Lagrangian Data Assimilation and Manifold Detection for a Point-Vortex Model

Mid-year Progress Report

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Today's Presentation

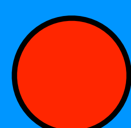
Background

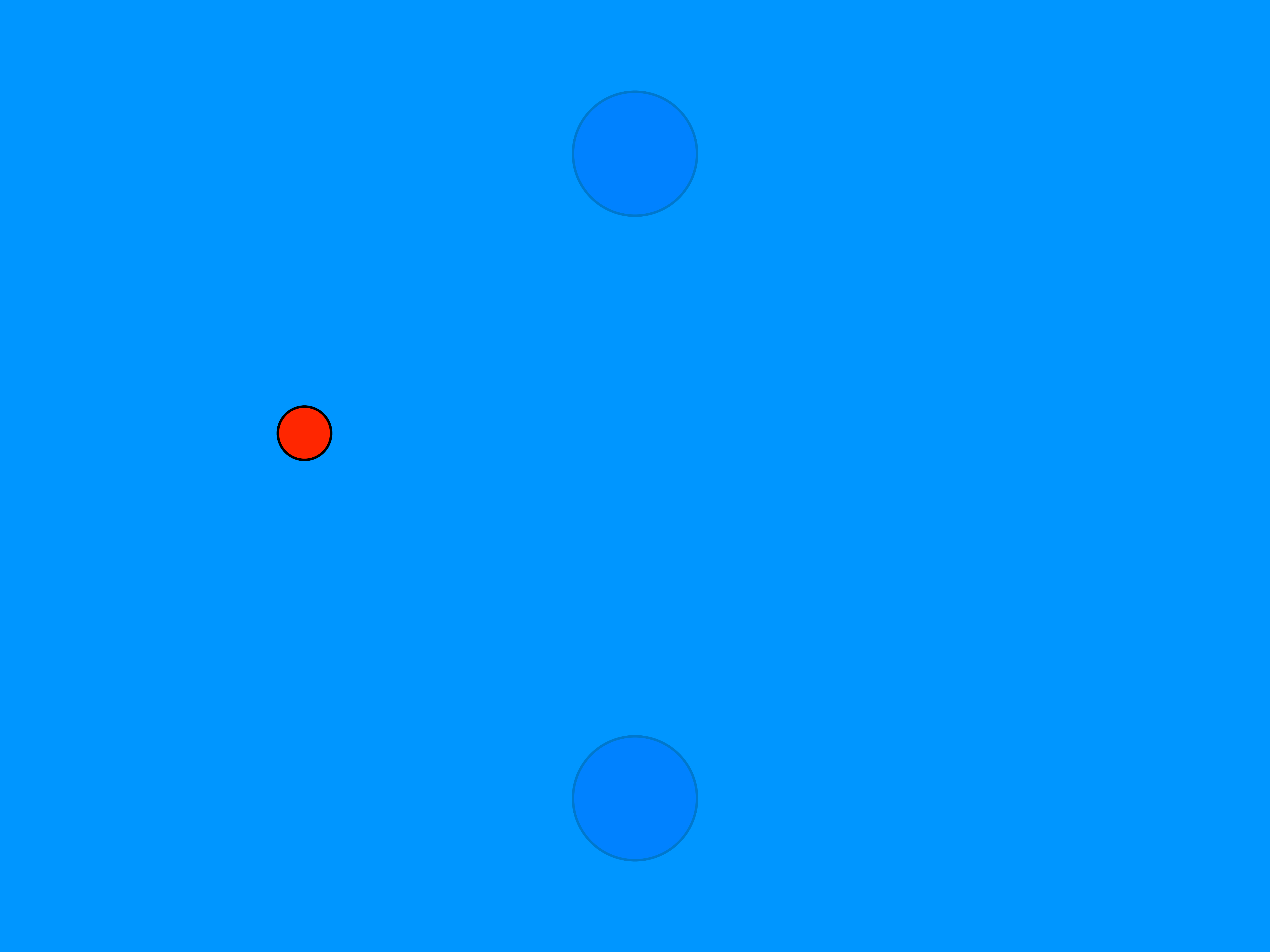
Database Generation

The EKF, Validation and Testing

The EnKF, Validation and Testing

Moving Forward

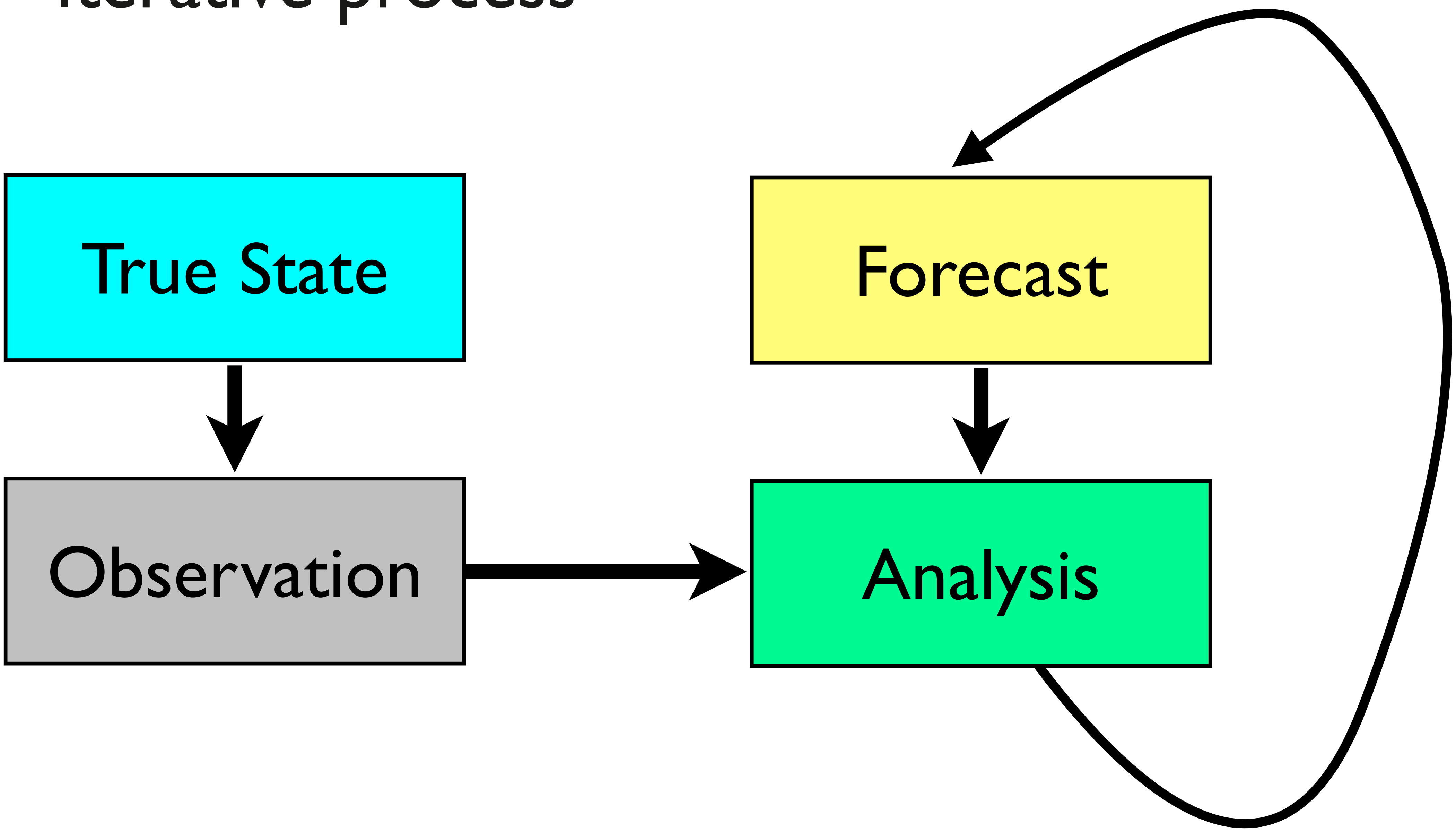




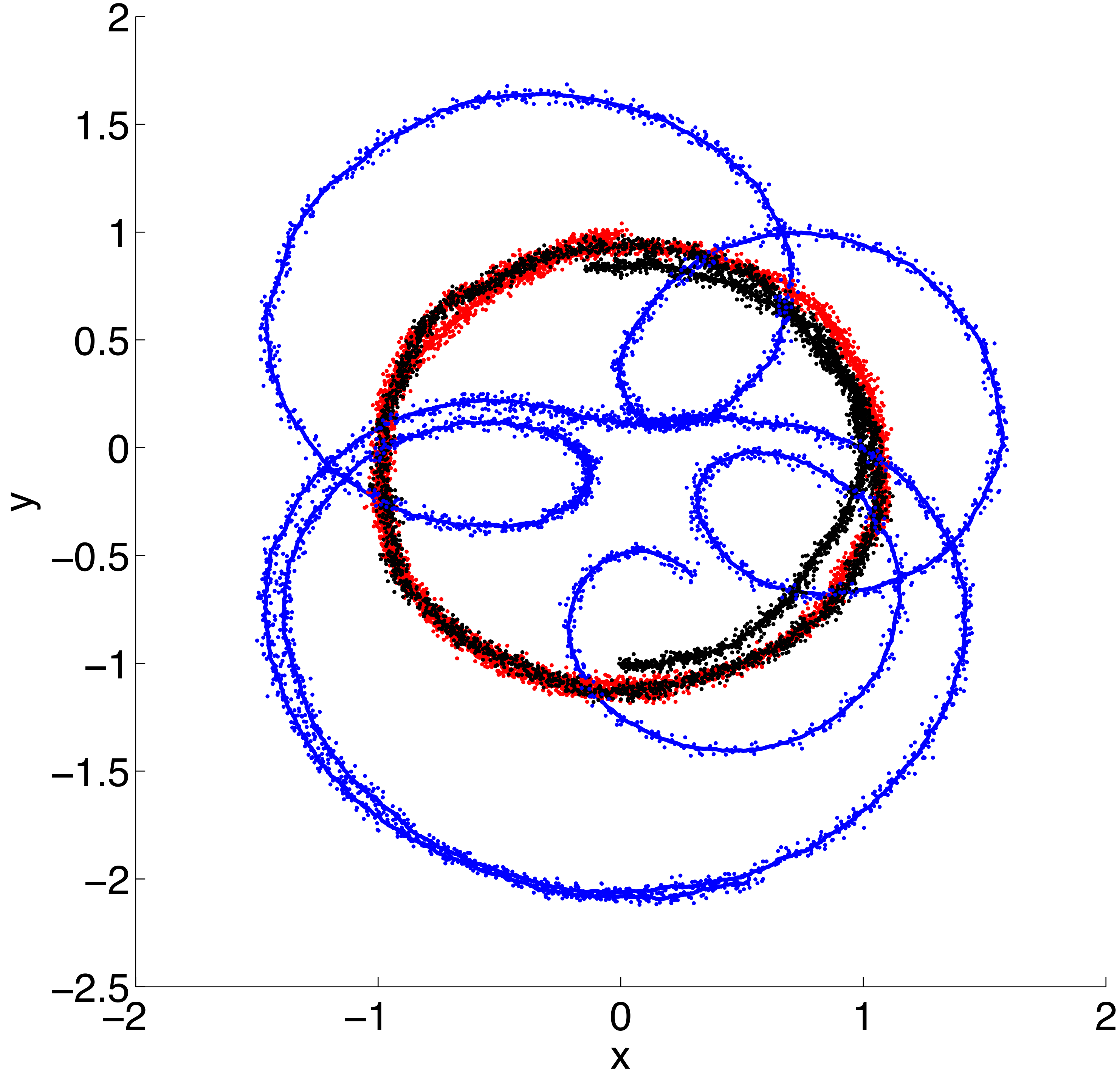
Background

