Introduction
Methods
Implementation
Validation
Application
Conclusions
Timeline
References

AMSC 664 Final Presentation: Lagrangian Analysis of 2D and 3D Ocean Flows from Eulerian Velocity Data

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Project Goals

Project goals:

- Develop tools for Lagrangian (particle-based) analysis of a 2D or 3D ocean flow from Eulerian (grid-based) velocity data
- Validate on a series of simple ODE systems with well-understood dynamics
- Validate against existing tools from ROMS (Regional Ocean Modeling System)
- Test on a dataset from the Chesapeake Bay

Introduction

Dynamics background:

- Given an ODE system $\dot{\mathbf{x}} = \mathbf{u}(t, \mathbf{x})$ ($\mathbf{u} = (u, v, w)$ in $\mathbb{R}^3$) with corresponding particle trajectories $\mathbf{X}(t, \mathbf{X}_0)$
- A *hyperbolic equilibrium point* is a point $\mathbf{x}^*$ for which $\mathbf{u}(t, \mathbf{x}^*) \equiv 0$ and all eigenvalues of the Jacobian $\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^*}$ have nonzero real part
  - *Stable manifold* of $\mathbf{x}^*$: $\{\mathbf{x} \in \mathbb{R}^n \mid \lim_{t\to\infty} \mathbf{X}(t, \mathbf{x}) = \mathbf{x}^*\}$
  - *Unstable manifold* of $\mathbf{x}^*$: $\{\mathbf{x} \in \mathbb{R}^n \mid \lim_{t\to-\infty} \mathbf{X}(t, \mathbf{x}) = \mathbf{x}^*\}$
- Corresponding concept when $\mathbf{x}^*$ is moving is that of a *distinguished hyperbolic trajectory*

Introduction

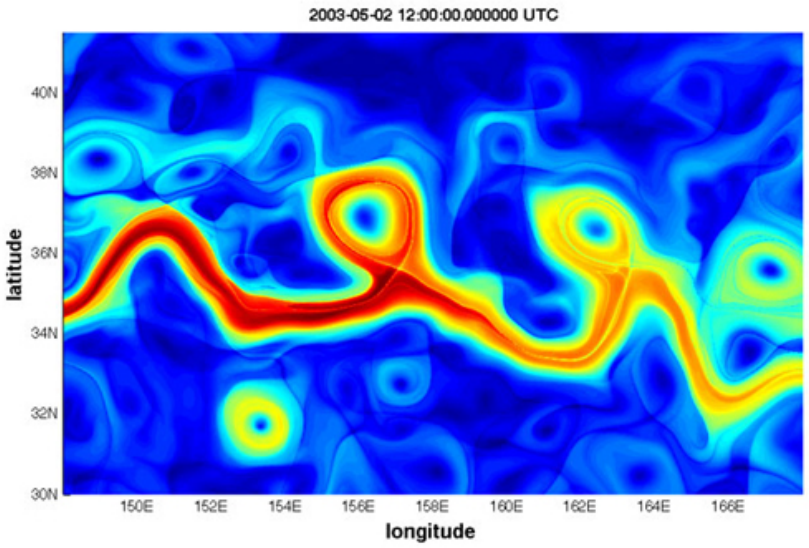
Stable and unstable manifolds:

- Act as boundaries between coherent structures in the flow (e.g. as rough barriers to pollutant transport in oceans)
- Can be found by one of two numerical methods: finite-time Lyapunov exponents (traditional) and arc lengths, also called M-function (newer)
- Each of these requires a thick soup of particle trajectories for calculation

Introduction

Example: M-function applied to dataset from the Kuroshio current, northwest Pacific Ocean [**?**]:

- Red fast, blue slow (on average)
- Thin yellow lines: stable and unstable manifolds



Methods: Overview

- Three main numerical tasks:
  - *Interpolate* velocities to off-grid particle locations
  - *Integrate* particle velocities to obtain trajectories
  - *Analyze* trajectories using numerical tools
- Implement and compare various versions of each of these

Methods: Interpolation

2D horizontal interpolation methods:

- Bilinear splines: Fit function of form

$$f(x,y) = \sum_{i,j=0}^{1} c_{ij} x^i y^j = c_{00} + c_{10}x + c_{01}y + c_{11}xy$$

  to given values of u at box corners

- Bicubic splines: Fit function of form

$$f(x,y) = \sum_{i,j=0}^{3} c_{ij} x^i y^j$$

  to given values of u, approximate values of u_x, u_y, u_{xy} at box corners (using second-order finite differences: two-sided for interior, one-sided for boundary)

Methods: Interpolation

Vertical and temporal interpolation methods:

- Linear: Fit linear function of z through two nearest vertical neighbors
- Cubic: Fit cubic polynomial in z through four nearest vertical neighbors
- Same algorithms for temporal interpolation

Intergration method:

- 4th-order Runge-Kutta

Methods: Analysis

Approaches:

- M-function (arc length over fixed time interval)
  - Forward: $M(\tau, \mathbf{X}_0) = \int_0^\tau |\mathbf{u}(t, \mathbf{X}(t, \mathbf{X}_0))| \, dt$
  - Backward: $M(\tau, \mathbf{X}_0) = \int_{-\tau}^0 |\mathbf{u}(t, \mathbf{X}(t, \mathbf{X}_0))| \, dt$
  - Both: $M(\tau, \mathbf{X}_0) = \int_{-\tau}^\tau |\mathbf{u}(t, \mathbf{X}(t, \mathbf{X}_0))| \, dt$
- Maximal finite-time Lyapunov exponent (FTLE) (maximal growth rate of distance between close trajectories):

$$\mathrm{FTLE}(\tau, \mathbf{X}_0) = \frac{1}{\tau} \ln \left(\sigma_{\max} \left(L(\tau, \mathbf{X}_0) \right) \right)$$

where $L(\tau, \mathbf{X}_0) = \frac{\partial \mathbf{X}(\tau, \mathbf{X}_0)}{\partial \mathbf{X}_0}$ is the transition matrix and $\sigma_{\max}$ is the largest singular value

Methods: Analysis

Calculating M and FTLE:

- M-function: Consider M as a state variable like u and v, integrate alongside u and v
- FTLE:
  - Track particles directly next to $\mathbf{X}_0$ up to time τ
  - Approximate $L = \frac{\partial \mathbf{X}}{\partial \mathbf{X}_0}$ using centered differences for $\Delta X_0, \Delta Y_0, \Delta Z_0$ and final locations for $\Delta X, \Delta Y, \Delta Z$
  - Calculate $\sigma_{\max}(L)$ as $\sqrt{\lambda_{\max}(L^T L)}$, where eigenvalues of $L^T L \in (\mathbb{R}^{2\times 2}$ or $\mathbb{R}^{3\times 3})$ are roots a quadratic or cubic polynomial

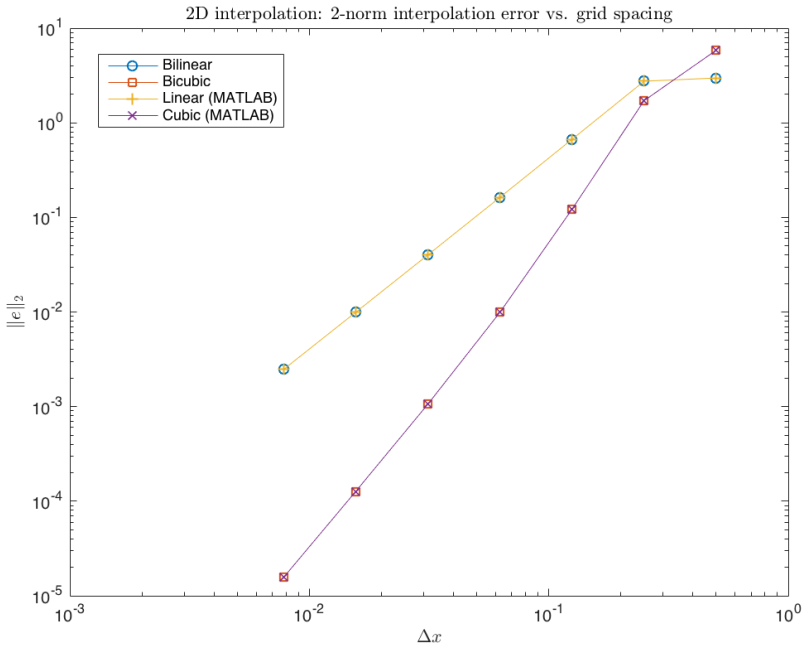
Implementation

Implementation details:

- Software: MATLAB
- Hardware:
  - Shorter runs (up to 6-hour dataset): MacBook Pro laptop, 2.6 GHz Intel Core i5, 8 GB 1600 MHz DDR3
  - Longer runs: Deepthought2
- Vectorization but no parallelization across particles
- Trajectories that leave domain set to `NaN`

Validation: 2D Interpolation

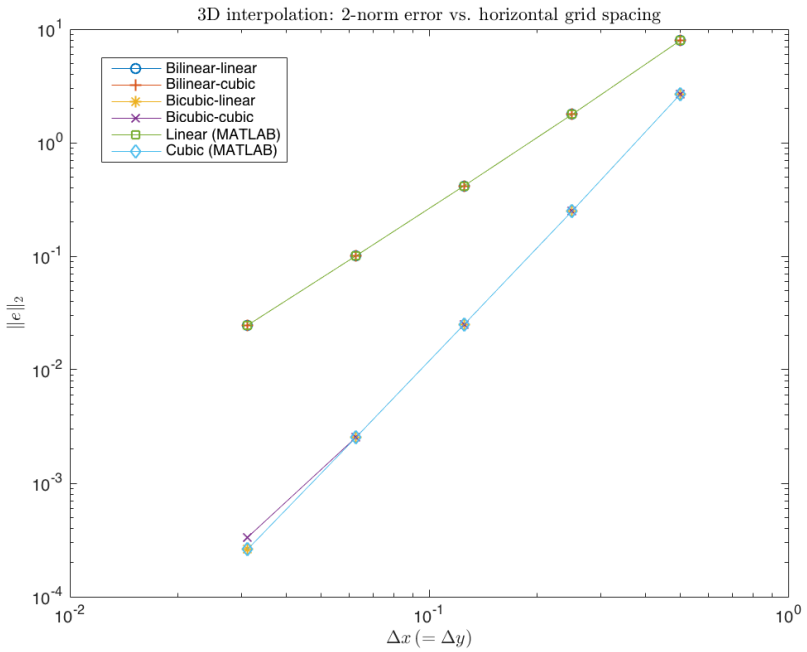
2D accuracy: $\|f_{\text{interp}} - f_{\text{semi-interp}}\|_2$ vs. Δx (interpolation mesh size) for $f(x, y) = e^x \cos(2\pi y)$ on $[-1, 1]^2$ for particle grid at 6x resolution



