centre bifurcations in the $xz$-plane, which then form closed loops with a pair of saddle–centre bifurcation points separating elliptic and hyperbolic segments, shown as the solid black circles in Fig. 4.10(a). These loops expand outward as $\tau$ increases, and eventually collide with the spherical boundary, as demonstrated in Fig. 6.5. Therefore each new period-1 line intersects the $y$-axis at a value $\tau = N\tau_0$, which also corresponds to the creation of a period-tripling bifurcation. At these values of $\tau$, a period-1 line intersects the $y$-axis tangentially, creating a single degenerate point at the origin. This degenerate point is unique because the period-3 lines also intersect the period-1 line and $y$-axis tangentially, meaning there is no reversal in the orientation of the triangular structures. The local rotation still reaches zero, but does not reverse in direction. For a small perturbation $\epsilon$ away from $\tau = N\tau_0$ the tangent intersections become

Figure 6.5: The path taken by the period-tripling bifurcation point with increasing $\tau$ (orange) shown with the corresponding period-1 lines at various values of $\tau$ (grey). The point where period-1 lines annihilate is marked as $A$. 

transverse, creating two period-tripling bifurcations that are symmetric about the $xz$-plane, and are orientation reversing. This is depicted in Fig. 6.6 for $N = 1$, showing the rotation angle $\alpha$ as a function of arc-length along the period-1 line starting from the $xz$-plane. Period-tripling bifurcations occur where the rotation angle $\alpha$ reaches $2\pi/3$. For $\tau < \tau_0$ there are no intersections of this period-1 line with the $y$-axis and therefore no period-tripling bifurcations, whereas for $\tau = \tau_0$ there is one intersection, and for $\tau > \tau_0$ there are two intersections. The reorientation periods $N\tau_0$ therefore correspond to local flow bifurcations.

The trajectory of the period-tripling bifurcation point on the first new period-1 line ($N = 1$) as $\tau$ is increased is shown in Fig. 6.5 by the orange curve. After appearing at the origin when $\tau = N\tau_0$, it moves up the $y$-axis, to the point where it reaches the spherical boundary. This occurs when $\tau$ is equal to the return time of the streamline on the spherical boundary, which has been scaled to be equal to 1, multiplied by the number of reinjections $N$, i.e. at $\tau = N$. This is also shown in Fig. 6.4(a) by the values of $\tau$ at $y^* = 1$. The period-tripling bifurcation point then moves off the $y$-axis, moving towards the $xz$-plane where it is annihilated. This path is traced out for each period-1 line that is created. The period-tripling bifurcation point is annihilated at approximately the same value of $\tau$ as when the period-1 line itself is annihilated, which occurs when the line reaches the point $A$ at the intersection of the $xz$-plane, spherical boundary and symmetry plane, shown in Fig. 6.5. To find the values of $\tau$ such that the point $A$ is a period-1 point, and hence when the period-1 lines are annihilated, consider the time $T_{AB}(\Theta)$ it takes for a particle to travel from the point $A$ to its reflection through the $xy$-plane, the point $B$ shown in Fig. 6.7. When $\tau = T_{AB} \approx 0.9333$, the map $Y_{\tau}^{\Theta}$ takes a particle

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**Figure 6.6:** The local rotation angle $\alpha$ given by the Jacobian at points a distance $d$ along the period-1 line from the $xz$-plane. Curves are shown for $\tau = 0.99\tau_0, \tau_0, 1.01\tau_0, 1.1\tau_0$. Degenerate points are marked by large dots, where $\alpha = 2\pi/3$. 
initially located at $A$ to the point $B$ under the steady dipole flow, then the particle is counter-rotated back to $A$, meaning the point $A$ is a period-1 point. Moreover, if the particle is reinjected any number of times through the dipole but still finishes at $B$ then the point $A$ will still be a period-1 point. As the streamlines on the spherical boundary have the longest return time, scaled to correspond to a value $\tau = 1$, $A$ is a period-1 point when $\tau = T_{AB} + j$ where $j$ is the number of times that the particle is reinjected. Combining this with the creation of period-tripling bifurcation points at values $\tau = N\tau_0$, the overall number of period-tripling bifurcation points $N_{1/3}$ within the 3DRPM flow is a linear function of $\tau$

\[ N_{1/3} \approx \frac{\tau}{\tau_0} - (\tau - T_{AB}) \approx 2.4\tau \] (6.5)

for $\tau \gg 0$. This shows that the number of period-tripling bifurcation points grows linearly with $\tau$, resulting in more of the stable pyramidal invariant tubes and more of the associated hyperbolic period-3 lines whose manifold intersections can drive chaos. By seeding a large number of particles on a grid in the domain it is observed that the total volume of the invariant tubes decreases as $\tau$ increases even though the total number of invariant tubes increases. It is likely that as $\tau \to \infty$ the total volume of the invariant tubes will approach zero, meaning an approach to global chaos.
6.1.4 Impact on transport and manifolds

The structures associated with period-tripling bifurcations can have a significant influence on the overall transport properties of a fluid flow, this is demonstrated in Fig. 6.8 where the period-tripling bifurcation at $\tau = 1.01\tau_0$ (Fig. 6.8(b)) destroys the invariant tori surrounding the period-1 line that exist at $\tau = 0.9\tau_0$ (Fig. 6.8(a)). The degenerate points associated with the bifurcation have three stable and three unstable directions, creating transport structures similar to hyperbolic points. These stable and unstable directions become the manifolds of the associated period-3 hyperbolic lines away from the bifurcation, as shown in Fig. 6.9. Also, surrounding the elliptic segments of the period-3 lines there exist invariant tori that join to create impenetrable barriers to particle transport. The locations of the outer-most invariant tori depend on the nature of the manifold intersections, tangential or transverse. If the stable and unstable manifolds intersect tangentially, as is the case at larger y-values (closer to white) in Fig. 6.9 and also in Fig. 6.8(b2), then the 1D manifolds form the outermost invariant tori. Descending down the y-axis, the manifolds become ‘wavy’, indicating transverse intersections of the stable and unstable manifolds and the existence of a chaotic region. Near the values of y that this first occurs, for example $y = 0.19$ (Fig. 6.8(b3)), particles in the chaotic region near the period-3 invariant tori are loosely trapped in a ‘sticky’ region. Descending further along the y-axis (Fig. 6.8(b4)), the ‘sticky’ region is also destroyed, giving way to wide-spread chaos. Therefore, period-tripling bifurcations can drive global chaos via transverse manifold intersections or create the boundaries for confining regions if the manifold intersections are tangent.

As well as a bifurcation in local stability, period-tripling bifurcations also create a bifurcation in the manifolds associated with the hyperbolic period-3 lines, as demonstrated in Fig. 6.10. The stable and unstable manifolds for single points on each of the period-3 lines are shown at values $y < y_0$ (left panel) and $y > y_0$ (right), where $y_0$ is the bifurcation point. The manifold pairs $W_{s,u}^*$ associated with each period-3 line are coloured with two shades of the same colour (e.g. stable - green, unstable - dark green etc.). It is observed that for $y > y_0$ (right) the manifolds form transverse homoclinic connections since the same colours intersect, whereas for $y < y_0$ (left) the connections become heteroclinic, and so while the orientation of the triangular island structures are reflected across the bifurcation point, the global arrangement of structures remains essentially the same. This is only possible if there is a change between heteroclinic and homoclinic connections across the bifurcation point. Considering the entire 2D unstable manifold $W_{2D}^*$ associated with only one of the period-3 lines, as in Fig. 6.9, there is a disconnection of the manifold sheet as
Figure 6.8: Poincaré sections generated by initially planar (parallel to the $xz$-plane) clusters of particles near the $y$-axis at various values of $y$. Period-1 and period-3 lines are colored according to stability, red - hyperbolic, blue - elliptic. (a1–a4) $\tau = 0.9\tau_0$. There are no period-3 lines, and invariant tori surround the elliptic period-1 line. (b1–b4) $\tau = 1.01\tau_0$. A period-tripling bifurcation occurs on the $y$-axis, that destroys tori, creates sticky regions, creates chaotic regions, alters topology and affects transport in a region of the domain that is vastly more extensive than just the ‘neighborhood’ of the bifurcation point.
Figure 6.9: (a–d) Four views of the 2D unstable manifold $W^u_{2D}$ for one of the period-3 lines for $\tau = 1.1 \tau_0$. The manifold consists of the disjoint union of 1D manifolds for points along the hyperbolic segment of the periodic line, colored according to the $y$-coordinate, $y = 0$ (dark red) to maximum (white). As in Fig. 6.3, the point $y_0$ on the $y$-axis – seen in (c) – is a period-tripling bifurcation point, and the 2D manifolds for $y < y_0$ and $y > y_0$ form disconnected sheets. The green point marks the location of a tangent saddle–centre bifurcation point, where the stability changes between elliptic and hyperbolic. In (d) it can be seen that close to the bifurcation point the 1D manifolds form parallel homoclinic connections, wrapping around the elliptic line, but at a critical distance away from the bifurcation point waves in the 1D manifolds begin to develop, indicating transverse intersections and chaos.
6.1. PERIOD-TRIPPING BIFURCATIONS

Figure 6.10: Bifurcation of stable/unstable manifolds caused by period-tripling bifurcation, which occurs at $y = y_0$ as in Fig. 6.3 for $(\Theta, \tau) = (2\pi/3, 1.01\tau_0)$. Manifold pairs associated with each period-3 line are shown as different shades of the same colour, e.g. green and dark green. (a) $y < y_0$, manifolds form heteroclinic connections. (b) $y > y_0$, manifolds form homoclinic connections.