Data Assimilation

Iterative process



Database Generation



Database Generation

True System Dynamics

$$d\mathbf{x}^t = M(\mathbf{x}^t, t)dt + d\boldsymbol{\eta}^t$$

$\mathbf{x}^t$ – system state

$\boldsymbol{\eta}^t$ – Brownian motion

$M(\cdot,\cdot)$ – deterministic evolution operator

Database Generation

Deterministic Dynamics

Point-Vortices

$$\frac{dx_i}{dt} = -\frac{1}{2\pi} \sum_{i'=1, i' \neq i}^{N_v} \frac{\Gamma_{i'}(y_i - y_{i'})}{l_{ii'}^2}$$

$$\frac{dy_i}{dt} = \frac{1}{2\pi} \sum_{i'=1, i' \neq i}^{N_v} \frac{\Gamma_{i'}(x_i - x_{i'})}{l_{ii'}^2}$$

$$l_{ii'}^2 = (x_i - x_{i'})^2 + (y_i - y_{i'}^2)$$

Database Generation

Deterministic Dynamics

Drifters

$$\frac{d\xi_i}{dt} = -\frac{1}{2\pi}\sum_{j=1}^{N_v}\frac{\Gamma_j(\eta_i - y_j)}{l_{ij}^2}$$

$$\frac{d\eta_i}{dt} = \frac{1}{2\pi}\sum_{j=1}^{N_v}\frac{\Gamma_j(\xi_i - x_j)}{l_{ij}^2}$$

$$l_{ij}^2 = (\xi_i - x_j)^2 + (\eta_i - y_j^2)$$

Database Generation

Scalar vs. Vector Case

Stochastic Differential Equation

$$dX(t) = f(X(t), t)dt + g(X(t), t)dW(t)$$
$$X(0) = X_0, 0 \leq t \leq T$$

$$d\mathbf{x}^t(t) = M(\mathbf{x}^t(t), t)dt + d\boldsymbol{\eta}^t(t)$$
$$\mathbf{x}^t(0) = \mathbf{x}_0^t, 0 \leq t \leq T$$

Database Generation

Numerical Solution

Runge-Kutta

$$h(X_j, \tau_j) = \left[f(X_j, \tau_j) - \frac{1}{2} g(X_j, \tau_j) \frac{\partial g(X_j, \tau_j)}{\partial X_j} \right] \Delta\tau + g(X_j, \tau_j)(W(\tau_j) - W(\tau_{j-1}))$$