	Convergence rate ($\|e\|_2 \sim h^p$)
Bilinear	$p \approx 2.0064$
Bicubic	$p \approx 3.0175$

Validation: 3D Interpolation

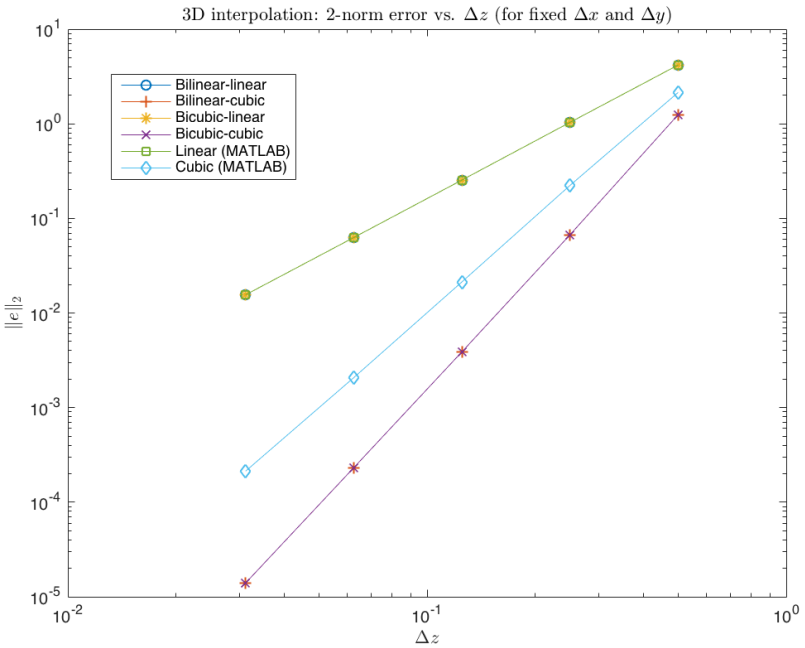
3D horizontal accuracy: $\|f_{\text{approx}} - f\|_2$ vs. $\Delta x = \Delta y$, Δz fixed, for $f(x, y, z) = e^x \cos 2\pi y \cos 2\pi z$ on $[-1, 1]^2$



Horizontal (-vertical) method	Convergence rate ($\|e\|_2 \sim h^p$)
Bilinear (-linear)	$p \approx 2.0253$
Bicubic (-linear)	$p \approx 3.2675$
Bicubic (-cubic)	$p \approx 2.9192$
MATLAB Cubic	$p \approx 3.2675$

Validation: 3D Interpolation

3D vertical accuracy: $\|f_{\text{interp}} - f_{\text{semi-interp}}\|_2$ vs. Δz, $\Delta x = \Delta y$ fixed



(Horizontal-)vertical method	Convergence rate ($\|e\|_2 \sim h^p$)
(Bilinear-)linear	$p \approx 2.0101$
(Bicubic-)cubic	$p \approx 4.0484$
MATLAB cubic	$p \approx 3.2836$

Validation: 2D Trajectory Calculation

2D test system: Undamped Duffing oscillator (1918) [**?**]:

- Simple nonlinear oscillator
- General case (forcing parameter ϵ):

$$\dot{x} = y$$
$$\dot{y} = x - x^3 + \epsilon \sin t$$

- Autonomous case ($\epsilon = 0$):
  - Hyperbolic equilibrium point at $\mathbf{x} = (0, 0)$
  - Stable and unstable manifolds both given by $y^2 = x^2 - \frac{x^4}{2}$ (figure-eight shape centered at origin)

Validation: 2D Trajectory Calculation

Autonomous Duffing oscillator:

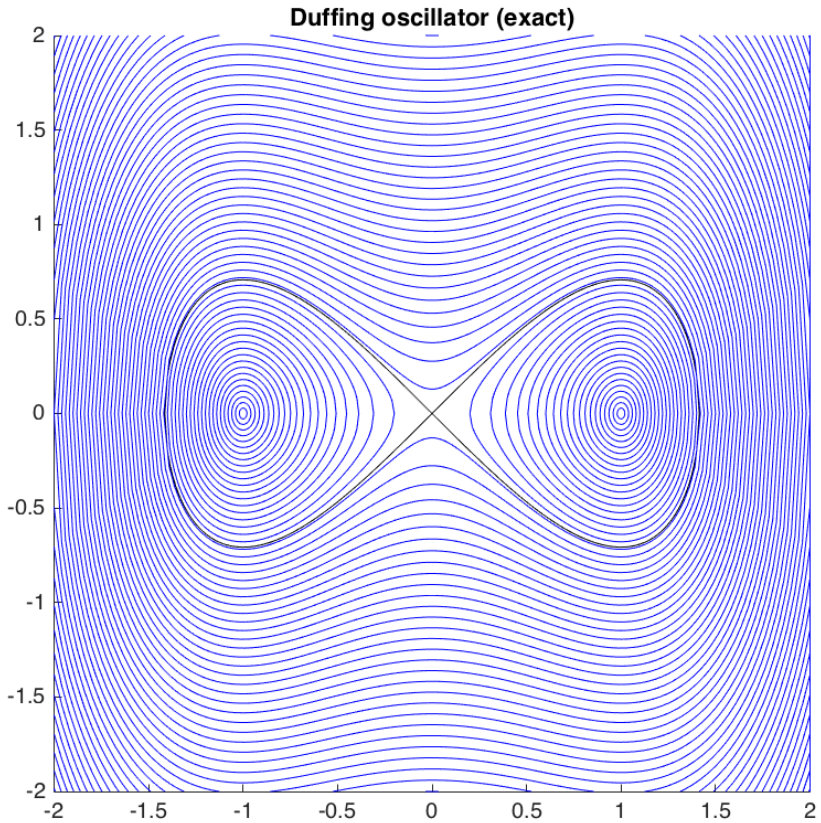
- Hamiltonian system with $H(x, y) = \frac{1}{2}y^2 - \frac{1}{2}x^2 + \frac{1}{4}x^4$ conserved along trajectories
- $x(t)$ and $y(t)$ can be computed explicitly via Jacobi elliptic functions [**?**], e.g. for $y_0 = 0$ we have

$$x(t) = x_0 \cdot \mathrm{cn}\left(t\sqrt{x_0^2 - 1}, \sqrt{\frac{x_0^2}{2(x_0^2 - 1)}}\right)$$

$$y(t) = -x_0\sqrt{x_0^2 - 1} \cdot \mathrm{sn}\left(t\sqrt{x_0^2 - 1}, \sqrt{\frac{x_0^2}{2(x_0^2 - 1)}}\right) \cdot \mathrm{dn}\left(t\sqrt{x_0^2 - 1}, \sqrt{\frac{x_0^2}{2(x_0^2 - 1)}}\right)$$

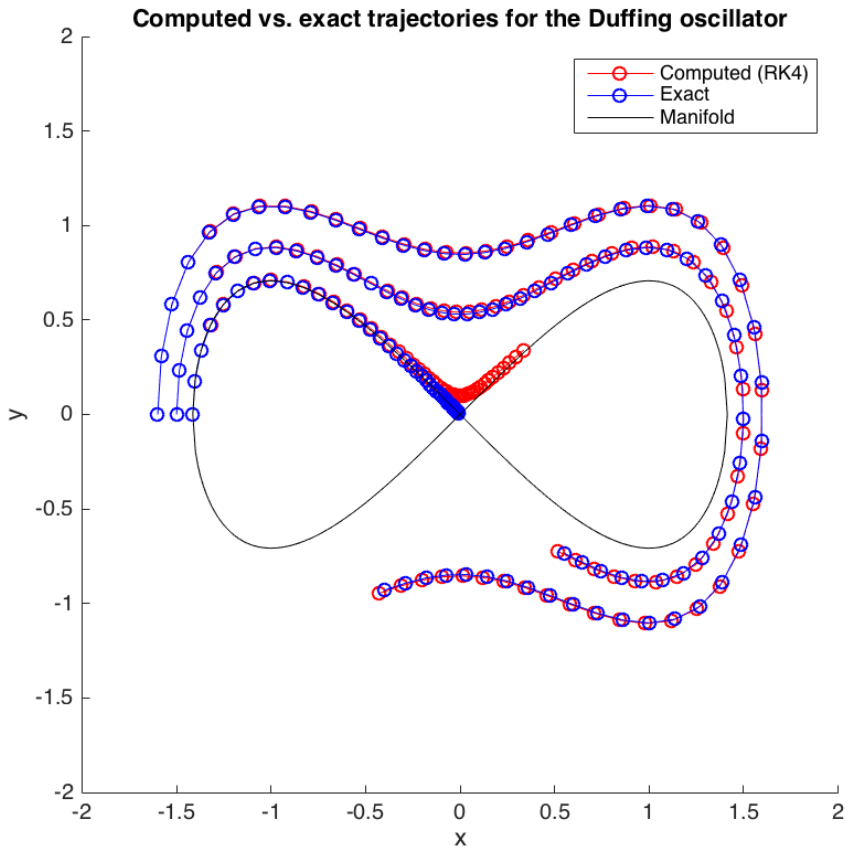
Validation: 2D Trajectory Calculation

Exact trajectories of autonomous Duffing (level sets of $H(x, y)$:)