The period-3 point crosses the bifurcation point. The bifurcation point can either be thought of as a point of discontinuity for the manifold sheet, or the two segments of the period-3 line, separated by the bifurcation point, can be considered as separate entities with their own manifold structures.

Therefore, the period-tripling bifurcation points themselves do not have a significant impact on global transport, as they occur as an isolated unstable point along an otherwise elliptic periodic line, but they organize vast transport structures that generate chaos and form barriers to transport.

For other values $\Theta = 2\pi m/n$ with $n$ odd similar behaviour is observed. Rather than period-tripling bifurcations they are $n$-tupling. Instead of three period-3 hyperbolic lines there are $n$ period-$n$ lines and the degenerate point has a Poincaré index of $1 - n$. These cases are analogous to the $2n$-roll mill, with the arc-length along the period-1 line acting as the control parameter $\omega$. 


### 6.2 Twist and twistless tori

Dullin *et al.* [DMS00] demonstrated that twistless tori are generic to period-tripling bifurcations in 2D systems, and used the bifurcation sequence of the Hénon map as an example. This bifurcation sequence is detailed at the start of this section, and it is then shown that the period-tripling bifurcations in the 3DRPM flow share similar properties, creating twistless tubes in a 2-action region.

#### 6.2.1 The Hénon map

Dullin *et al.* [DMS00] present the Hénon map as an example of an area-preserving map that displays twistless tori and reconnection bifurcations. The map is given by

\[
H : (x, y) \mapsto (y - k + x^2, -x)
\]  

(6.6)

and it can be shown that any quadratic area-preserving map of the plane can be written in this form [Hen69]. Solving \( H(x) = x \) reveals a pair of fixed points when \( k \geq -1 \) located at \( x^\pm = (x^\pm, y^\pm) \), such that \( x^\pm = -y^\pm = 1 \pm \sqrt{1 + k} \), and whose local stability is determined by the deformation tensor

\[
D H \bigg|_{x^\pm} = \begin{pmatrix} 2x^\pm & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} 2(1 \pm \sqrt{1 + k}) & 1 \\ -1 & 0 \end{pmatrix}.
\]

(6.7)

For \(-1 < k < 3\) the eigenvalues for the fixed point \( x^- \)

\[
\lambda_{1,2}^- = x^- \pm \sqrt{1 + k - 2\sqrt{1 + k}}
\]

(6.8)

form a complex conjugate pair with unit modulus and hence the fixed point is elliptic. Whereas for \( k > 3 \) the eigenvalues \( \lambda_{1,2}^- \) are reciprocal real numbers and the fixed point is hyperbolic. The other fixed point \( x^+ \) has eigenvalues

\[
\lambda_{1,2}^+ = x^+ \pm \sqrt{1 + k + 2\sqrt{1 + k}}
\]

(6.9)

which are real for all values of \( k > -1 \). Hence the fixed point \( x^+ \) is always hyperbolic.

The fixed point \( x^- \) is elliptic when \(-1 < k < 3\), and has a rotation number given by

\[
\omega = \frac{1}{2\pi} \arccos \left( 1 - \sqrt{1 + k} \right) = \frac{1}{\pi} \arcsin \left( \frac{1 + k}{4} \right)^{1/4}.
\]

(6.10)

which is a monotonically increasing function of \( k \). Therefore the parameters \( \omega \) and \( k \) can be used interchangeably as the system parameter in this range. By computing the twist, Dullin *et al.* show that the Hénon map has a twistless torus for \( 9/16 < k < 1 \), with the twistless torus coinciding with the fixed point \( x^- \) when
As $k$ increases the twistless torus moves radially outward from the elliptic fixed point, and at $k = 1$ three period-3 saddle–centre bifurcations occur on the twistless torus. At this point the twistless torus becomes the manifold connections associated with the period-3 hyperbolic points. This bifurcation sequence is depicted in Table 6.1 and Fig. 6.11. In the sequence from $\omega_0$ to $\omega_5$ the twistless torus has rotation number that passes through infinitely many rational numbers $m/n$, and each time it is expected that a reconnection bifurcation will occur resonant to $m/n$, i.e. two chains of period-$n$ points will reconnect via a sequence of saddle–centre bifurcations. This is illustrated in the sequence $\omega_1-\omega_4$ for the $3/10$ resonance, which is the lowest-order rational (smallest denominator) in the range of values taken by the rotation number of the twistless torus. Note that the values $\omega_1-\omega_4$ are very close so the bifurcation occurs in a very small window.

To elaborate on the bifurcation sequence shown in Fig. 6.11 the phase portraits shown in Fig. 6.12 have been produced. These figures fit into the sequence as

$$(a) < \omega_0 < \omega_4 < (b) < (c) < (d) = \omega_5 < (e) < (f) < \omega_6.$$  

(6.11)

In each case the tori surrounding the elliptic fixed point $x^-$ are coloured according to their rotation number $\Omega$, where red is the maximum and purple is the minimum. In each case the torus with the highest rotation number is shown in thick black, which for Fig. 6.12(b-d) corresponds to the twistless torus, and for Fig. 6.12(e,f) is the torus chosen closest to the manifold connections associated with the period-3 hyperbolic points (red). Note that tori are chosen at equally spaced radii ($\Delta r = 0.005$) along

<table>
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<th>Bifurcation</th>
<th>Label</th>
<th>$\omega$</th>
<th>$k$</th>
</tr>
</thead>
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<td>Twistless</td>
<td>$\omega_0$</td>
<td>0.2902153</td>
<td>9/16</td>
</tr>
<tr>
<td>sc(3/10)</td>
<td>$\omega_1$</td>
<td>0.2995432</td>
<td>0.7063832</td>
</tr>
<tr>
<td>sc(3/10)</td>
<td>$\omega_2$</td>
<td>0.2995438</td>
<td>0.7063926</td>
</tr>
<tr>
<td>Reconnection</td>
<td>$\omega_3$</td>
<td>0.2995444</td>
<td>0.70640121</td>
</tr>
<tr>
<td>Decoupling</td>
<td>$\omega_4$</td>
<td>3/10</td>
<td>0.7135255</td>
</tr>
<tr>
<td>sc(1/3)</td>
<td>$\omega_5$</td>
<td>0.3179717</td>
<td>1</td>
</tr>
<tr>
<td>Tripling</td>
<td>$\omega_6$</td>
<td>1/3</td>
<td>5/4</td>
</tr>
</tbody>
</table>

Table 6.1: Bifurcation sequence for the Hénon map. Here sc($m/n$) refers to a saddle–centre bifurcation with resonance $m/n$. Reproduced with permission from H. R. Dullin, J. D. Meiss, and D. Sterling. Generic twistless bifurcations. Nonlinearity, 13(1):203, 2000 [DMS00], Copyright IOP Publishing & London Mathematical Society. All rights reserved.
Figure 6.11: Bifurcation diagram for the Hénon map. The twistless torus appears at the centre of the elliptic point at \( \omega_0 \). Between \( \omega_1 \) and \( \omega_4 \) a 3/10 reconnection bifurcation occurs on the twistless torus. At \( \omega_5 \) a period-3 saddle–centre bifurcation occurs and finally at \( \omega_6 \) a period-tripling bifurcation occurs. Reproduced with permission from H. R. Dullin, J. D. Meiss, and D. Sterling. Generic twistless bifurcations. *Nonlinearity*, 13(1):203, 2000 [DMS00], Copyright IOP Publishing & London Mathematical Society. All rights reserved.
6.2. TWIST AND TWISTLESS TORI

