Chapter 1

Introduction

This thesis investigates flows defined by the system of ordinary differential equations,

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t), t)\,. \tag{1.1}$$

The flows to be studied arise in a wide array of applications. Of particular interest in this work are geophysical fluid flows including global oceanic circulation, and the intense atmospheric flows of hurricanes. We shall also study flow generated in the phase space of a second order dynamical system, such as three bodies under mutual gravitational attraction, or a chain of coupled oscillators.

The approach will be geometric and qualitative. We are not so concerned about the motion or accurate description of an individual trajectory, as we are about uncovering global structures that govern the motion of entire regions in the flow.

In satelite imagery of geophysical fluid flows, it is plain to see that, despite the manifestly turbulent flow of the ocean and atmosphere, large-scale coherent structures are present – the imagery of hurricanes in the Atlantic being a declarative case in point. The visual evidence for coherent structures begs for a deeper understanding of their dynamical properties. How should these coherent structures be described from a dynamical systems perspective? Given that the imagery of intense cloud bands indicates the presence of a hurricane, what are the corresponding structures in the underlying velocity field that delineate the hurricane's dynamical structure? Can we uncover structures in the flow that define the mechanisms by which fluid is transported in and around the hurricane? For aperiodic flows, even the simplest of questions can have ill-defined answers. For example, "How do we define the dynamically relevant boundary of a hurricane?".

These questions can be applied equally well to eddies in the global ocean. Important questions that are not yet well-understood by the oceanography community include: "What process controls the rate of mixing at the ocean surface?", and "Why are eddies leaky?" Nascent Lagrangian analysis of ocean flows is starting to yield answers; however, the studies most commonly involve direct visualization of tracer trajectories. Nevertheless, the insight that Lagrangian descriptions provide is now more widely recognized, and experiments are underway to directly observe Lagrangian evolution of dye patches and regularly spaced grids of drifters in the ocean in order to uncover the important dynamic transport structures.

Over the last several years, varied techniques have been developed within the dynamical systems community to study coherent structures in aperiodic flows. The underlying goal of these methods is to identify key structures within the flow that govern transport and mixing. For the purposes of the present study, we will adopt the FTLE-LCS method first proposed by [Haller 2000, Haller 2001], which uses Finite Time Liapunov Exponents (FTLE) to identify Lagrangian Coherent Structures (LCS). A precise definition of the method and an initial discussion of the properties of the LCS is provided by [Shadden 2005] and [Lekien 2007].

The underlying premise of the FTLE-LCS approach is that coherent structures in a flow are best represented by visualizing the surfaces of greatest separation. Defined in this way, the LCS act as barriers to transport, and parse the flow into regions with different dynamical behavior and outcomes. Most important for our purposes, the motion of the time-dependent LCS reveals the mechanisms that mediate transport from one region of the flow to another. The method has several variants, including the Finite Size Liapunov Exponent (FSLE) approach [Aurell 1997, d'Ovidio 2004], but all are in the same spirit. A different method, that is not used in this thesis, is the Distinguished Hyperbolic Trajectory approach, which identifies coherent structures as the most hyperbolic trajectories emanating from "instantaneous stagnation points"

[Ide 2002].

The utility of the FTLE-LCS method lies in the fact that it can be applied without impediment to flows with arbitrary time-dependence. The flows in question may arise from an analytical model, or a finite data set of discrete flow data originating from a numerical simulation (a direct simulation of Navier-Stokes equation, for example), or from observations of the flow (such as radar measurements of ocean surface currents) that may be interpolated to determine the velocity field during the period of interest.

The number of applications to which the FTLE-LCS method is now being applied is steadily increasing. Recent studies include bio-mechanics [Shadden 2008, Tanaka 2008], bio-locomotion[Shadden 2007, Peng 2009], laboratory flows, naval search and rescue, and oil spill mitigation.