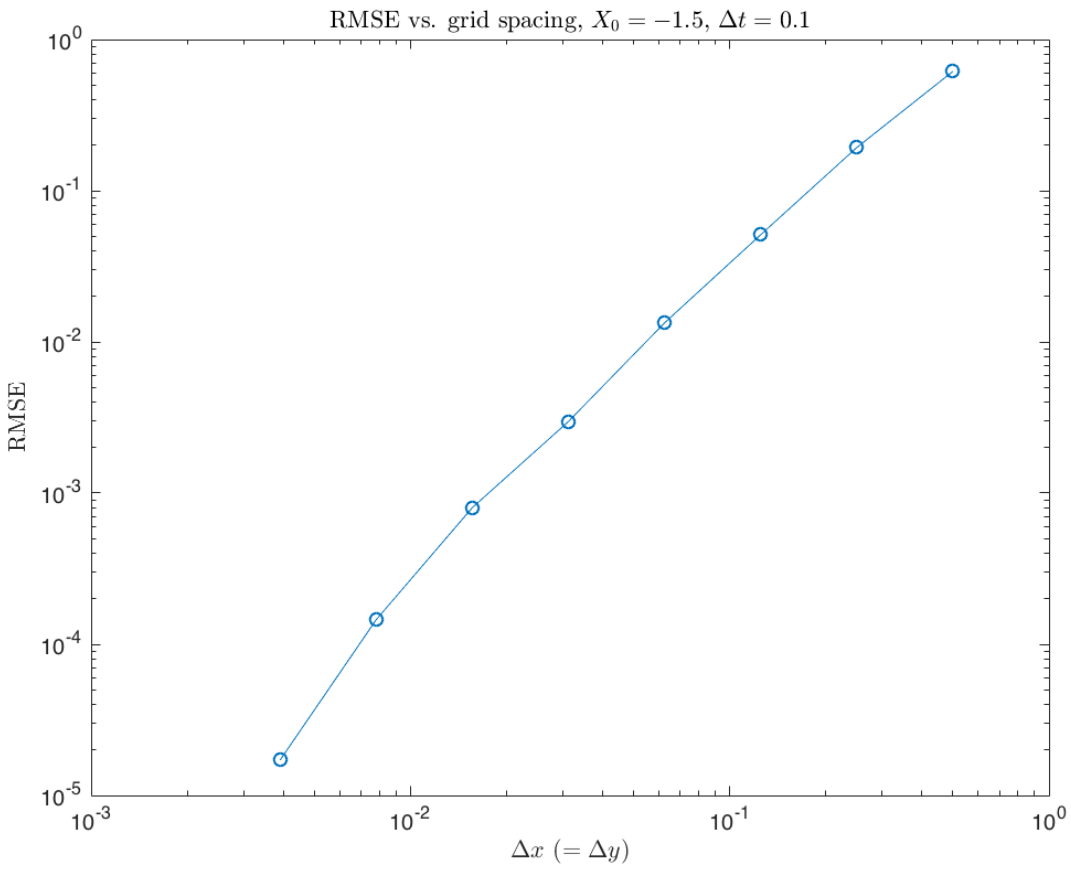
Validation: 2D Trajectory Calculation

Visual validation: A few computed vs. exact trajectories for Duffing oscillator (RK4, bilinear, $\Delta x = \Delta y = 0.1$, $\Delta t = 2^{-3}$, $t_f = 6$):



Validation: 2D Trajectory Calculation

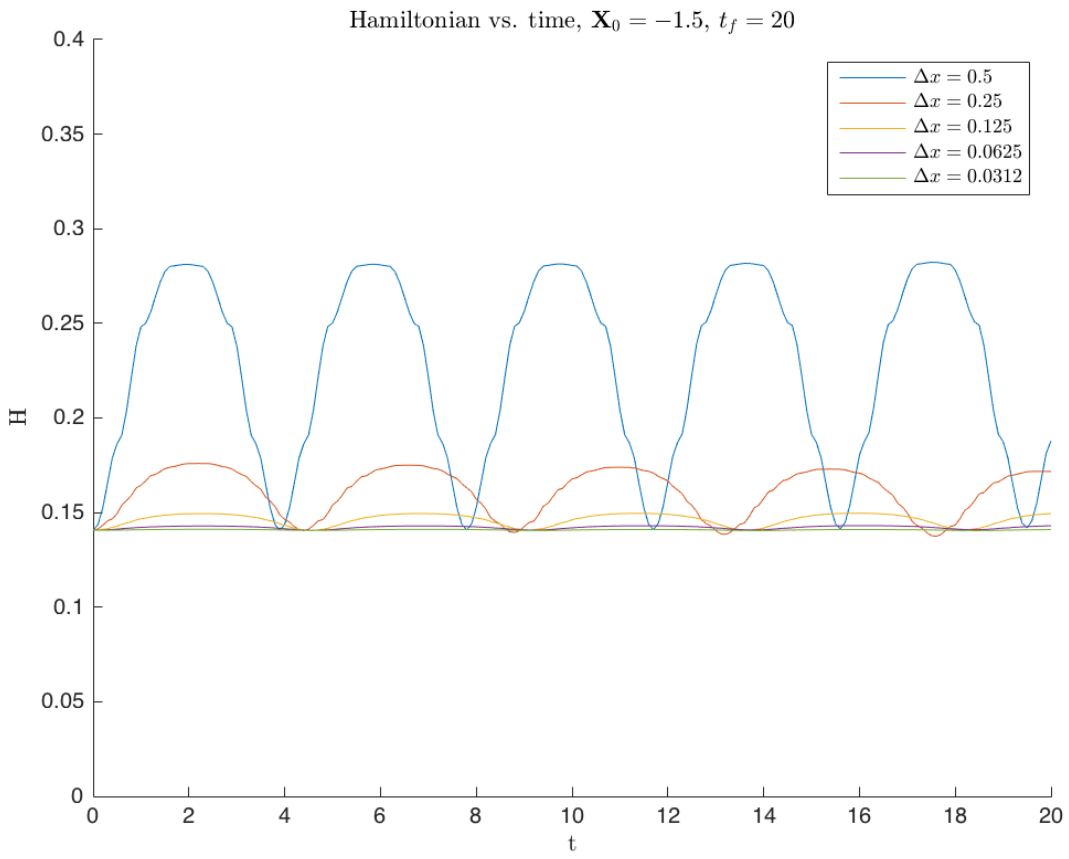
RMSE vs. interpolation Δx for individual trajectory with $\mathbf{X}_0 = (-1.5, 0)$, $\Delta t = 0.1$, $t_f = 6$:



Validation: 2D Trajectory Calculation

Hamiltonian vs. time for $\mathbf{X}_0 = (-1.5, 0)$, $t_f = 20$:

- Hamiltonian becomes constant as $\Delta x \to 0$



Visual Validation: 2D Lagrangian Tools

Autonomous Duffing oscillator: M-function, forwards and backwards, $\tau = 10$

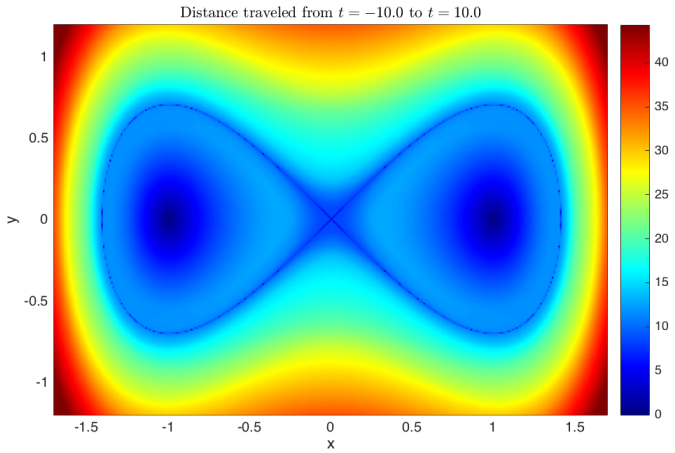


Figure: My results

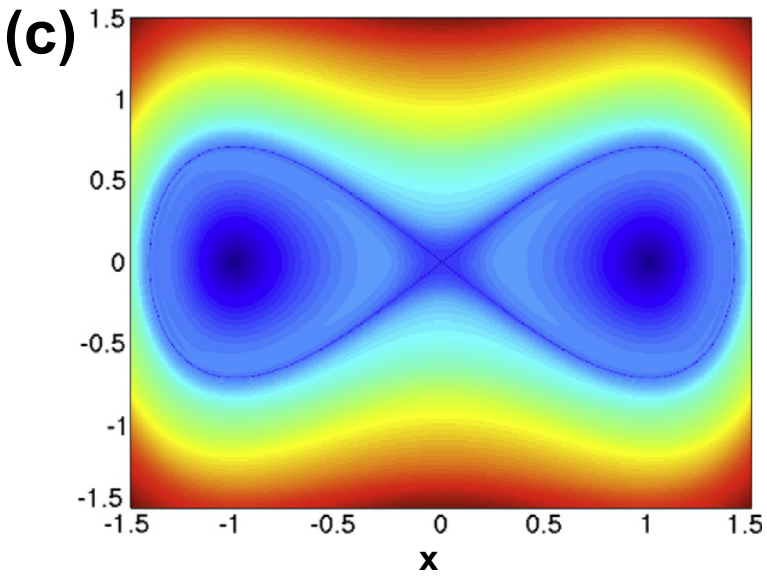


Figure: Mancho et al results [?]

Visual Validation: 2D Lagrangian Tools

Autonomous Duffing oscillator: FTLE, forwards, $\tau = 10$

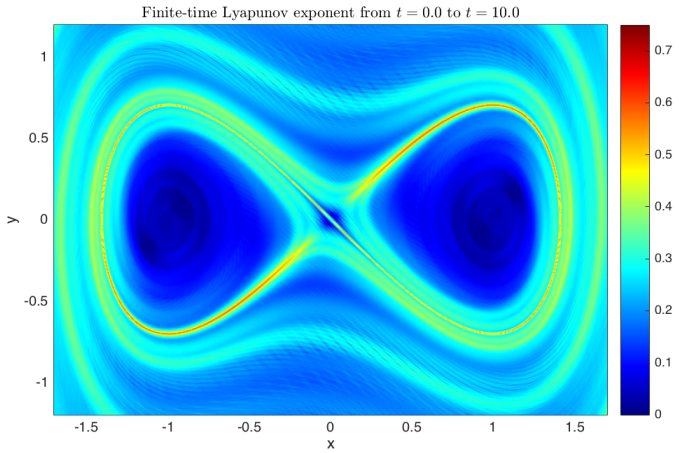


Figure: My results

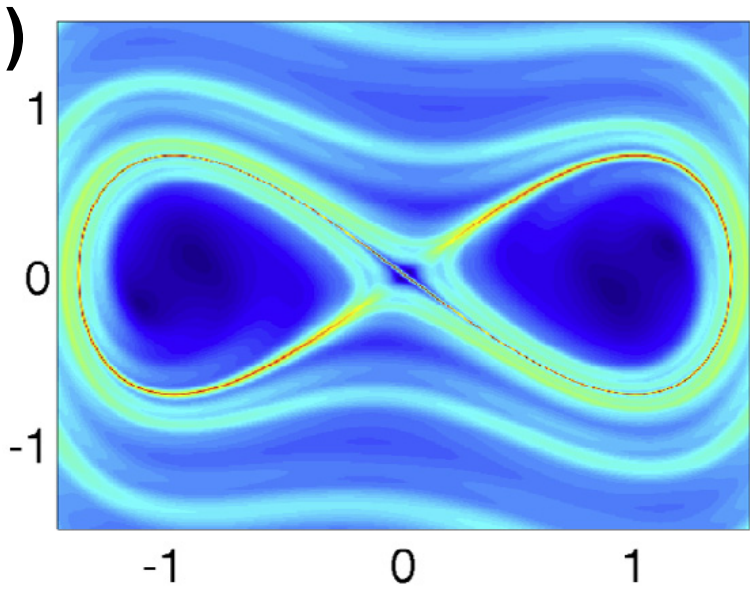


Figure: Mancho et al results [**?**]