Figure 6.12: Phase portraits for the Hénon map at various values of the system parameter $k$. In each plot the tori surrounding the elliptic fixed point (blue) are coloured according their rotation number $\Omega$ (red: maximum, purple: minimum) and the torus with the maximum rotation number is shown in thick black, representing the twistless torus for $9/16 \leq k \leq 1$. Non-periodic trajectories are coloured light grey (most evident in (f)). The period-3 elliptic and hyperbolic fixed points that are created by the $1/3$ saddle–centre bifurcation are shown as the blue and red points in (e,f).

the symmetry line $y = -x$, so the black torus is not exactly the twistless torus but is the closest torus in the finite set to it. The rotation number $\Omega$ of each torus is determined by mapping a single point on the torus for 200,000 iterations, then finding the peak in the Fourier spectrum of the $x$-coordinate time-series. With 200,000 iterations the rotation number $\Omega$ is determined with an uncertainty of $1/200,000 = 5 \times 10^{-6}$. This degree of accuracy was required to distinguish the difference in rotation number between neighbouring tori, in particular distinguishing the torus with maximal rotation number corresponding to the twistless torus.

To visualise the trajectory and transitions of the twistless torus, for each of the phase portraits in Fig. 6.12 the rotation number $\Omega$ is determined as a function of the radial distance of tori from the elliptic fixed point along the symmetry line $y = -x$ in the negative $x$ direction, denoted as $r$. This parameter $r$ uniquely determines the set
of tori and can be thought of as the action coordinate in the 1-action system eq. (2.6).
Therefore, Ω can be expressed as a function of $r$ and $k$, the contours of which are shown in Fig. 6.13. The position of the twistless torus corresponds to locations where $\partial \Omega / \partial r = 0$, i.e. the contours are horizontal, and are shown as black points. For $k > 1$ ($\omega > \omega_5$) the rotation number $\Omega$ diverges logarithmically [DMS00] approaching the manifold connections associated with the period-3 hyperbolic points, hence there is no maximum value of $\Omega$, but in the finite set of equally spaced tori there is still a maximum, shown as the blue connected squares. For each value of $k$ these indicate the torus closest to the manifold connections amongst the finite set. As expected from the bifurcation diagram, the twistless torus only appears for $k > 9/16$ and at $k = 1$ the twistless torus becomes the manifold connection. Additionally, from this plot the range of rotation number taken by the twistless torus can be determined, and hence the rational resonances $m/n$ and corresponding values $k$ for which reconnection bifurcations are expected to occur can also be determined.

![Figure 6.13](image)

Figure 6.13: Contours of the rotation number $\Omega$ as a function of the system parameter $k$ and the radial distance of the torus from the elliptic fixed point along the line $y = -x$ in the negative $x$ direction ($r$). The twist is zero where the contours become horizontal, shown by the connected black points, and the connected blue points show the tori that are closest to the manifold connection.
6.2.2 Twistless tori in the 3DRPM flow

One concern when translating the idea of twist and twistless tori to 3D is that twist is fundamentally a 2D concept. In 2D systems twist is defined as the derivative of the rotation number $\Omega$ with respect to the action coordinate $J$, and this has been extended to 1-action 3D systems by Dullin and Meiss [DM12] (see §2.6.1), however in a 2-action 3D system there are two action coordinates $J_1, J_2$ in addition to the angle coordinate $\theta$, so there are infinitely many directions in which twist can be defined. If there is a natural global invariant of the system (restricting particle motion to a set of 2D nested surfaces) the twist for each of the nested 2D systems can be defined as

$$\tau(J_1; J_2) = \frac{\partial \Omega}{\partial J_1} (J_1, J_2)$$ (6.12)

where $J_2$ is the global invariant. Here the 3D system is viewed as a set of 2D systems, each with a different value of the parameter $J_2$. However, many systems do not admit a global invariant, including the 3DRPM flow, making a meaningful definition of twist more difficult, if not impossible. However, in the 3DRPM it has been shown in §3.2.5 that transport is loosely confined to 2D surfaces of revolution (about the $y$-axis). Therefore, the adiabatic invariant $G_R$ defined in eq. (3.28) is a natural choice of the coordinate $J_2$ in the definition of twist, with $G_R = 0$ corresponding to the $xz$-plane and $G_R = 1$ corresponding to the outer sphere.

As an example, the 3DRPM with $\tau = 0.29637 = 1.01\tau_0$ is considered, for which it is known there exists a period-tripling bifurcation at the point where the period-1 line meets the $y$-axis (Fig. 6.8(b1–b4)). Poincaré sections are used to perform similar analysis as for the Hénon map in the previous section. The initial points for each Poincaré section are chosen on an iso-surface of the adiabatic invariant $G_R$, equally spaced ($\Delta r = 0.005$) along the curve given by the intersection of the level surface $G_R = c$ and the symmetry plane $z = \tan(-\Theta/2)x$, starting from the elliptic periodic line. Each particle is advected for 20,000 iterations, yielding either a closed curve (torus) around the elliptic period-1 line or a chaotic orbit. For each torus the rotation number is computed using the same method as for the Hénon map: finding the peak in the Fourier spectrum of the $x$-coordinate time series. Projecting the Poincaré sections onto the $xz$-plane (Fig. 6.14) similar phenomena are seen as in the phase portraits of the Hénon map (Fig. 6.12), except here the system parameters are fixed and it is the adiabatic invariant $G_R$ that acts as the bifurcation parameter for approximately 2D transport. With the tori coloured according to their rotation number, and the torus with maximum rotation number coloured black, it is seen that a twistless torus appears between a $G_R$ value of 0.28634 and 0.28186 (Fig. 6.14(a,b)). It then moves radially outward as $G_R$ decreases (moving towards the $xz$-plane) until
Figure 6.14: Poincaré sections for the 3DRPM flow with $\tau = 0.29637 = 1.01\tau_0$ and $\Theta = 2\pi/3$ around the elliptic period-1 line. Each plot is a projection onto the $xz$-plane. As in Fig. 6.12 the tori are coloured according to their rotation number $\Omega$ (red: maximum, purple: minimum), and the torus with the maximum rotation number is shown in black, representing either the twistless torus (a-e) or the torus closest to the manifold connection (f-h).
it becomes the manifold connections associated with the period-3 lines.

Combining the Poincaré section plots in Fig. 6.14 across a larger set of $G_R$ values, a contour plot of the rotation number $\Omega$ is created as a function of torus intersection location in the symmetry plane $z = \tan(-\Theta/2)x$. As for the Hénon map (Fig. 6.13) the twistless torus connects with the manifold connections associated with the period-3 hyperbolic lines. However, this structure exists in 3D, so there is a ‘twistless tube’ that is formed by connecting all the twistless tori, shown in green in Fig. 6.15. This is the first time that a twistless tube has been reported in a 2-action system, and similarly interesting transport organisations is expected to occur in the vicinity of the twistless tube as for the twistless tori in 2D systems. For example, reconnection bifurcations are expected to occur near any point where the rotation number becomes rational. Unlike the Hénon map, the value $3/10$ does not fall in the range of values taken by the rotation number of the twistless tube (approximately 0.324174 to 0.330379), and the lowest order rational number in this range is $12/37 \approx 0.324324$. The associated reconnection bifurcation is expected to occur in a very small region of the flow domain due to the high order of this resonance, making it difficult to detect.

As discussed in §2.6, in 2D systems a twistless torus can create a leaky barrier to transport, even when the system is perturbed to the point that the twistless torus is destroyed. Similar behaviour is expected to occur in the 3DRPM flow under perturbation, with regions of low transmissivity (transverse transport) along the twistless tube. This could have a significant impact in 3D systems that possess twistless tubes, creating loosely trapped regions and impeding the transport of fluid.

Figure 6.15: The twistless tube (green) that exists in the 3DRPM flow with $(\Theta, \tau) = (2\pi/3, 1.01\tau_0)$. The period-1 (P1) and period-3 (P3) lines are also shown, with elliptic and hyperbolic segments coloured blue and red respectively.
6.3 Tangent bifurcations

Turning attention to other types of bifurcation that occur in the 3DRPM flow, saddle–centre and period-doubling, these can be classified as ‘tangent bifurcations’.