Database Generation

Numerical Solution

Runge-Kutta

$$K_1 = h(X_j, \tau_j)$$

$$K_2 = h(X_j + \frac{1}{2}K_1, \tau_j + \frac{1}{2}\Delta\tau)$$

$$K_3 = h(X_j + \frac{1}{2}K_2, \tau_j + \frac{1}{2}\Delta\tau)$$

$$K_4 = h(X_j + K_3, \tau_j + \Delta\tau)$$

$$X_{j+1} = X_j + \frac{1}{6}(K_1 + 2K_2 + 2K_3 + K_4)$$

Database Generation

Numerical Solution

Runge-Kutta

$$K_1 = h(X_j, \tau_j)$$

$$K_2 = h(X_j + \frac{1}{2}K_1, \tau_j + \frac{1}{2}\Delta\tau)$$

$$K_3 = h(X_j + \frac{1}{2}K_2, \tau_j + \frac{1}{2}\Delta\tau)$$

$$K_4 = h(X_j + K_3, \tau_j + \Delta\tau)$$

$$\boxed{X_{j+1} = X_j + \frac{1}{6}(K_1 + 2K_2 + 2K_3 + K_4)}$$

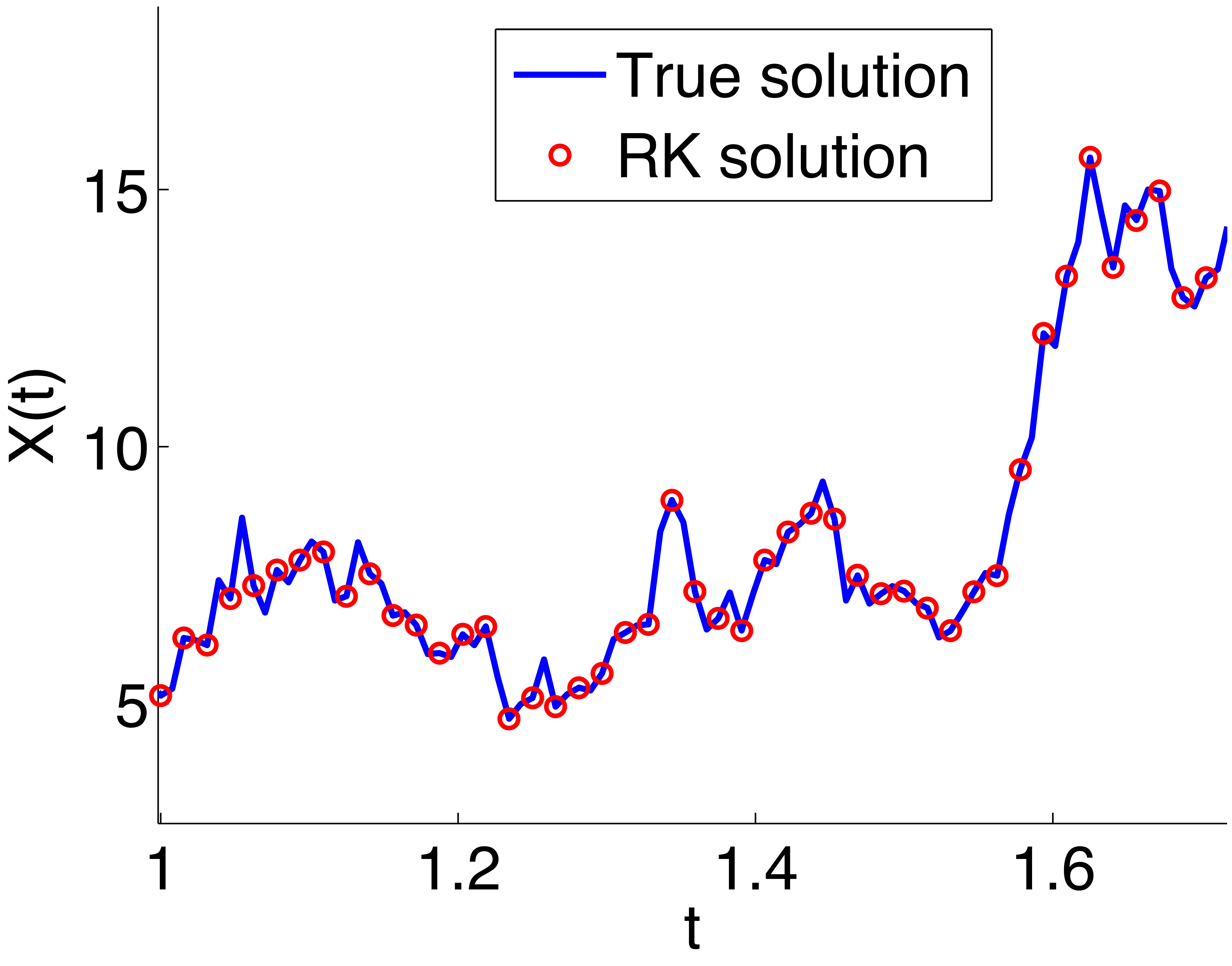
Database Generation

Simple Scalar Case

Validation

$$dX(t) = \lambda X(t)dt + \mu X(t)dW(t)$$
$$X(0) = X_0$$

$$X(t) = X_0 \exp\left[\left(\lambda - \frac{1}{2}\mu^2\right)t + \mu W(t)\right]$$