Visual Validation: 2D + Time Lagrangian Tools

Forced Duffing oscillator ($\epsilon = 0.1$): M-function, forwards and backwards, $\tau = 10$

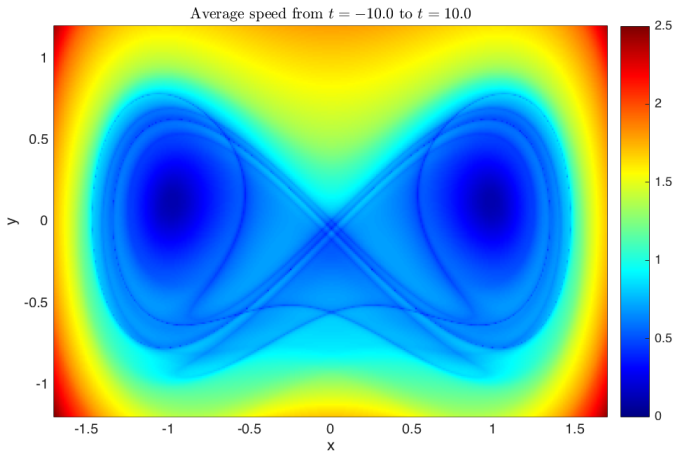


Figure: My results

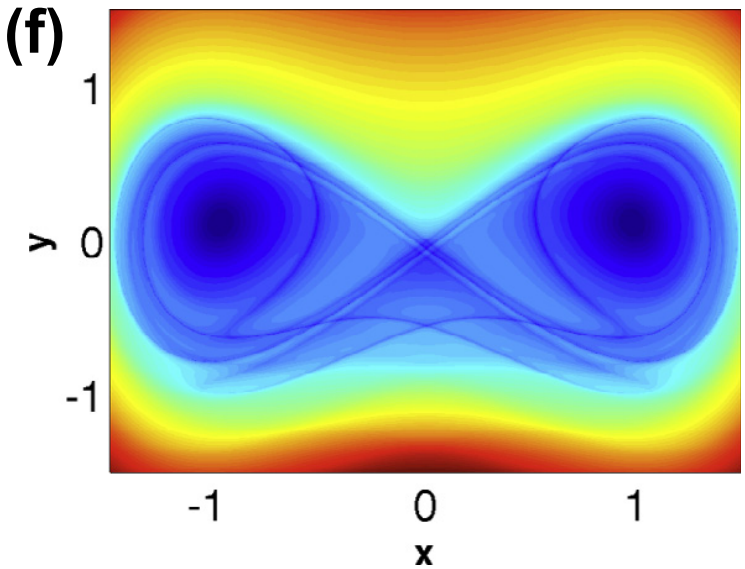


Figure: Mancho et al results [?]

Visual Validation: 2D + Time Lagrangian Tools

Forced Duffing oscillator: FTLE, forwards, $\tau = 10$

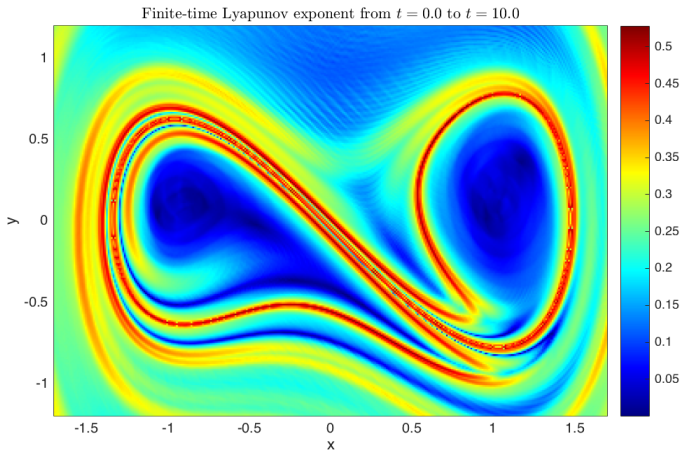


Figure: My results

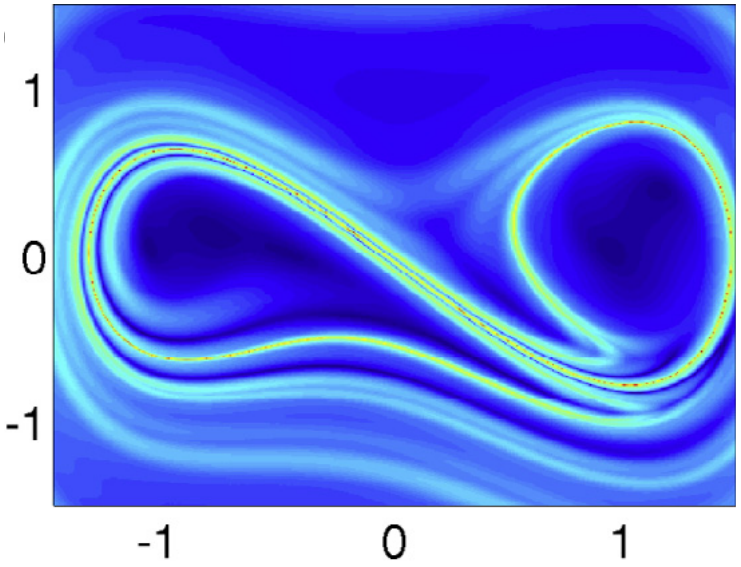


Figure: Mancho et al results [**?**]

Visual Validation: 2D + Time Lagrangian Tools

Finding manifolds: M vs. FTLE, forwards, $\tau = 10$

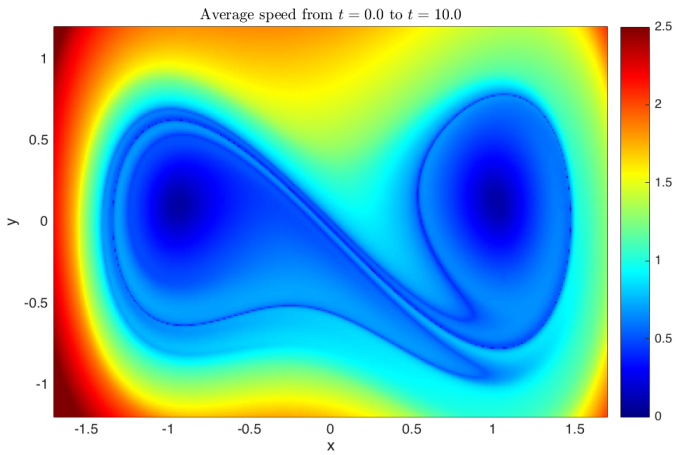


Figure: M-function

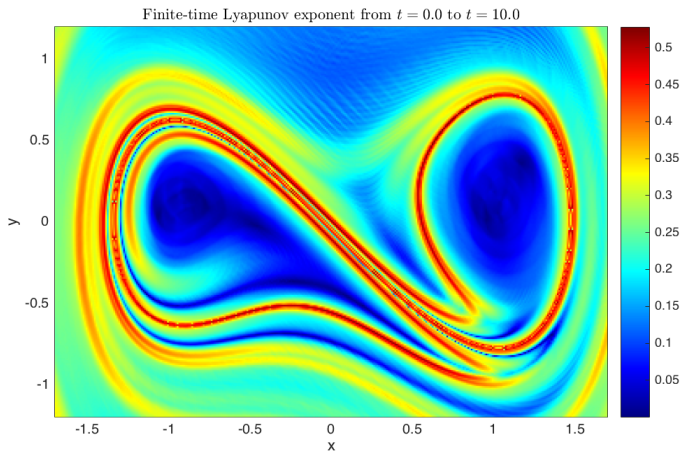


Figure: FTLE

Validation: 3D Trajectory Calculation

3D test case: Hill's spherical vortex (1894) [**?**]

- Simple model of axisymmetric flow around and inside a sphere of radius a
- Cartesian ODE system:

$$\dot{x} = -\frac{3Uxz}{2a^2}$$
$$\dot{y} = -\frac{3Uyz}{2a^2}$$
$$\dot{z} = \frac{3U(2x^2 + 2y^2 + z^2 - a^2)}{2a^2}$$

Validation: 3D Trajectory Calculation

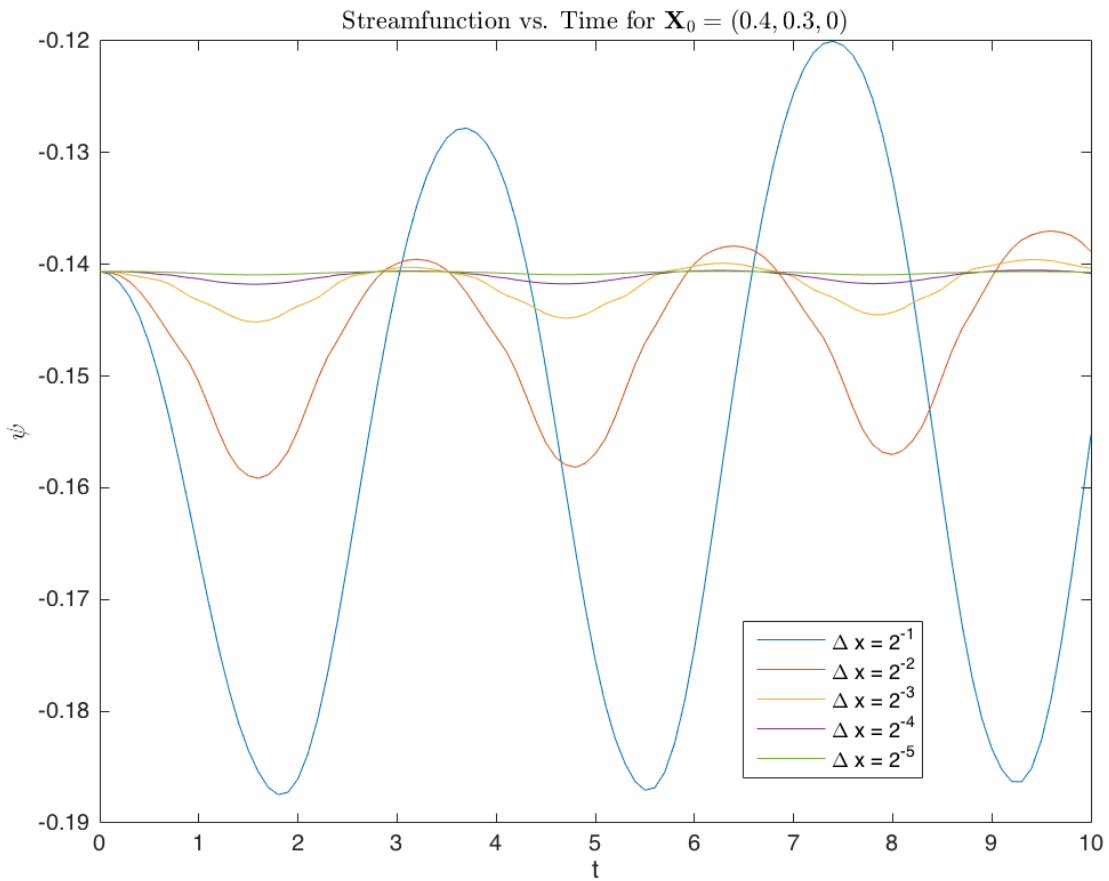
- Hyperbolic fixed points: $\mathbf{x}_1^* = (0, 0, -a)$, $\mathbf{x}_2^* = (0, 0, a)$
- Stable/unstable manifolds consist of sphere and vertical line through center of sphere
- Streamfunction (conserved along trajectories):

$$\psi(r, \theta) = -\frac{3}{4} U r^2 \left(1 - \frac{r^2}{a^2}\right) \sin^2 \theta$$