Tangent bifurcations occur in 3D systems when the null direction ($v_3$) of the Jacobian becomes tangent to the plane spanned by the other two eigenvectors ($v_{1,2}$). Formally a point $x_0$ is a tangent bifurcation point if the vectors $w_{1,2,3}$ are linearly dependent, where

$$w_i = \lim_{x \to x_0, x \in P_1 \text{ line}} v_i(x).$$  \hspace{1cm} (6.13)

There are infinitely many possibilities for the different types of tangent bifurcations, based on the periodicity of the periodic line that becomes tangent, for instance saddle–centre bifurcations occur when a period-1 line becomes tangent and period-
doubling bifurcations occur when a period-2 line becomes tangent*. By plotting the eigenvectors with the periodic line, tangent bifurcations can be identified as points where the span of the non-null eigenvectors becomes tangent to the periodic line, as demonstrated in Fig. 6.17. Alternatively, in systems which admit a global invariant, tangent bifurcations occur at points where periodic lines become tangent to an invariant surface. When the null direction becomes tangent to an invariant surface the three eigenvectors are linearly dependent, and hence no longer distinct. For incompressible flows the product of the eigenvalues is always equal to 1, so there are only two possibilities for the eigenvalues: \( \lambda_{1,2} = \pm 1 \) and \( \lambda_3 = 1 \). This means that these tangent points are necessarily degenerate, resulting in bifurcations of local stability. This provides a simple diagnostic to determine the locations of some degenerate points in systems with an invariant. In systems that do not admit a global invariant, such as the 3DRPM flow, the flow becomes essentially 2D near the periodic line, according to eq. (4.30), and so the variable \( \xi_3 \) is a local invariant. Like global invariants, tangent bifurcations occur where a periodic line becomes tangent to isosurfaces of the local invariant.

Conservation of the Poincaré index constrains the possible types of bifurcation that can occur via tangent bifurcations. Two of the possibilities are illustrated in Fig. 6.18: a saddle–centre bifurcation (left) and a period doubling bifurcation.

*Note that for each periodicity, there may be multiple types of tangent bifurcations, e.g. there may exist bifurcations other than saddle–centre bifurcations when a period-1 line becomes tangent.
(right), both of which occur in the 3DRPM flow (Fig. 4.10). Note that saddle–centre bifurcations are sometimes also referred to as tangent bifurcations in the context of 2D systems, but here the term is used to refer to the broader class of bifurcations for 3D systems that includes saddle–centre bifurcations. In each case the bifurcation point must occur where the periodic lines become tangent to the invariant surfaces $\xi_3 = c$, otherwise the Poincaré index $\Sigma$ would not be conserved. These constraints allow us to make a priori deductions with limited information, for example:

- If there is a point on a periodic line that lies tangent to an invariant surface, and no other periodic lines intersect at the same point, then the tangent point must be a saddle–centre bifurcation point separating elliptic and hyperbolic segments, as demonstrated in Fig. 6.18(a).

- Additionally, if there exists a saddle–centre bifurcation point on a periodic line, then the tangent to the periodic line at that point forms one of the tangent vectors of the local/global invariant.

- If there is a point on a periodic line that is tangent to invariant surfaces, and the periodic line has the same stability on each side of the tangent point e.g. both elliptic, then there must exist another periodic line (possibly of different periodicity) that also intersects at the tangent point. This is the case for the period-2 line in the period-doubling bifurcation, as in Fig. 6.18(b).

Considering the impact that tangent bifurcations have on transport, here the primary focus is on saddle–centre bifurcations as they provide a complete picture for the bifurcation sequence that occurs near period-tripling bifurcations in the 3DRPM flow. At a critical value $y > y_0$, the period-3 lines associated with the period-tripling bifurcation undergo saddle–centre bifurcations, dividing them into elliptic and hyperbolic segments, as seen in Figs. 6.2(b), 6.9. While not the focus of this study, period-doubling bifurcations are equally important for transport. Cascades of period-doubling bifurcations are a common route to chaos in 2D systems [Fei79] and similar behaviour is expected for 3D systems, though the chaos may be restricted to approximately 2D structures.

Saddle–centre bifurcations are commonly found in 2D conservative systems, resulting in the creation of a pair of periodic points, one elliptic and one hyperbolic. For 3D conservative systems the third dimension can act as the control parameter for essentially 2D transport. Thus saddle–centre bifurcations in 3D conservative systems create elliptic and hyperbolic segments of periodic lines. Enclosing the elliptic segment is an invariant tube, yielding an isolated non-mixing region. At the
6.3. TANGENT BIFURCATIONS

saddle–centre bifurcation point the elliptic segment and hence the invariant tube converges to a point, creating a ‘cap’ for the tube. For the 3DRPM flow the cap is formed by the tangent connections of the 2D stable and unstable manifolds $W_{2D}^{s,u}$, as seen in Fig. 6.9. However at a critical distance away from the bifurcation point the 2D manifolds intersect transversally, indicated by the ‘wavy’ pattern that appears at smaller $y$ values (closer to red) in Fig. 6.9(d). This transverse intersection means the 2D manifolds no longer form the outer boundary of the invariant tube, but rather there is a bounding ergodic region. This phenomenon is expected to be generic, as the distance from the bifurcation point in the transverse direction $\xi_3$ to the essentially 2D transport can act as a perturbation parameter.

Therefore the framework of tangent bifurcations, in particular the restrictions imposed by conservation of the Poincaré index, provide a simple diagnostic tool for the analysis of periodic lines. For each periodicity there exists at least one distinct type of tangent bifurcation, e.g. saddle–centre bifurcations occur when a period-1 line becomes tangent, and period-doubling bifurcations occur when a period-2 line becomes tangent. These different types of tangent bifurcations can have vastly different impacts on transport. For instance, saddle–centre bifurcations yield both isolated non-mixing regions and the possibility of locally chaotic regions, whereas period-doubling bifurcations can create regions of chaos via period-doubling cascades, though possibly only two-dimensional chaos.
6.4 Conclusions

In Chapter 5 it was demonstrated that discontinuous deformations play a significant role in the organisation of transport in systems with extraction and reinjection of fluid. In this chapter it has been shown that the transport structures created by smooth deformations play an equally important role. Studying these structures via the methods of classical periodic point analysis reveals a kinematic template governing the transport of particles in their vicinity.

In many systems, including the 3DRPM flow, it is found that periodic points generically occur as periodic lines, with segments of elliptic and hyperbolic periodic points that connect at degenerate periodic points. These elliptic and hyperbolic segments indicate regions of stability and chaos respectively, and here it is shown the degenerate points that connect them are particularly important, representing bifurcations in local transport stability. In the 3DRPM flow with reorientation angle \( \Theta = \frac{2\pi}{3} \) these commonly occur as period-tripling bifurcations due to the degeneracy that occurs when a point on the \( y \)-axis (the axis of reorientation) is periodic. For rotation angles of the form \( \frac{2\pi m}{n} \) with \( n \) odd these bifurcations become \( n \)-tupling bifurcations. While these bifurcations occur as a single unstable point along an otherwise stable elliptic segment of the periodic line, they control vast transport structures that create stable regions, chaotic regions, and 'sticky' regions, resulting in a large influence on global transport behaviour. Also generically associated with period-tripling bifurcations in 2D systems are twistless tori that produce reconnection bifurcations not predicted by KAM theory. By extending the notion of twist to 3D 2-action systems, it has been shown that twistless tubes are created in 3D systems associated with period-tripling bifurcations.

It is also shown that period-doubling and saddle–centre bifurcations occur in the 3DRPM flow, and these can be grouped into the broader class of 'tangent bifurcations', i.e. those for which the eigenvectors become linearly dependent. These tangent bifurcations are easily found in systems that admit a global invariant, occurring at points where periodic lines become tangent to iso-surfaces of the invariant. There are infinitely many types of these tangent bifurcations, based on the periodicity of the periodic line that becomes tangent, however they are topologically constrained by conservation of the Poincaré index.

Enclosing elliptic segments of the periodic line are invariant tori that create topological barriers to particle transport. These tori also do not (and cannot) interact with the Lagrangian discontinuity, otherwise they would be destroyed. On the other hand, hyperbolic segments of the periodic lines drive chaos through the transverse intersections of their associated stable and unstable manifolds, and these structures
do interact with the Lagrangian discontinuity, resulting in the same intermittent convergence of the Lyapunov exponent demonstrated in the previous chapter for the 2DRPM flow.