True solution
RK solution
X(t)
t
5
10
15
1
1.2
1.4
1.6

Database Generation

True Dynamics

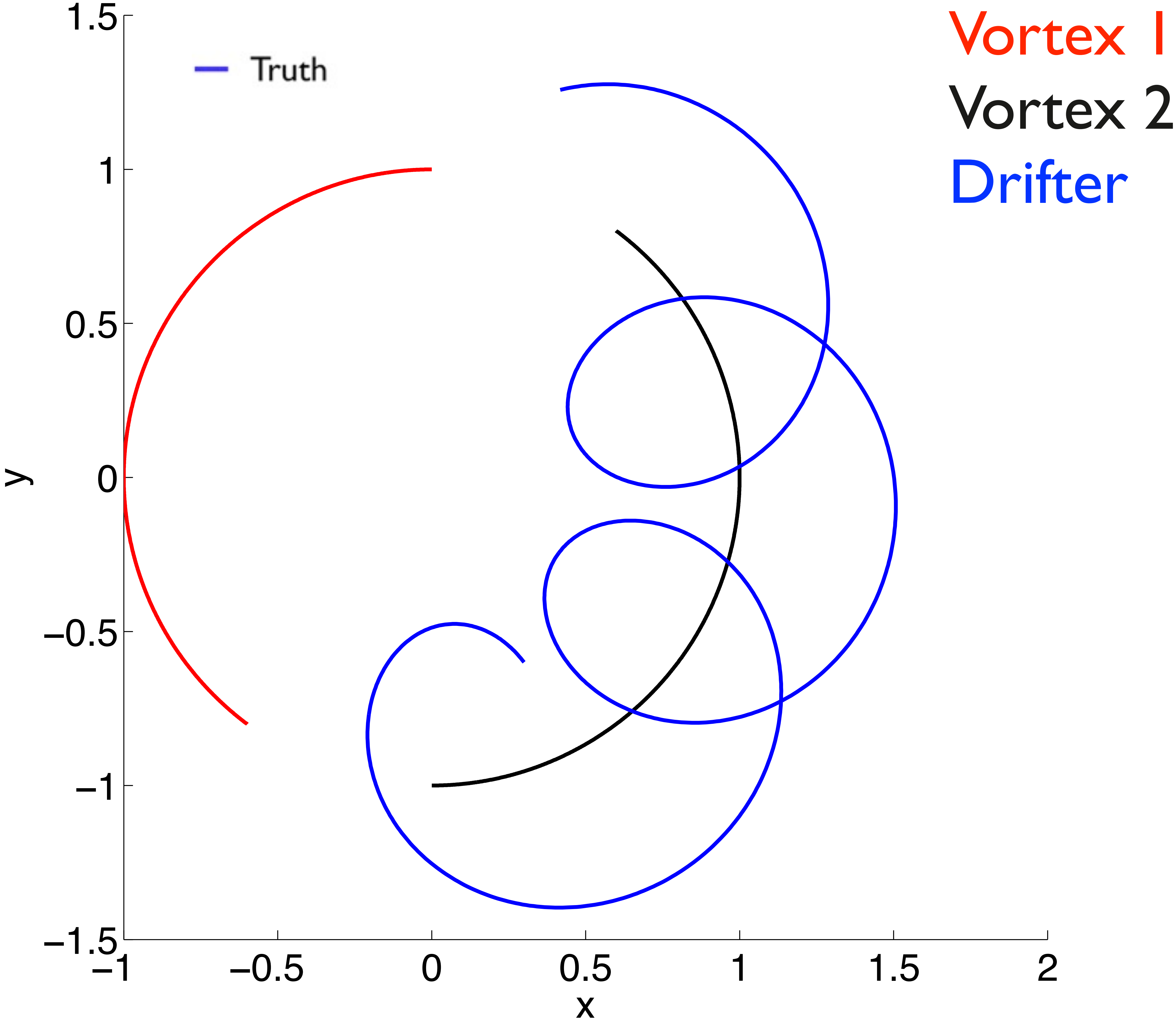
Stochastic Differential Equation