Validation: 3D Trajectory Calculation

Hill's spherical vortex: Streamfunction ψ vs. time for various interpolation Δx, $\mathbf{X}_0 = (0.4, 0.3, 0)$, $\Delta t = 0.1$, $t_f = 10$

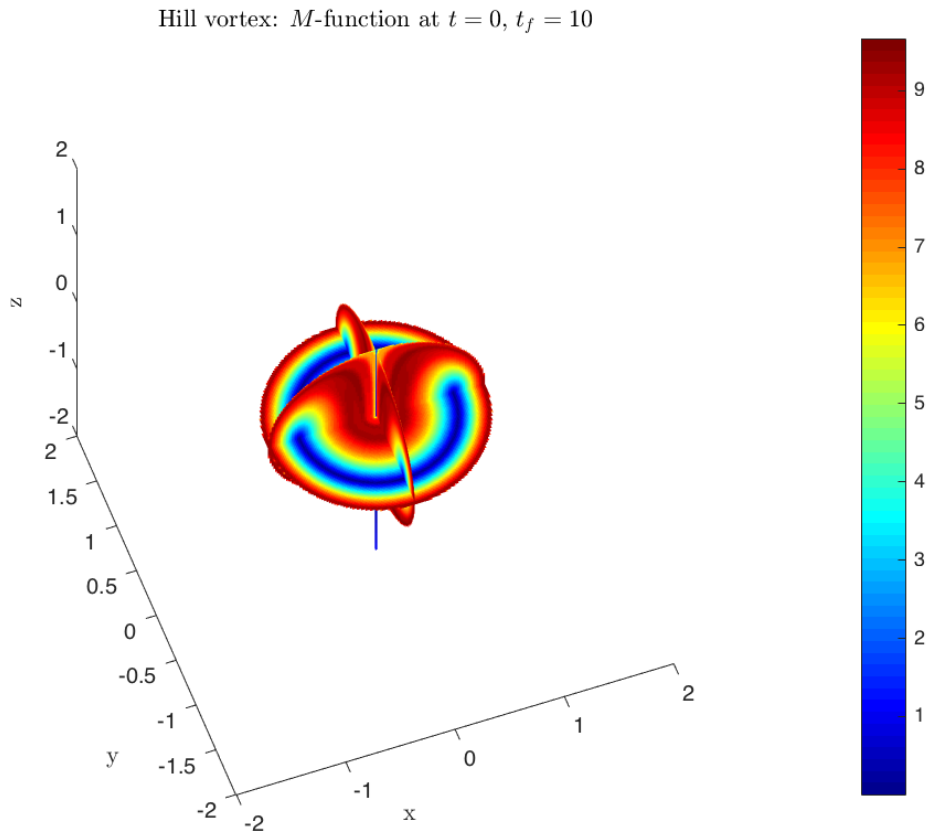
- ψ becomes more constant as $\Delta x \to 0$



Visual Validation: 3D Lagrangian Tools

Hill's vortex: M-function, $t_f = 10$:

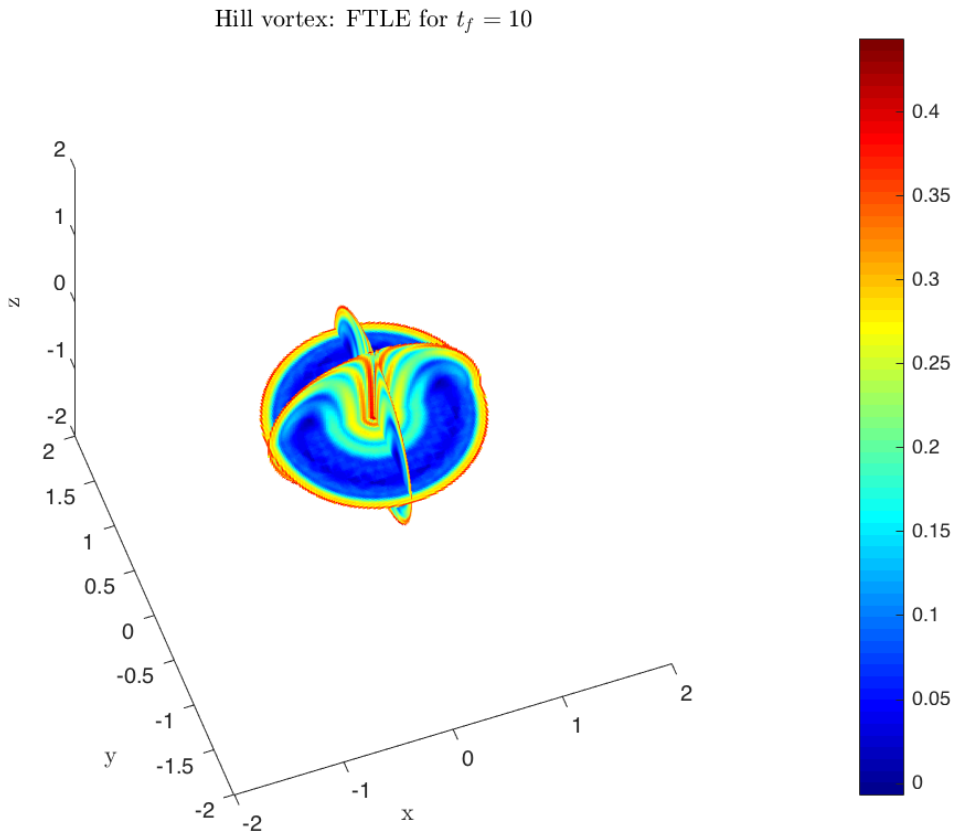
- Spherical + z-axis manifold clearly visible



Visual Validation: 3D Lagrangian Tools

Hill's vortex: FTLE, $t_f = 10$:

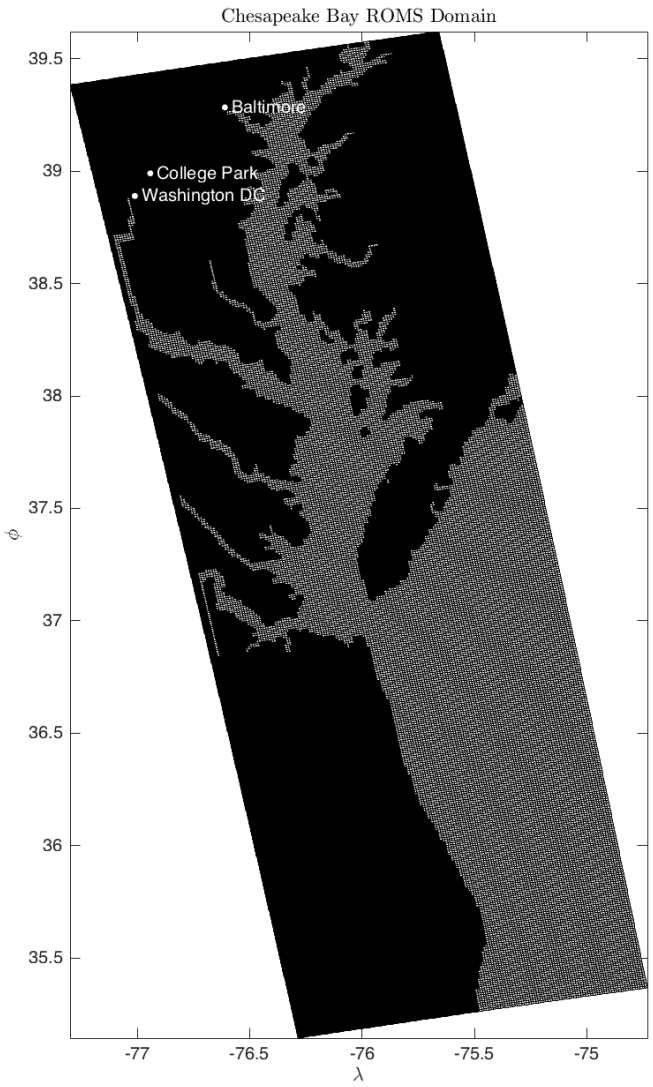
- Spherical manifold clearly visible



Application: Chesapeake Bay ROMS Dataset

Chesapeake Bay ROMS (Ches-ROMS) domain:

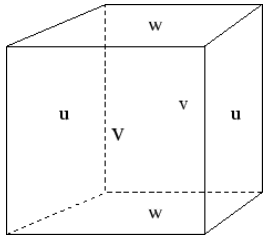
- Dimensions: $\sim$ 84 mi x 300 mi x 2.5-50 ft
- Discretized to 150 x 480 x 20 grid (terrain-following vertical coordinate)



Application: Chesapeake Bay ROMS Dataset

ChesROMS velocity data:

- Grid indexed by (ξ, η) instead of (i, j)
  - Arakawa C-grid, so (ξ_u, η_u) staggered from (ξ_v, η_v)



- Physical velocity components u_ξ, u_η, v_ξ and v_η proscribed at grid points (in m/s), also longitude (λ) and latitude (ϕ)
- Velocity given every two minutes on spatial grid