### 6.4.1 Future work

Future work in this area should focus on:

- **Finding reconnection bifurcations near the twistless torus.** Finding these bifurcations would confirm that the definition of twist is appropriate to 3D systems.

- **Perturbations of the 3DRPM flow,** to see whether the twistless tube forms a region of low transmissivity once destroyed, as occurs in the Standard Non-twist Map [SJCL+09]. This is important for any experimental implementation of the RPM flows since the presence of additional physics such as inertia or heterogeneity in the porous medium can be thought of as a perturbation of the purely advective model, and could provide an explanation for any regions of low transmissivity encountered.

- **Generalisation to arbitrary reorientation angles** $\Theta$, in particular when $\Theta = 2\pi m/n$ with $n$ even, and when $\Theta/\pi$ is irrational. Fundamentally different behaviour is expected in these cases due to the difference in the degenerate fixed point at the origin in the asymptotic limit $\tau \to 0$ of the 2D and 3D RPM flows. The nature of the degenerate points that occur as the intersection of period-1 lines and the $y$-axis share are of the same type as the one at the origin in the asymptotic limit $\tau \to 0$, and these are fundamentally different for the odd and the even or irrational cases since in the odd case the dipole positions do not ‘cancel’ each other out.

- **Introduce more complex reorientation protocols.** Along with changing the reorientation angle $\Theta$, there are many other ways to change the reorientation protocols, for instance by rotating the dipole about two different axes rather than just the $y$-axis. A natural extension of the 3DRPM flow with dipole rotation about the $y$-axis studied here is to consider a rotation axis slightly perturbed from the $y$-axis. This would break many of the symmetries of the flow, including the reflection symmetry that makes the $xz$-plane invariant. Therefore a small perturbation would result in a small degree of particle transport through the $xz$-plane.
Chapter 7

Transition to Fully 3D Transport

In 3D fluid flows that admit an invariant, particles are confined to 1D or 2D structures, and the theory of Hamiltonian systems applies. Therefore, 3D fluid flows are most interesting when particles are able to travel fully three-dimensionally, described as 3D transport. As discussed in §2.3, most studies on 3D transport consider perturbations away from systems with 1D or 2D transport, and this study follows a similar approach. In the limit as $\tau \to 0$ the 3DRPM flow becomes steady (§3.2.4), and particles are trapped to 1D streamlines. Therefore, $\tau$ acts as a perturbation parameter away from this limiting case, and in this chapter it is shown that increasing $\tau$ leads to a transition from 1D to 3D transport.

Here it is shown that the Lagrangian discontinuity created by dipole reorientation in the 2DRPM flow (Chapter 5) extends to the 3DRPM flow, and creates a new mechanism for 3D transport, albeit a mechanism that is similar in effect to RID. Particles follow approximately 1D trajectories, and when they approach the Lagrangian discontinuity surface they are kicked off their current streamline to a new one. Unlike past studies on RID, this streamline jumping is not created by the ‘slowing down of angle variables’, but rather sensitivity of particle trajectories caused by discontinuous deformation.

7.1 Transition from 1D to 3D transport

For a fixed reorientation angle $\Theta$ (here $2\pi/3$), the Poincaré sections reveal a transition from 1D transport at low $\tau$ to fully 3D transport at high $\tau$, as seen in Fig. 7.1. At very small values of $\tau$, particle trajectories shadow the streamlines of the steady flow corresponding to the limit as $\tau \to 0$ (see §3.2.4). These particles experience small perturbations away from the streamlines in a manner similar to that of the 2DRPM flow in Chapter 5 (Fig. 7.1(a-d)). Hence, particle transport is approx-
imimately 1D at these low values of $\tau$, though there is a fractal structure at very small length scales. Conversely, at large values of $\tau$ particles can undertake fully 3D transport throughout a volume, as shown in Fig. 7.1(f). This transition from 1D to 3D transport can be quantified by computing the fractal dimensions $D_f$ of Poincaré sections for various values of $\tau$ across this transition. This has been carried out for $\tau = 2^{n/2} \times 10^{-5}$, with $n = 0,1,\ldots,37$, i.e. $\tau \in [10^{-5}, 3.707]$, each using the Poincaré sections for 514 equally spaced initial particle locations to give a representative measure of the entire domain. For each initial location, a particle is advected for 200,000 iterations, producing a Poincaré section (such as those shown in Fig. 7.1), and the fractal dimension of the Poincaré section is computed numerically via the algorithm described in §4.2.1. The results of this computation are shown as a density histogram in Fig. 7.2, where a darker shading means more points have that fractal dimension. It is clear that at very small values of $\tau$ all the Poincaré sections have a fractal dimension close to 1. At large values of $\tau$ particles either have a fractal dimension close to 3, signifying fully 3D transport, or fractal dimension close to 1, which occurs when a particle is trapped inside an invariant tube. This transition from 1D to 3D transport is fairly smooth, with 2D transport observed at intermediate values of $\tau$, corresponding to Poincaré sections similar to Fig. 7.1(e).

The transition from 1D to 2D transport occurs via a similar mechanism that of the 2DRPM flow, being played out on each iso-surface of the adiabatic invariant $G_R$, and therefore it is not discussed here any further. The remainder of this chapter focuses on the mechanisms that drive the transition from 2D to 3D transport. This latter transition occurs for $\tau$ values in the order $10^{-2} - 10^{-1}$, and a key tool in studying the transition is the adiabatic invariant $G_R$, which can be used to detect significant 3D transport transverse.

7.2 Transverse jumps created by the Lagrangian discontinuity

In this section it is demonstrated that the same Lagrangian discontinuity discussed in §5 for the 2DRPM creates a mechanism that is responsible for a large portion of the transverse transport in the 3DRPM flow, especially in the range of $\tau$ values where the transition from 2D to 3D transport occurs. While in 2D the Lagrangian discontinuity occurs along the curve $t_{\text{sink}}(x) = \tau$, in 3D this equation describes a surface (shown as orange in Fig. 7.3), separating points that are advected through the sink in the next advection step from those that are not. Due to axisymmetry of
Figure 7.1: Typical Poincaré sections in the 3DRPM flow with $\Theta = 2\pi/3$. (a-d) $\tau = 5 \times 10^{-4}$. (e) $\tau = 0.02$. (f) $\tau = 5$. (a,b) The particle is trapped in an invariant tube and its orbit is a 1D closed curve. (c,d) The particle is in the chaotic region.
7.2. 3D JUMPS CREATED BY THE LAGRANGIAN DISCONTINUITY

Figure 7.2: Evolution of the fractal dimension $D_f$ of Poincaré sections in the 3DRPM flow with $\Theta = 2\pi/3$ and varying $\tau$. For each value of $\tau$, 514 Poincaré sections are generated using equally spaced initial particle locations and 200,000 flow periods each. The distribution of the fractal dimensions of these Poincaré sections is represented as a density histogram, darker meaning more particles produced a Poincaré section with fractal dimension in that range.

the steady dipole flow about the $z$-axis, this surface of Lagrangian discontinuity is also axisymmetric. While the gross nature of the cutting mechanism is the same for 2D and 3D, as seen by the similarity between Fig. 7.3 and Fig. 5 from [SRLM16] (§5.1 here), it will be shown that this Lagrangian discontinuity also creates a mechanism for 3D transport.

### 7.2.1 Correlation between transverse jumps and proximity to the Lagrangian discontinuity

Applying the time series zoning method described in §4.6 to several of the particle trajectories used to create Fig. 7.2, the times, locations and magnitudes of jumps transverse to the adiabatic invariant $G_R$ can be detected, as shown in Figs. 4.20–4.22. Note that the magnitude $|\Delta G_R|$ of each jump is calculated as the change in the piecewise constant approximation given by the median of each zone, shown as the orange curves in Figs. 4.20–4.22. Combining the locations of these jumps for several particles over 200,000 iterations (see Table 7.1 for the number of particles used for each value of $\tau$), Fig. 7.4 shows that these jumps occur when particles are close to
Figure 7.3: The Lagrangian discontinuity illustrated in the 3DRPM flow for \((\Theta, \tau) = (2\pi/3, 4.096 \times 10^{-2})\). The black set of particles initially straddles the surface of Lagrangian discontinuity (orange), given by \(t_{\text{sink}} = \tau\), and lies on the surface \(G_R = 0.5\) (the mesh lines on the surface are intersections of the Lagrangian discontinuity and the \(G_R\) iso-surfaces). This set of particles experiences a Lagrangian discontinuity that is evident at \(t = 4\tau\). This is the 3D analogue of Fig. 5 in [SRLM16] (§5.1).

