Chapter 10

Numerical Considerations

The FTLE calculations presented in this thesis were computed using recently developed research software, called `Newman`. One of the the most important contributions of the new software is that the calculations can be performed in parallel, thus dramatically decreasing computation times. As an example, calculations of the FTLE for the global ocean at a grid resolution of 4096×4096 that would require days to compute with first-generation single processor codes, can now be computed in minutes on a parallel cluster. A further advantage of the new software is that it can be compiled for computations in flows of any dimension, whereas previous codes were restricted to two-dimensional flows.

10.1 FTLE Computation

The core algorithm for computing the FTLE follows that of [Lekien 2003], and involves approximating the flow map by integrating trajectories from a uniform grid of initial conditions. The derivatives of the flow map needed in the definition of the FTLE are then obtained by finite differencing the approximate flow map. In principle, the numerical algorithm is very simple, and the pseudo-code barely fills a hand-written page; however, the software can become somewhat complex (a few thousand lines of code) in order to cover all possible contingencies. These include memory constraints, velocity data provided on non-uniform grids or nested grids, arbitrarily shaped domains including domains with islands, varying input and output formats, choices of integration schemes, integration in Cartesian space or on the sphere, etc.

By far the most computationally expensive part of the algorithm is integration of individual drifter trajectories. As mentioned, this task can be trivially parallelized, thus reducing the computation time. Although not pursued as part of this thesis, opportunities still remain to design a more efficient algorithm beyond straightforward parallelization. Possibilities include adaptive refinement of the grid of initial conditions in regions that track the LCS, as well as reusing results of drifter integrations from previous time frames to inform integration of drifters in the current frame. Further ideas include using the evolution equations for the LCS to numerically track the motion of the LCS, or approximating the motion of the LCS using flux minimizing curves.

10.2 Features of the `Newman` Software

`Newman` was specifically designed for large-scale parallel computations of geophysical flows. In particular it contains the following features:

1. **N-Dimensional Code:** The underlying code in `Newman` is dimension independent. When the code is compiled, a user-supplied flag indicates the desired dimensionality. In this way, the code is more easily maintained, and no sacrifice in efficiency is required.

2. **Parallel Implementation:** The code is written using the Message Passing Interface for use on either a single processor or a parallel cluster. Currently, parallel computations are performed routinely on several hundreds of processors in the Geophysical and Planetary Sciences supercluster at Caltech.

3. **Fast and Modular C++ Structures:** `Newman` is written in C++ to ensure computational speed and modularity of code. Users can easily implement their own additions to the code by editing or replacing individual modules.

4. **Light-Weight Data Structures:** `Newman` can handle large data sets and high-resolution computations through efficient memory usage. All input and output

are performed in binary format for fastest retrieval over the internet.

5. **Geophysical Applications:** `Newman` has many features specifically intended for geophysical applications. These include the ability to compute and plot FTLE on the sphere in 2D and 3D, or on a Mercator longitude-latitude-altitude projection; track the center of a tropical storm so that FTLE may be computed in storm-centered coordinates; use velocity data computed on multiple moving nested grids as is common for hurricane simulations; and interpolate data provided on non-uniform Cartesian grids.

6. **Fast Treatment of Boundaries:** `Newman` can quickly integrate trajectories for flows with arbitrarily shaped boundaries and multiple islands and appropriately compute the FTLE.

7. **Library of Integration Algorithms:** `Newman` uses the GNU Scientific Library for integration of trajectories and linear algebra calculations. The user can choose from several different integration schemes available.

8. **Miscellaneous Features:** `Newman` allows the user to produce plots of the FTLE, drifter trajectories, and velocity fields both forward and backward in time at a temporal resolution that is independent of the temporal spacing between frames in the data set. Data sets can be specified as periodic along any spatial dimension and in time.

`Newman` is freely available for download over the internet at www.cds.caltech.edu:∼/pdutoit/software. A manual that describes installation, including all the parameters the user may select, is provided in Appendix A.