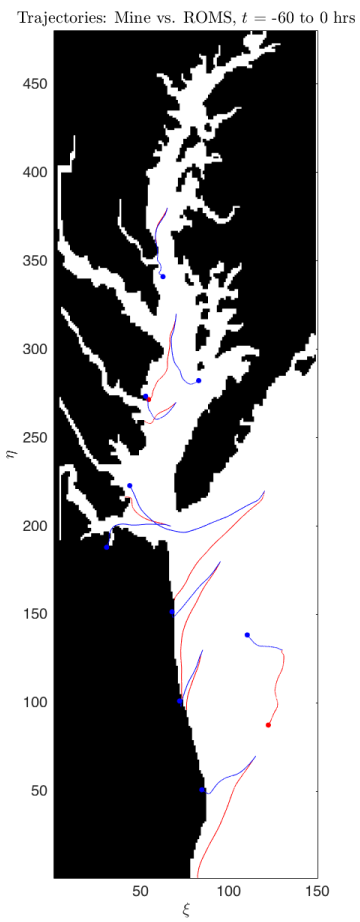
Application: Chesapeake Bay ROMS Dataset

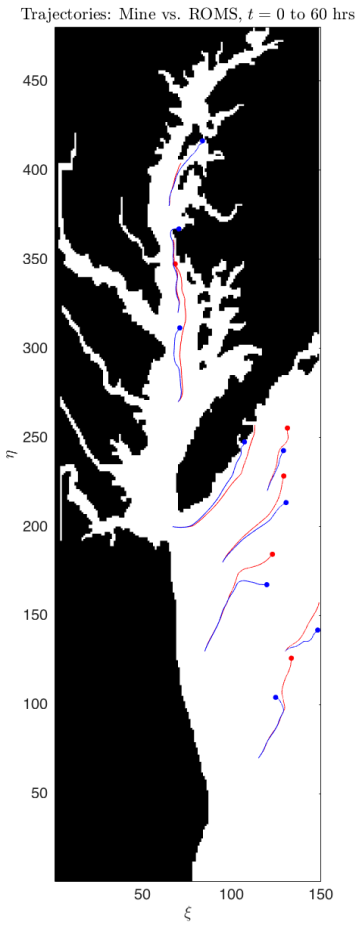
ROMS implementation details:

- Interpolation done in (ξ, η)-space (linear and bilinear only)
- Velocities normalized to index space (s^{-1}), integration done there
- M-function calculated in physical space (m)
- FTLE calculated from physical x and y displacements, estimated from λ and ϕ

Application: Chesapeake Bay ROMS Dataset

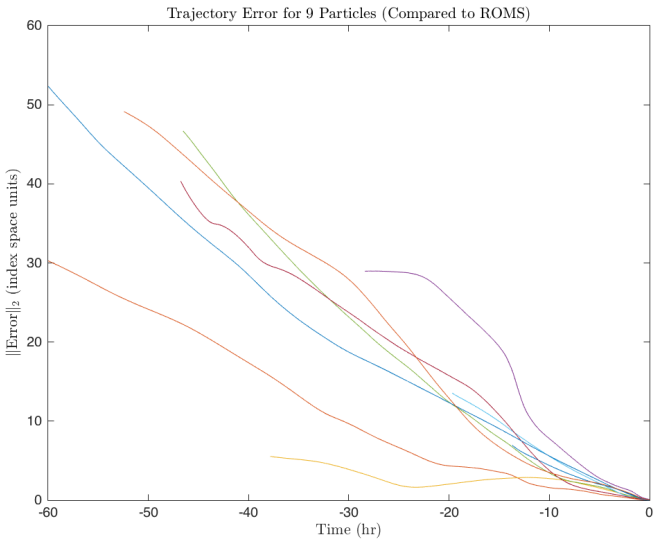
Validating Chesapeake trajectories: Mine vs. ROMS-generated, backwards (left) and forwards (right) 60 hrs, static flow field

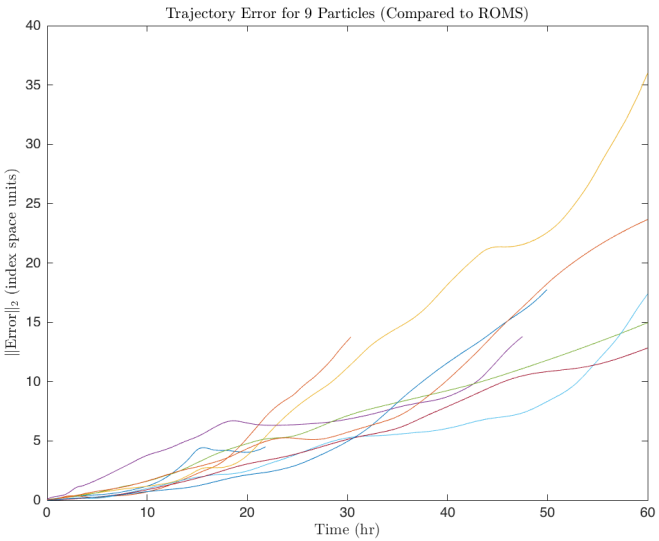




Application: Chesapeake Bay ROMS Dataset

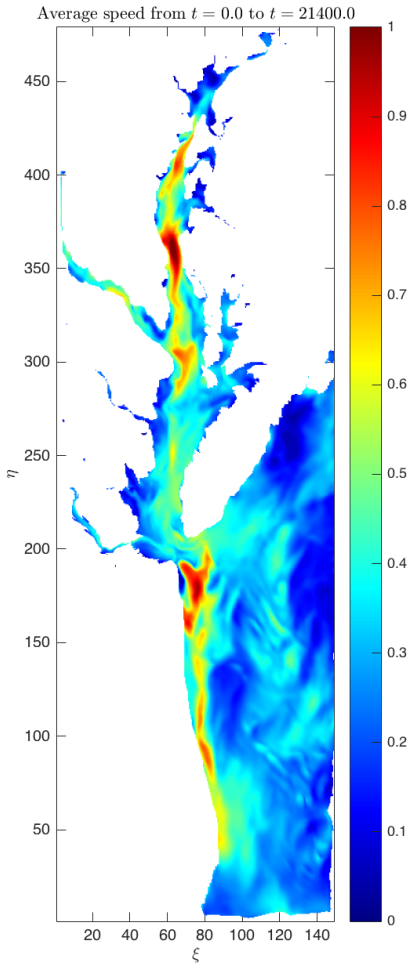
Trajectory error vs. time (2-norm in index space), backwards and forwards 60 hrs

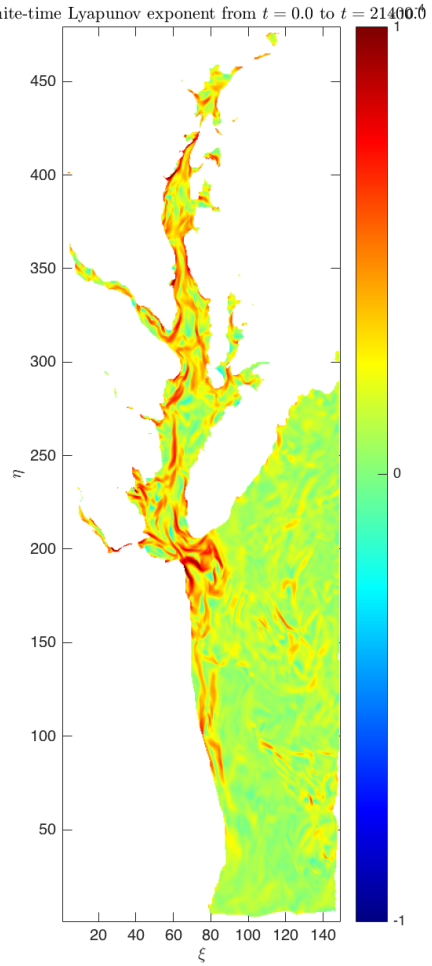




Application: Chesapeake Bay ROMS Dataset

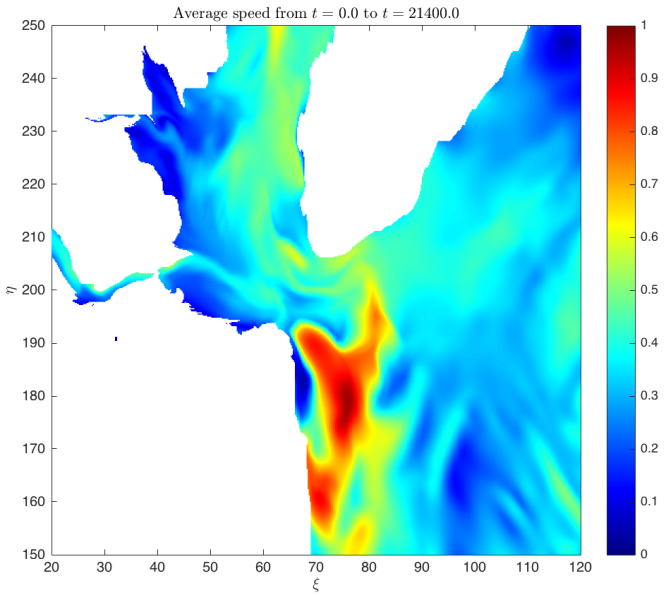
Average speed in m/s ($= \frac{M}{\tau}$) and FTLE, $\tau \approx 6$ hr, forward in time

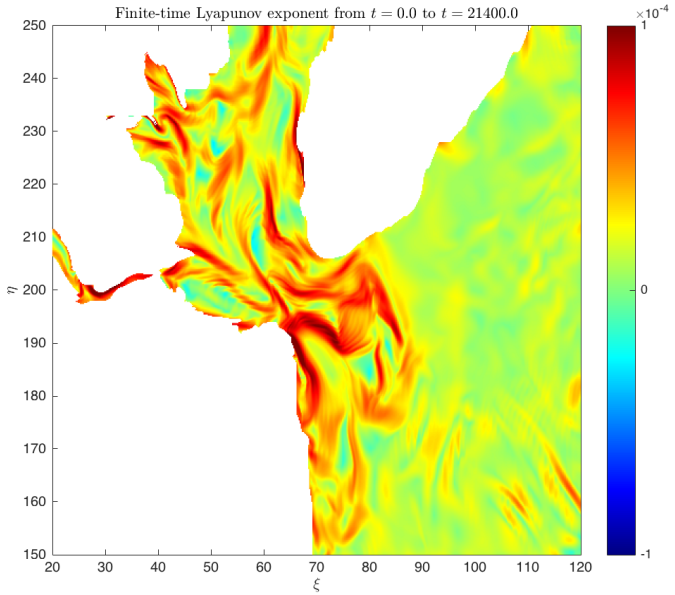




Application: Chesapeake Bay ROMS Dataset

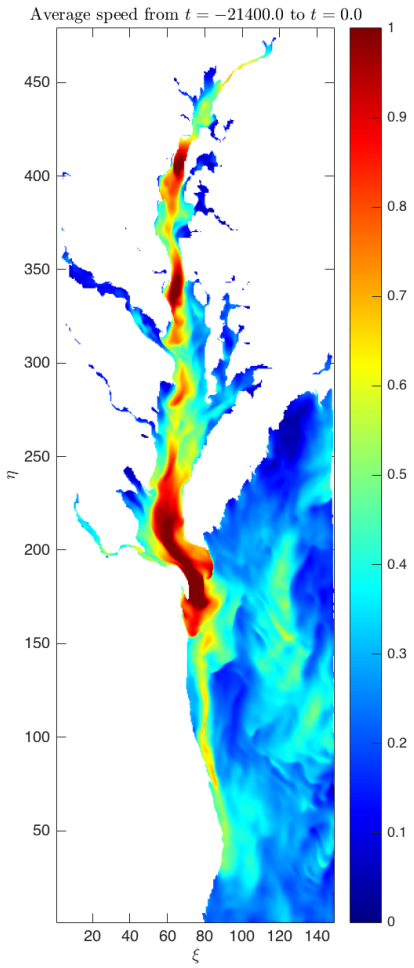
Average speed in m/s and FTLE, $\tau \approx 6$ hr, forward in time