Furthermore, the jumps illustrated in Fig. 7.4 are mostly positive (red, moving toward the spherical boundary) on the side of the surface where \(t_{\text{LD}} > 0\), i.e. those points not advected through the sink, and the jumps are mostly negative (blue, moving toward the \(xz\)-plane) on the side of the Lagrangian discontinuity where
Figure 7.4: Locations of the transverse jumps, $\Delta G_R$, projected onto the cylindrical coordinate $\rho z$-plane for the $\tau$ values in Table 7.1. (a) $\tau = 1.024 \times 10^{-2}$. (b) $\tau = 4.096 \times 10^{-2}$ (c) $\tau = 0.1159$. (d) $\tau = 0.3277$. In each plot the jump locations are coloured according to the value of $\Delta G_R$. Note the different scales on each legend, with smaller jumps at lower $\tau$. Also shown is the projected iso-surface $t_{\text{sink}} = \tau$ (solid black), representing the Lagrangian discontinuity, and the projected iso-surfaces $t_{\text{sink}} = \tau \pm \delta^\pm$ (dashed black), indicating the approximate region in which the jump locations are contained.
<table>
<thead>
<tr>
<th>$\tau$</th>
<th>No. initial particles (200,000 iterations each)</th>
<th>No. jumps</th>
<th>Jump frequency (jumps/iteration)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1.024 \times 10^{-2}$</td>
<td>190</td>
<td>40,757</td>
<td>$1.073 \times 10^{-3}$</td>
</tr>
<tr>
<td>$4.096 \times 10^{-2}$</td>
<td>58</td>
<td>77,684</td>
<td>$6.697 \times 10^{-3}$</td>
</tr>
<tr>
<td>0.1159</td>
<td>12</td>
<td>64,090</td>
<td>$2.670 \times 10^{-2}$</td>
</tr>
<tr>
<td>0.3277</td>
<td>15</td>
<td>79,781</td>
<td>$2.659 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

Table 7.1: The number of particles used, the number of jumps detected, and their frequency for four $\tau$ values near the transition between 2D and 3D transport.

Figure 7.5: Density histograms (darker means more data points in that box) showing the correlation between the reciprocal of the advection time from the Lagrangian discontinuity, $t_{LD}$, and the magnitude of the time series jumps, $|\Delta G_R|$, for a range of $\tau$ values.

$t_{LD} < 0$\(^*\). This is also shown in Fig. 7.6, where only the data points with $t_{LD} > 0$ are plotted, and it is seen that the vast majority of jumps are positive. Likewise, restricting the data to points with $t_{LD} < 0$, Fig. 7.7 shows that the majority of the jumps are negative. These correlations are strongest at the lower values of $\tau$. At $\tau = 0.3277$ the jumps still occur close to the Lagrangian discontinuity, however there is a weaker correlation between the sign of the jump and the sign of $t_{LD}$. A possible cause of this is the existence of the first reinjected period-tripling bifurcation discussed in Chapter 6, and its associated structures. This bifurcation exists for $\tau > \tau_0 = 0.29344$, and creates complex transport structures that are likely to significantly affect the distribution of transverse jumps. In addition, the nature of the cutting mechanism changes at larger values of $\tau$. Referring to Fig. 7.3, at larger values of

\(^*\)There are exceptions on each side of the Lagrangian discontinuity, however these are caused by limitations of the zoning method, i.e. zones added where they should not exist, and zones not added where they should. It is difficult to determine all the ‘bad’ zones without manually checking all 260,000 zone boundaries.
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![Graphs showing 3D jumps created by the Lagrangian discontinuity](image)

Figure 7.6: Similar to Fig. 7.5, except only the data points with $t_{LD} > 0$ are used. In the first row $\Delta G_R$ is used as the vertical axis to show that predominantly positive jumps occur when $t_{LD} > 0$, and in the second row $\log_{10}|\Delta G_R|$ is used as the vertical axis to further demonstrate the correlation.

$\tau$ particles originally located near the Lagrangian discontinuity at $t = 0$ may pass through the dipoles in their reoriented positions in the time $\tau < t < 3\tau$. This means fluid may not recombine, even in an approximate sense, after $t = 4\tau$, and more complex phenomena can occur.

While Fig. 7.4 shows that the transverse jumps occur near the Lagrangian discontinuity, they are not evenly distributed over the axisymmetric surface $t_{LD} = 0$, as shown by the histograms in Fig. 7.8 of the azimuthal angle $\theta$ of the jump locations ($x = \rho \cos \theta, y = \rho \sin \theta$). At low values of $\tau$ (Fig. 7.8(a,b)), the jumps occur approximately symmetrically about $\theta = \pi/2$, corresponding to the $yz$-plane, with a peak near $\theta = \pi/2$. This peak corresponds to particles whose trajectories are similar to the streamlines in the limit as $\tau \to 0$, and come close to the period-tripling bifurcation structures near the $y$-axis. On each pass near the Lagrangian discontinuity, they are kicked off their current streamline and onto a new one, and since they come close to the period-1 point, these particles take a large number of iterations to reach the Lagrangian discontinuity again. Therefore, in this region the mechanism for 3D transport is similar to RID, as the motion of particles can be described as 2-action (eq. (2.4)), with essentially 1D trajectories, and the Lagrangian discontinuity creates streamline jumping like the resonance regions in RID.

Conversely, particles away from the $yz$-plane still experience jumps, although much less frequently. In these regions particles are loosely trapped in sticky regions.
near a dense tiling of invariant tubes, analogous to the tiling of invariant tori in the 2DRPM flow demonstrated in [SRLM16] (§5.1). Particles within these invariant tubes follow exactly 1D trajectories (closed curves), such as the orbit in Fig. 7.1(a,b), and thus experience zero net transverse transport, though they may oscillate over a small range of $G_R$ shells. Therefore particles in the sticky chaotic regions close to invariant tori - whose orbits are similar to those of their nearest invariant torus for long periods of time - experience quasi-periodic transverse transport, as demonstrated by the first 600 iterations in Fig. 4.22. In these regions particles jump much less frequently than those near the $yz$-plane. Particles are able to move between the sticky region and the more frequent jumping region, as occurs after approximately 600 iterations in Fig. 4.22. At $\tau = 0.1159$ (Fig. 7.8(c)), there is still a peak in the number of jumps near $\theta = \pi/2$, however it is more spread out, and there is less symmetry between the jump locations on each side of the Lagrangian discontinuity (red and blue). However, for $\tau = 0.3277$ (Fig. 7.8(d)), there is no single peak, and a much more complicated relationship between the jump locations and the azimuthal angle $\theta$. Again, this could be related to the period-tripling bifurcation that occurs, creating complex transport structures, as well as the difference in the cutting mechanism.

### 7.2.2 The mechanism for transverse transport

The cause of the transverse jumps can be directly attributed to the discontinuous deformations produced by the dipoles and slip boundaries. Considering fluid that initially straddles the Lagrangian discontinuity (Fig. 7.3 and Fig. 7.9), after the

![Figure 7.7: The same as Fig. 7.6, except only the data points with $t_{LD} < 0$ are used.](image)
first flow period, at $t = \tau$, the fluid becomes disconnected by the dipole, and the two disconnected pieces move independently. In the following two flow periods ($\tau < t < 3\tau$) the dipoles are in their reoriented positions, and each disconnected piece of fluid experiences transverse transport in opposite directions. Therefore, when the dipole returns to its initial position ($3\tau < t < 4\tau$), the fluid is advected through the dipole, and there is a discontinuous difference in shell number $G_R$ as well as the slip deformation observed in the 2D flow.

Furthermore, tracking a set of particles that evenly cover an adiabatic shell ($G_R = 0.2, 0.5, 0.8$), and measuring the transverse displacement $\Delta G_R$ of each particle from their initial value, Fig. 7.10 shows that the transverse displacement has a discontinuous distribution, with sharp interfaces between positive (red) and negative (blue) displacement. These discontinuous interfaces correspond to the preimages of the curve given by the intersection of the surface of Lagrangian discontinuity with the corresponding adiabatic shell ($G_R = 0.2, 0.5, 0.8$). These are cross-sections of the 3D ‘web of preimages’ ([SRLM16], §5.1 here), shown as black in Fig. 7.10(c,f,i), which
further demonstrate the role of the Lagrangian discontinuity in creating transverse transport. Likewise, the ‘web of images’ would be revealed by tracking the particles backwards in time, and is given by the reflection of the web of preimages through the symmetry plane $z = \tan(-\Theta/2)x$ due to the reflection reversal symmetry eq. (3.27).