The overarching advantage of the FTLE-LCS method is that it systematically and succinctly encodes Lagrangian data into a single visualization. Whereas human temporal perception struggles with untangling chaotic trajectories in a turbulent flow, the FTLE-LCS presents the same Lagrangian information in a single intuitive image. Without access to the FTLE, researchers are often tempted to use the Eulerian velocity field, or streamlines to determine coherent structures; however, this yields very little insight into Lagrangian transport mechanisms, and can often lead to erroneous conclusions about flow structure (the time-dependence plays havoc with Eulerian conclusions!). Furthermore, an attempt to uncover Lagrangian information about the flow by simply integrating particle trajectories at different locations and times very quickly leads to "spaghetti" plots that are also not helpful. In contrast, the LCS method provides a systematic and concise approach for analyzing aperiodic flows and extracting the coherent structures that govern transport.

1.1 Main contributions of this thesis

This thesis continues the development of the FTLE-LCS method for studying aperiodic flows. In summary, the main contributions are as follows:

- The FTLE-LCS method is applied to several example flows yielding insight into the major structures that guide transport. The example flows include coastal oceans, planetary atmospheres, laboratory flows, and the three-body problem. (Chapter 3)

- The FTLE-LCS method is used to demonstrate that homoclinic tangles and the attendant transport mechanism of 'lobe dynamics' are a dominant transport structure in *aperiodic* geophysical flows – most notably in hurricanes, and mesoscale ocean eddies. (Chapters 5, 6, and 7).

- A study of global conformation change in a system of coupled oscillators provides a method for model reduction so that the statistics of the full system with many degrees of freedom are adequately described by a reduced system with one and a half degrees of freedom. (Chapter 8).

- The structures that govern transport from one conformation to another in the previously mentioned coupled oscillator model are visualized using surfaces of greatest separation (a slight modification of the FTLE-LCS method) and provides the appropriate reduced coordinates in which to reveal the presence of lobe dynamics and a homoclinic tangle in the high-dimensional flow. (Chapter 8).

- A study is made of the relationship between FTLE-LCS and stable/unstable manifolds of classical dynamical systems theory. A criterion is proposed for determining when FTLE-LCS and stable/unstable manifolds coincide. (Chapter 9).

- An algorithm is provided for determining evolution equations for the LCS. In light of this result, the motion of the LCS can be thought of as 'deterministic' (the result of an underlying evolution equation written in terms of the given velocity field), rather than 'emergent' (the result of extracting the LCS motion from multiple visualization frames in time). (Chapter 9).

- Software has been developed for large-scale computations of FTLE in flows of any dimension on parallel processors at unprecedented resolution. The software provides many features especially designed for analyzing geophysical flows. (Chapter 10).

1.2 Research topics not covered in this thesis

The central penetrating theme of this thesis is the discovery of transport mechanisms, and in particular the homoclinic tangle, in aperiodic flows. The author's research interests, however, are not as narrowly defined, and during my graduate research, I have pursued several unrelated research areas. A brief summary of this research that is not included in the body of the thesis is presented here.

1.2.1 Fast parallelized particle methods for PDEs

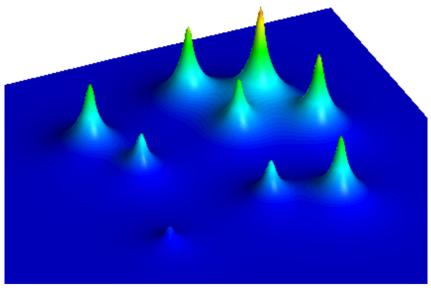
A particle method is developed for obtaining numerical solutions of the EPDiff-equation – the Euler-Poincaré equation associated with the diffeomorphism group [Chertock 2009]. For vectors in $\mathbb{R}^n$, the EPDiff-equation is

$$\frac{\partial \mathbf{m}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{m} + \nabla \mathbf{u}^T \cdot \mathbf{m} + \mathbf{m}(\operatorname{div} \mathbf{u}) = 0. \tag{1.2}$$