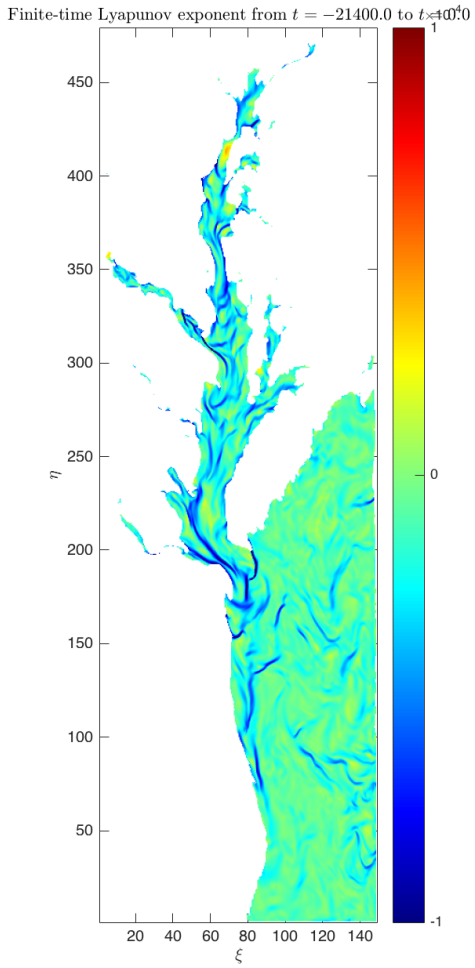




Application: Chesapeake Bay ROMS Dataset

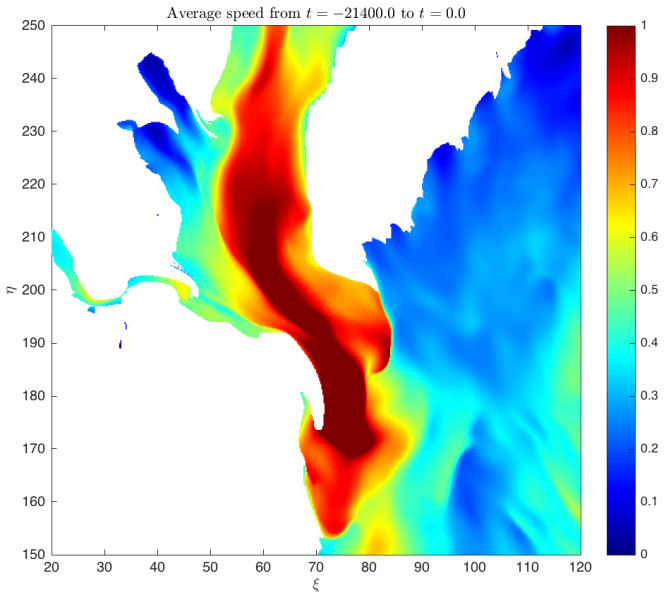
Average speed in m/s and FTLE, $\tau \approx 6$ hr, backward in time

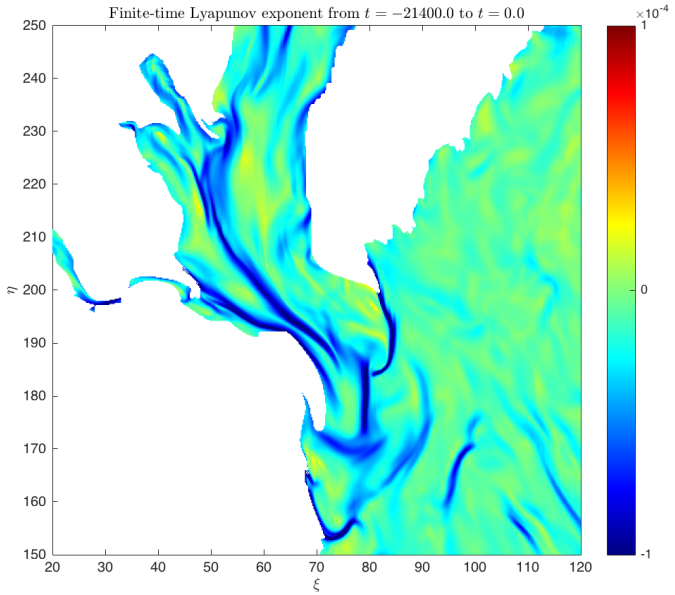




Application: Chesapeake Bay ROMS Dataset

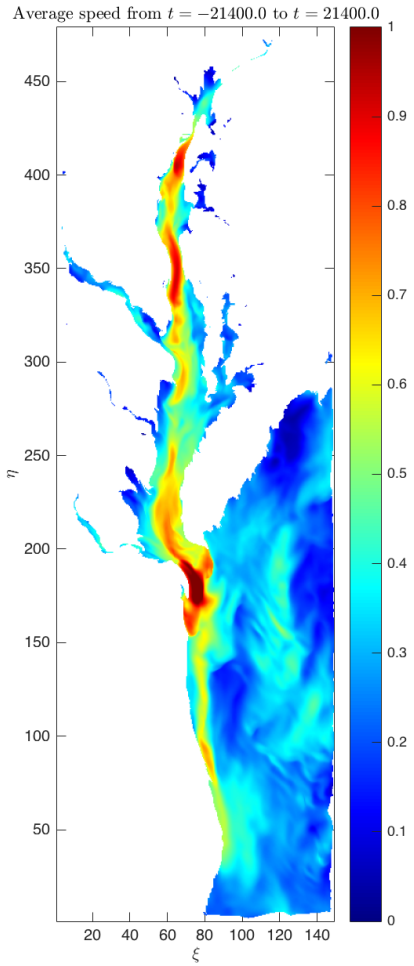
Average speed in m/s and FTLE, $\tau \approx 6$ hr, backward in time

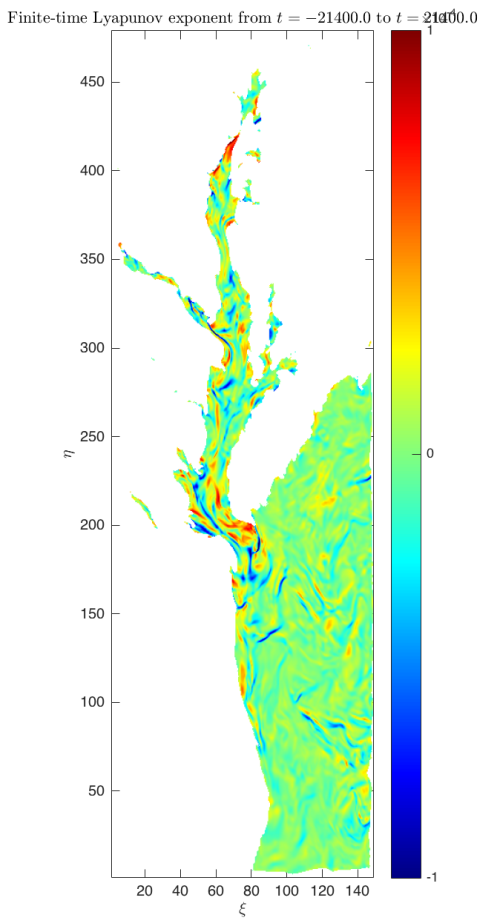




Application: Chesapeake Bay ROMS Dataset

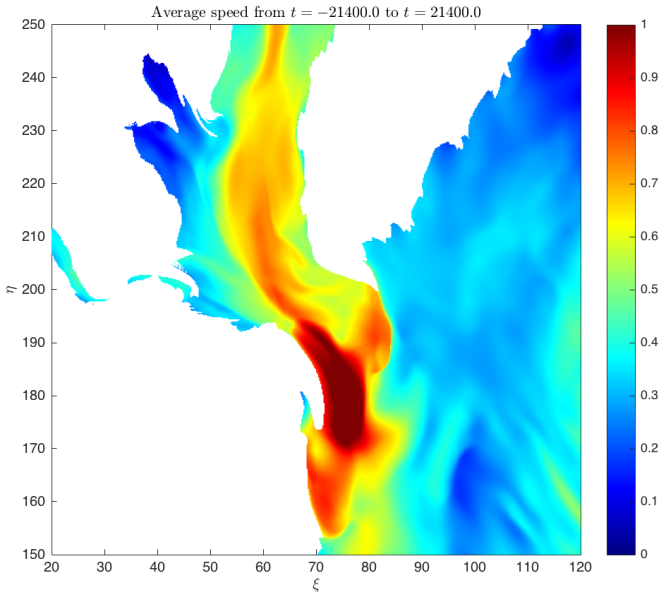
Average speed in m/s and FTLE, $\tau \approx 6$ hr, forward and backward in time