Note also that while the regions near the outer circle in Fig. 7.10 exhibit high $|\Delta G_R|$, this transverse displacement does not persist, as particles experience quasi-periodic orbits, and these regions oscillate between large positive and negative $\Delta G_R$ values. These quasi-periodic oscillations are created by nearby elliptic orbits, and their large amplitude stems from the regions near the circle $x^2 + z^2 = 1$ with a large difference in $G_R$ after one advection step (Fig. 3.10). On the other hand, jumps that occur as a result of the Lagrangian discontinuity near the line $x = 0$ are less affected by the elliptic orbits, and so these transverse jumps persist as indicated by the peak near $\theta = \pi/2$ in Fig. 7.8(b).
Figure 7.10: Transverse displacement of particles evenly distributed on adiabatic shells \((G_R = 0.2, 0.5, 0.8)\) in the 3DRPM flow with \((\Theta, \tau) = (2\pi/3, 4.096 \times 10^{-2})\), after (a,d,g) \(N = 4\), and (b,e,h) \(N = 20\) iterations. In each figure the particles are projected onto the \(xz\)-plane and the initial particle location is coloured according to the transverse displacement \(\Delta G_R\). (c,f,i) The transverse displacement after \(N = 20\) iterations combined with 20 preimages of the curve given by the intersection of the surface of Lagrangian discontinuity with the corresponding adiabatic shell \(G_R = 0.2, 0.5, 0.8\).
7.2.3 Rates of transverse transport produced by the Lagrangian discontinuity

While the Lagrangian discontinuity exists for all values of $\tau$, and therefore creates 3D transport at all values of $\tau$, the rate of transverse transport is controlled by $\tau$. By considering the frequency of jumps (jumps per iteration, Fig. 7.11(a)), and the average magnitude of the jumps (Fig. 7.11(b)), the rate of transverse transport can be defined as their product, and increases significantly from $\tau = 1.024 \times 10^{-2}$ to $\tau = 0.1159$, as shown in Fig. 7.11(c). This large increase is caused by increases in both the jump frequency and average jump magnitude, and explains the transition from 2D to 3D transport that occurs over this range.

In contrast, from $\tau = 0.1159$ to $\tau = 0.3277$ the average jump magnitude still increases, but the frequency slightly decreases, resulting in a relatively small increase in the rate of transverse transport. This also could be caused by the first reinjected period-tripling bifurcation (discussed in Chapter 6) and its associated structures. In particular, the bifurcation yields sticky chaotic regions near the $y$-axis, as seen in Fig. 6.8(b3). Particles in this sticky region are trapped for a long time without approaching the Lagrangian discontinuity, resulting in a reduced jump frequency. It has also been demonstrated in Fig. 7.4 and Fig. 7.8 that the distribution of the jumps at this value of $\tau$ are more complex, and it is likely that other structures not related to the discontinuous deformations also play a role in the generation of transverse transport.

![Figure 7.11](image-url)

Figure 7.11: The frequency, average magnitude, and rate of transverse transport associated with the jumps caused by the Lagrangian discontinuity calculated for the values of $\tau$ in Table 7.1.
7.3 Conclusions

In Chapter 5 it was seen that the presence of discontinuous deformations can significantly alter the arrangement of transport structures in 2D systems, and here it is shown that they can have an even greater impact in 3D systems, providing a mechanism for 3D transport. In the 3DRPM flow discontinuous deformations not only produce slip deformations parallel to the adiabatic invariant, but also produce discontinuous transverse transport. This results in a new mechanism for 3D particle transport, similar in effect to RID, where particles follow approximately 1D trajectories, but are kicked off streamlines by the Lagrangian discontinuity. In contrast to RID, there is no resonance of angle variables, and the jumps are produced by transverse discontinuous deformation.

Despite the existence of discontinuous deformations that produce 3D transport at all values of $\tau$, only 1D and 2D transport is observed at low values of $\tau$. This apparent contradiction is caused by decreases in both the frequency and the average magnitude of the transverse jumps as $\tau$ decreases, meaning 3D transport still occurs, but at a much slower rate.

On the other hand, once the transition from 2D to mostly 3D transport has concluded at $\tau \approx 0.1$, the organisation of transport becomes more complex, with a greater contribution from stretching and folding mechanisms, and the birth of reinjected period-tripling bifurcations for $\tau > 0.29344$. This results in a slight decrease in the frequency of transverse jumps from $\tau = 0.1159$ to $\tau = 0.3277$, though an increase in the average magnitude of jumps means the rate of transverse transport still increases. A likely cause of this decrease in frequency is the presence of the first reinjected period-tripling bifurcation point and its associated structures, in particular the ‘sticky’ chaotic regions near the $y$-axis that loosely trap particles near the $y$-axis, away from the Lagrangian discontinuity.

7.3.1 Future work

Future work should focus on:

- **A 3D analogue of the CSS map**: The effect of the Lagrangian discontinuity was revealed at a fundamental level by the simple CSS map. Can a similar formulation be used in 3D to gain a deeper understanding of the transverse transport mechanism? This could possibly be achieved by using three shears instead of two, with an additional shear for the direction transverse to the original two, and an additional transverse cut map may also be required.
• **Generalisation to arbitrary reorientation angles** $\Theta$, and more complex reorientation protocols: The Lagrangian discontinuity is created by the slip boundary and the dipole, so any choice of reorientation protocol will produce discontinuous deformation, and could produce new and interesting phenomena.

• **Further analysis of the complex interaction between transport structures at higher values of** $\tau$: Understanding all the mechanisms that contribute to 3D transport and how they interact.

• **Further analysis of discontinuous deformations in 3D systems**: Similar phenomena are expected in all 3D time-dependent extraction-reinjection systems, and the presence of discontinuous deformations will produce an infinite array of transport phenomena that have yet to be explored.
Chapter 8

Conclusions

While mixing and particle transport is well understood in 2D area-preserving fluid flows due to their correspondence with Hamiltonian systems, much less is known about mixing in 3D volume-preserving flows. In this study, a periodically reoriented dipole flow, the 3DRPM flow, is considered as a case study to uncover some of the general mixing and particle transport properties of 3D volume-preserving flows and potential flows. As an unexpected consequence, it is found that the periodic extraction and reinjection of fluid results in discontinuous deformation akin to cutting and shuffling. This discontinuous deformation couples with smooth stretching and folding type deformation to produce complex mixing and transport phenomena, with novel behaviour in both 2D area-preserving and 3D volume-preserving flows.

In 2D area-preserving flows, such as the 2DRPM flow, the presence of discontinuous deformation invalidates Hamiltonian theory, even when the base flow is a Hamiltonian system. This introduces many more possibilities for the behaviour of particle transport, such as the creation of ‘pseudo-periodic’ points that correspond to true periodic points that are ‘destroyed’ by the discontinuous deformation, and can either enhance or impede the rate of mixing. These phenomena are expected to occur in all systems with a combination of discontinuous and smooth deformation, including other flows with extraction and reinjection of fluid, granular flows, and deformations of shear-banding materials.

When discontinuous deformation is present in 3D volume-preserving flow, such as the 3DRPM flow, the impact is even greater. Not only does the addition of a third dimension creates more possibilities for novel transport phenomena, but also the cutting and shuffling mechanism can kick particles between streamlines, resulting in fully 3D particle transport. This provides a novel mechanism for transverse transport, though similar in effect to Resonance Induced Dispersion, that is likely to occur in other 3D extraction-reinjection flows, as well as 3D granular flows and
3D deformations of shear-banding materials.

While discontinuous deformations play a significant role in the organisation of mixing and particle transport in the 3DRPM flow, the effect of smooth deformations cannot be ignored. Periodic points and lines are generic to all volume-preserving flows, and create an organisational template for particle transport in their vicinity. The transverse intersections of manifolds associated with hyperbolic periodic points generate chaos, whereas elliptic periodic points create impenetrable barriers to transport. In some systems, including the 3DRPM flow, periodic points occur as periodic lines, with segments of hyperbolic and elliptic points separated by degenerate type periodic points. These degenerate periodic points are particularly important for the organisation of particle transport, representing bifurcations between unstable and stable regions, and it is demonstrated here that they can organise vast transport structures.