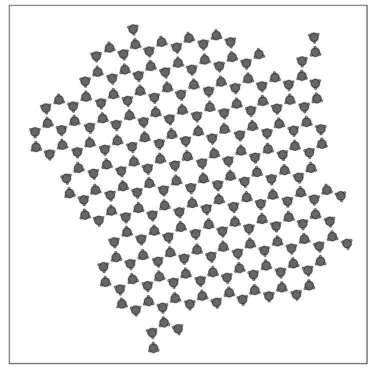
Here the momentum $\mathbf{m}$ and velocity $\mathbf{u}$ are vector functions of space and time, and are related by the second-order Helmholtz operator,

$$\mathbf{m} = \mathbf{u} - \alpha^2 \Delta \mathbf{u}, \tag{1.3}$$

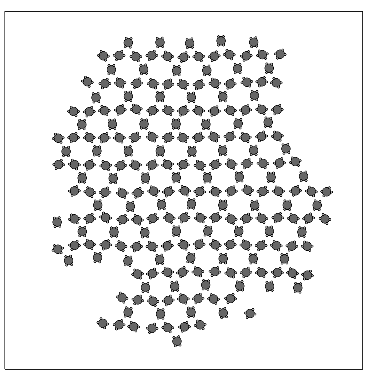
where α is a constant parameter. As shown in [Holm 2005], the particle approach reduces the partial differential equation to a finite-dimensional Hamiltonian system that can be implemented with geometry-preserving integrators that respect the symmetries of the particle system. The particle method is efficiently implemented on a parallel computing cluster using a spatial decomposition method that scales linearly with the number of particles. As depicted in Figure 1.1(a), the extremely low



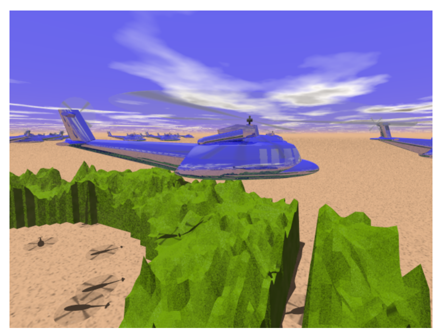
(a) Nonlinear interactions between peakons in the EPDiff-equation are simulated using an efficient particle method.



(b) An interaction potential is designed so that a honeycomb lattice forms via self-assembly as the system of particles is cooled.



(c) The use of anisotropic potentials allows for the formation of the kagome lattice.



(d) Underactuated vehicles with uncertain sensors perform a coordinated search over complex terrain.

Figure 1.1: Some of the applications addressed in my current research.

numerical diffusion of the particle method allows for sharp reproduction of *peakon* solutions, as well as interesting nonlinear *peakon-peakon* interactions. *Peakons* are solitary traveling wave solutions that are distinguished from soliton solutions by a discontinuity in their derivative that leads to a sharp peak at the crest of the wave.

1.2.2 Self-Assembly by design

Self-Assembly is the process by which constituents organize *themselves* into a globally ordered configuration without the influence of external factors [Whitesides 2002]. Order in the global superstructure is predicated on the local interactions between the individual constituents. Studies of self-assembly have typically examined the types of ordered superstructures that arise from a given fixed interaction potential; however, recent interest in fabrication of nanomaterials and photonic crystals with desired material properties motivates the inverse problem: *design* the short-range interaction in order to induce self-assembly of the components into a target lattice structure. We consider the specific problem of designing short-range pairwise interaction potentials between particles on a planar surface so that the particles self-assemble into a desired lattice.

New methods (a fast geometric method as well as a robust trend optimization method based on the rigorous Surrogate Management Framework [Booker 1999]) have been developed for the design of isotropic interaction potentials that lead to the formation of high quality honeycomb lattices as the system of particles is cooled (as shown in Figure 1.1(b)) [Du Toit 2009b]. The geometric method is also extended to the case of anisotropic potentials which allow for the formation of the more exotic kagome lattice (Figure 1.1(c)).

1.2.3 Coordinated Search with under-actuated vehicles

Motivated by recent advancements in unmanned aerial vehicles, we have considered the problem of using multiple vehicles equipped with sensors to find a target in a large complex terrain. An important feature of the problem description is that the vehicles are modeled as rigid bodies with *under-actuated* helicopter dynamics and limited control authority, and that the sensors are uncertain with probabilities for both missed detection and false alarm (Figure 1.1(d)). Hence, there is strong coupling between the vehicle dynamics and the design of the search strategy to be employed. We have developed a framework for vehicle control that uses motion primitives to dynamically generate trajectories that are consistent with the under-actuated dynamics of the search vehicle. The vehicle trajectories are updated dynamically as the sensors receive measurements using a Bayesian scheme to locally maximize the likelihood of target detection [Du Toit 2009c]. The algorithm is robust to changes in the terrain, limited communication range, and vehicle failure.