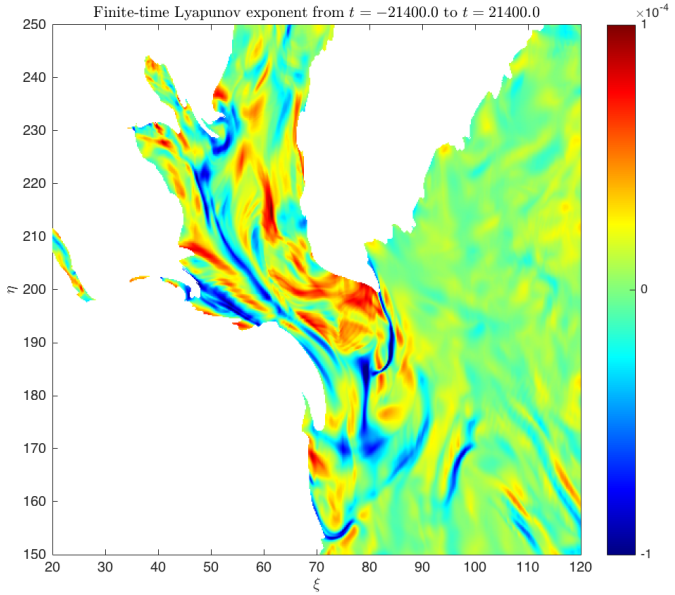




Application: Chesapeake Bay ROMS Dataset

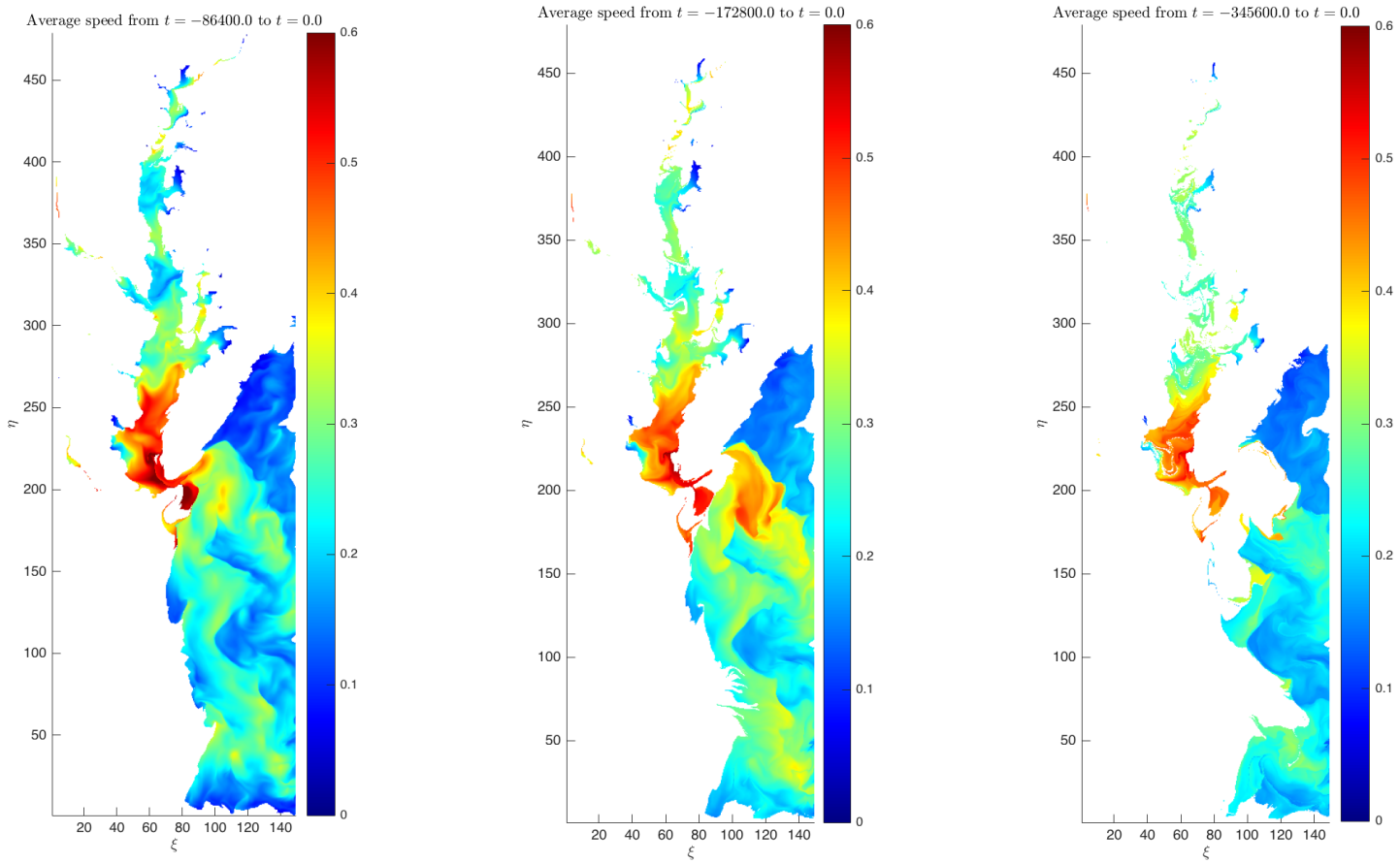
Average speed in m/s and FTLE, $\tau \approx 6$ hr, forward and backward in time





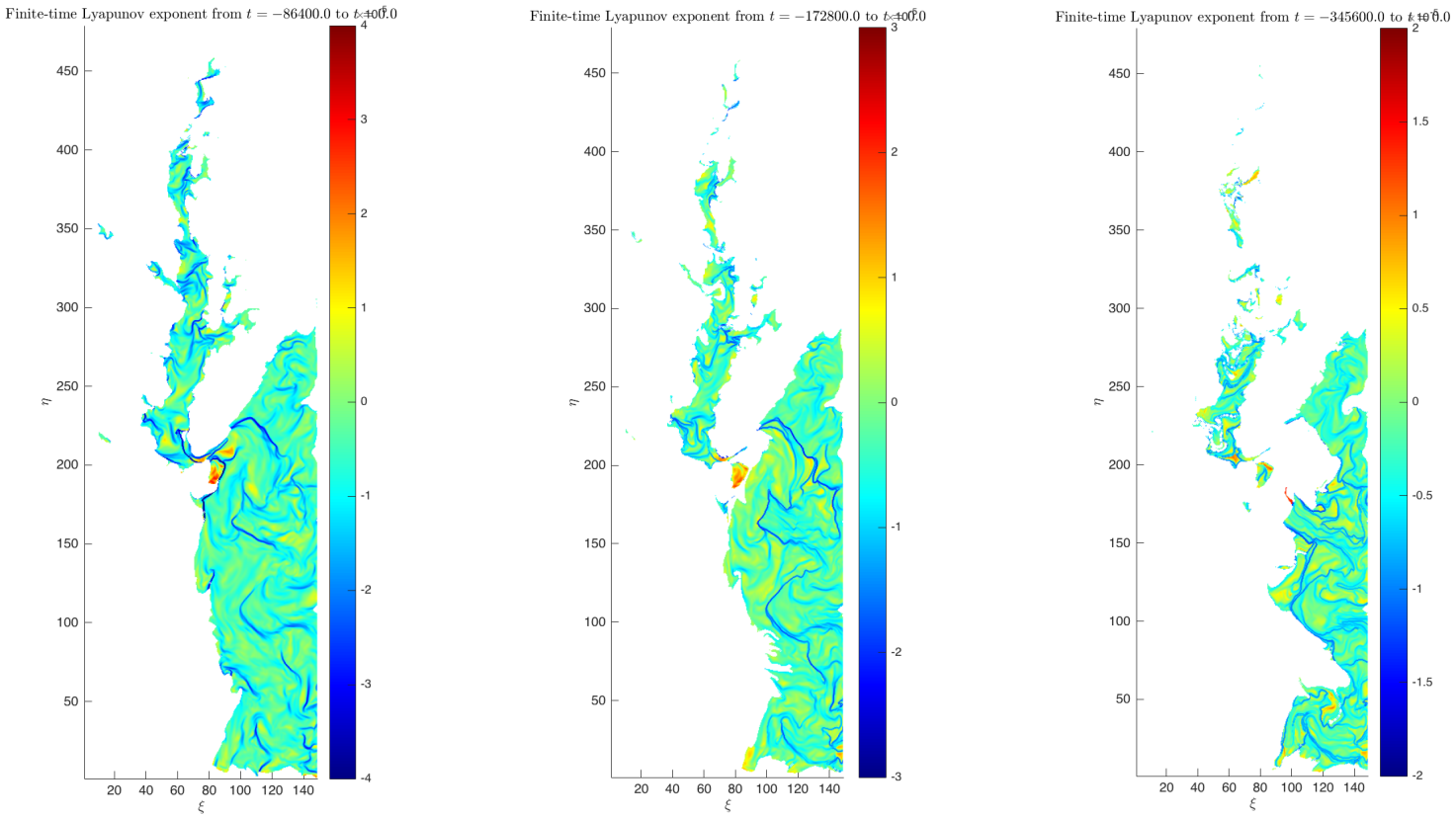
Application: Chesapeake Bay ROMS Dataset

Average speed in m/s, $\tau \approx 1$ (left), 2 (center), and 4 (right) days, backward in time



Application: Chesapeake Bay ROMS Dataset

Average speed in m/s, $\tau \approx 1$ (left), 2 (center), and 4 (right) days, backward in time (changing scale)



Conclusions

Conclusions:

- Both M-function and FTLE reveal coherent structures in an ocean flow
- Boundaries of coherent structures given by large gradients in M, ridges and troughs of FTLE
- Boundary conditions important: some version of no-slip or free-slip preferable to nothing
- Interpretation somewhat sensitive to color scale, especially for FTLE

Timeline

- October - Mid-November
  - Project proposal presentation and paper ✓
  - 2D and 3D interpolation ✓
- Mid-November - December
  - 2D trajectory implementation and validation ✓
  - M function implementation and validation ✓
  - Mid-year report and presentation ✓
- January - February
  - 3D trajectory implementation and validation (mostly)
  - FTLE implementation ✓
  - Tailor all existing code to work with ROMS data (mostly)
- March - April
  - Apply tools to Chesapeake ROMS dataset (mostly)
  - Final presentation and paper (in progress)

References

[1] Georg Duffing. *Erzwungene Schwingungen bei veränderlicher Eigenfrequenz und ihre technische Bedeutung*. Number 41-42. R, Vieweg & Sohn, 1918.

[2] Micaiah John Muller Hill. On a spherical vortex. *Proceedings of the Royal Society of London*, 55(331-335):219–224, 1894.

[3] Ana M Mancho, Stephen Wiggins, Jezabel Curbelo, and Carolina Mendoza. Lagrangian descriptors: A method for revealing phase space structures of general time dependent dynamical systems. *Communications in Nonlinear Science and Numerical Simulation*, 18(12):3530–3557, 2013.

[4] Carolina Mendoza and Ana M Mancho. Hidden geometry of ocean flows. *Physical review letters*, 105(3):038501, 2010.

[5] Alvaro H Salas. Exact solution to duffing equation and the pendulum equation. *Applied Mathematical Sciences*, 8(176):8781–8789, 2014.