Overall, even simple flow regimes, such as a periodically reoriented dipole flow, can create a surprising degree of complexity. This is exacerbated when the flow has complex interactions between smooth and discontinuous deformations.

8.1 Future work

Along with the more specific future areas of work mentioned at the end of Chapters 5-7, further study is needed to gain a better understanding of the interaction between smooth and discontinuous deformation. These interactions will occur in a broad array of applications, and it has been demonstrated here that they have a significant impact on transport and mixing. Future directions for research include generalisations of the CSS map in both 2D and 3D, with the goal of a complete classification of the possible transport structures that can be created by combined smooth and discontinuous deformation. In addition, there is a need for more fundamental studies on systems that include both smooth and discontinuous deformations, such as granular flows and other extraction-reinjection fluid flows.

More generally, further study is required to gain a better understanding of mixing and particle transport in 3D volume-preserving flows. While this study has examined some of the possibilities, there is still a vast gap in the understanding of volume-preserving flows, in particular the possible mechanisms for fully 3D transport.
Appendices
Appendix A

Frames of Reference

A.1 Rotation of the dipole about the y-axis

Considering the simple case of rotation of the dipole about the y-axis. The initial starting position of the dipole is always with the sink at $z_- = (0, 0, -1)$ and the source at $z_+ = (0, 0, 1)$. The 3DRPM flow has two control parameters, the rotation angle $\Theta$ and the period $\tau$ for which the dipole stays at each reorientation angle. If the angle $\Theta$ is commensurate with $2\pi$, i.e. $\Theta = \frac{2\pi m}{n}$ for some integers $m, n$, then the dipole will return to its starting position after $n$ rotations, and so the flow is periodic with period $n\tau$.

For $\Theta = \frac{2\pi m}{n}$, the advection of a particle over the full flow period $n\tau$ is given by

$$Y = Y^{\tau(n-1)\Theta} \cdots Y^{2\Theta} Y^{\Theta} Y^{0}. \quad (A.1)$$

Note that we can evaluate $Y^{\alpha}(x)$ by first counter-rotating the particle back to the base frame with the dipole at $z_-, z_+$ and then integrating it in this frame, followed by rotating the particle back to the original frame. In algebraic terms

$$Y^{\alpha}_\tau = R^y_\alpha Y^{0}_\tau R^{-y}_\alpha \quad (A.2)$$

where $R^y_\alpha$ denotes rotation by angle $\alpha$ about the y-axis. Therefore the periodic map $Y$ can be computed as

$$Y = (R^y_\Theta Y^{0}_\tau R^{-y}_\Theta)(R^y_\Theta Y^{0}_\tau R^{-y}_\Theta)(R^y_\Theta Y^{0}_\tau R^{-y}_\Theta) \cdots \left( R^y_\Theta Y^{0}_\tau R^{-y}_\Theta \right)(R^y_\Theta Y^{0}_\tau R^{-y}_\Theta) (Y^{0}_\tau)
= (R^y_\Theta Y^{0}_\tau)^n \quad (A.3)$$

which shows that it is equivalent to counter-rotate the particle by $\Theta$ after each integration in the base frame. Each iteration of the map $Z = R^y_{-\Theta} Y^\tau_0$ tracks the
particle in the dipole frame, i.e. the frame in which the dipole is fixed and the
particles counter-rotate around it. After \( n \) iterations the dipole frame and laboratory frame coincide and so every \( n \) iterations of \( Z \) gives the real location of the particle. Therefore, the successive iterations of the map \( Z \) can be thought of as tracking \( n \) different particles in the laboratory frame, with starting locations \( x, Z(x), Z^2(x), \ldots, Z^{n-1}(x) \) respectively.

In order to convert the position of a particle from the dipole frame to the laboratory frame after \( k \) iterations of \( Z \), it is necessary to rotate the particle by \( k\Theta \), i.e. \( R_{x\Theta}^k Z^k \) will track the particle in the laboratory frame.

### A.1.1 Poincaré sections

There are two natural Poincaré sections that could be considered based on the two periodic maps \( Y \) and \( Z \). The stroboscopic maps of \( Y \) and \( Z \) perform sections in the time domain in the laboratory frame and dipole frame respectively. A key difference is that \( Y \) has period \( n\tau \) whereas \( Z \) has period \( \tau \). The overall structures of each Poincaré section are identical, but using the map \( Z \), i.e. tracking in the dipole frame has two advantages. First, any reorientation angle \( \Theta \) can be considered, whether rational or incommensurate with \( \pi \), whereas for the map \( Y \) only rational reorientation angle can be used. Also, since the iterates of \( Z \) are equivalent to tracking \( n \) particles in the laboratory frame, it takes \( n \)-times less computational time to develop Poincaré sections with the same number of data points.
Appendix B

Quintic equations describing the
3DRPM flow

A pseudo-analytic solution to the advection equation was able to be found for the
2DRPM flow using a coordinate transformation \((x, y) \leftrightarrow (\phi, \psi)\) from cartesian co-
ordinates to potential and streamfunction coordinates. This reduced the system to
one-dimension as \(\psi'(t) = 0\). When attempting a similar approach for the 3DRPM
flow, it is necessary to solve

\[
\Psi(\rho, z) = \psi \tag{B.1}
\]

for \(\rho\) in terms of \(\psi, z\), and \(z\) in terms of \(\rho, \psi\). However, when expanding eq. (B.1)
into the form of a polynomial, the solutions for \(\rho\) and \(z\) satisfy the quintic equations

\[
\sum_{i=0}^{5} a_i(\psi, z)\rho^{2i} = 0, \tag{B.2}
\]

\[
\sum_{i=0}^{5} b_i(\psi, \rho)z^{2i} = 0, \tag{B.3}
\]

where the functions \(a_i(\psi, z)\) and \(b_i(\psi, \rho)\) are the polynomials

\[
a_0 = (4\pi^2\psi^2 - 1) (z^2 - 1)^4 (z^2 - 4\pi^2\psi^2)
\]

\[
a_1 = 4 (z^2 - 1)^2 (-z^4 - 16\pi^4\psi^4 (z^2 + 1) + z^2 + \pi^2\psi^2 (5z^4 + 2z^2 + 1))
\]

\[
a_2 = 8\pi^2\psi^2(z - 1)(z + 1) (5z^4 + 2z^2 + 1) - 6z^2 (z^2 - 1)^2 - 32\pi^4\psi^4 (3z^4 + 2z^2 + 3)
\]

\[
a_3 = 8\pi^2\psi^2 (5z^4 - 1) - 64\pi^4\psi^4 (z^2 + 1) - 4z^2 (z^2 - 1)
\]

\[
a_4 = -16\pi^4\psi^4 + 4\pi^2\psi^2 (5z^2 + 1) - z^2
\]

\[
a_5 = 4\pi^2\psi^2,
\]
and

\begin{align*}
b_0 &= 4\pi^2 (\rho^2 + 1)^3 \psi^2 \left( (\rho^2 - 1)^2 - 4\pi^2 (\rho^2 + 1) \psi^2 \right) \\
b_1 &= -64\pi^4 (\rho^2 + 1)^2 (\rho^2 - 1) \psi^4 - (\rho^2 - 1)^4 + 4\pi^2 (5\rho^8 - 2\rho^4 - 3) \psi^2 \\
b_2 &= -4 (\rho^2 - 1)^3 - 32\pi^4 (3\rho^4 - 2\rho^2 + 3) \psi^4 + 8\pi^2 (5\rho^6 - 3\rho^4 + \rho^2 + 1) \psi^2 \\
b_3 &= -64\pi^4 (\rho^2 - 1) \psi^4 - 6 (\rho^2 - 1)^2 + 8\pi^2 (5\rho^4 - 4\rho^2 + 1) \psi^2 \\
b_4 &= 4 \left( \pi^2 (5\rho^2 - 3) \psi^2 - \rho^2 - 4\pi^4 \psi^4 + 1 \right) \\
b_5 &= 4\pi^2 \psi^2 - 1.
\end{align*}

By the Abel–Ruffini Theorem, there cannot exist a general solution for quintic equations in terms of radicals. Hermite and Klein have since found solutions using elliptic modular functions and hypergeometric functions respectively, however these are untenable in the context of this problem. Even if the functions \( \rho(\psi, z) \) and \( z(\psi, \rho) \) are found in terms of inverse elliptic functions, it is still necessary to solve the advection equation in these coordinates.
Bibliography