$$d\mathbf{x}^t = M(\mathbf{x}^t, t)dt + d\boldsymbol{\eta}^t$$

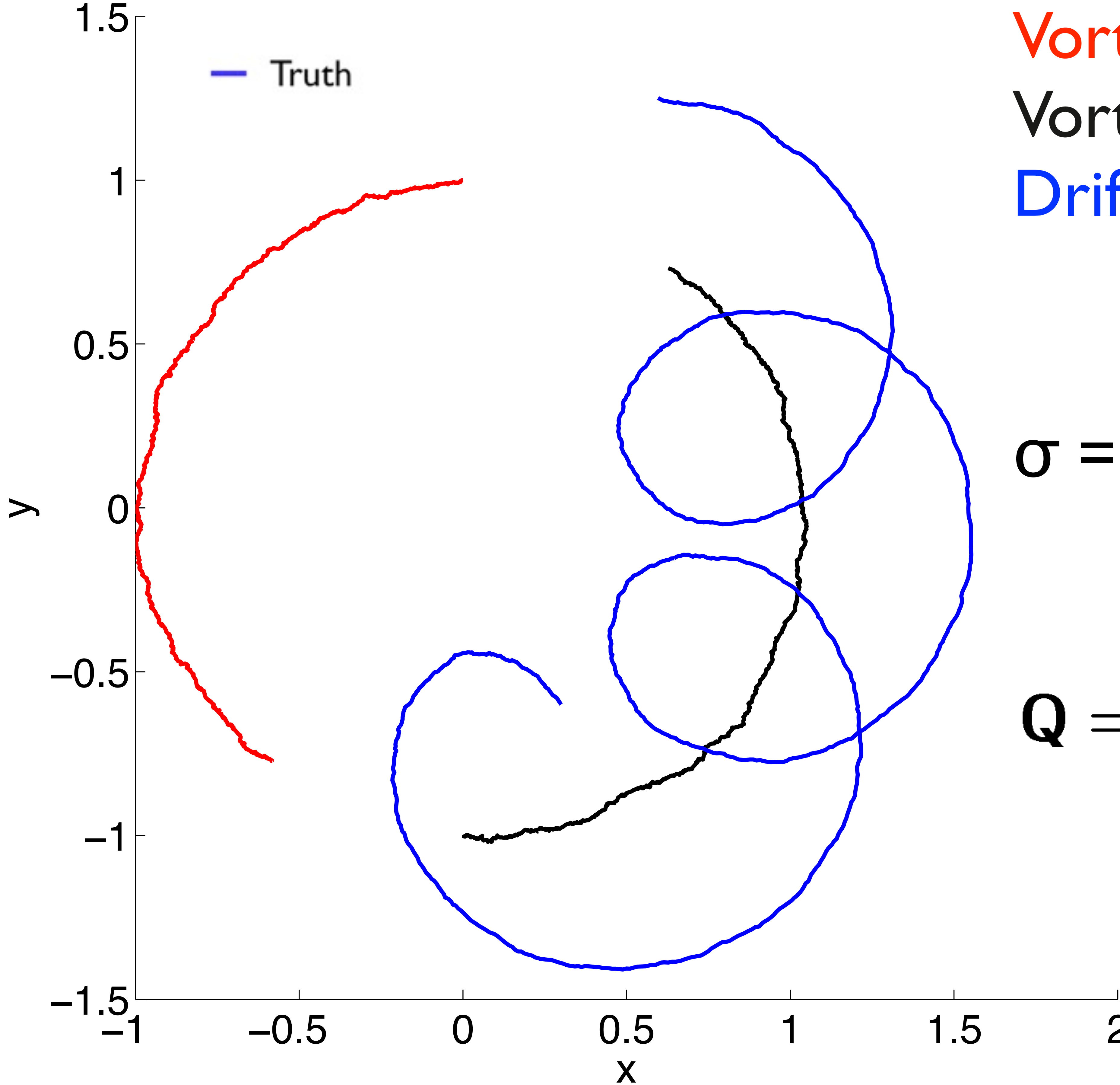
$$d\mathbf{X} = \mathbf{f}(\mathbf{X}, t)dt + \mathbf{g}(\mathbf{X}, t)d\mathbf{W}(t)$$

$$\mathbf{f}(\mathbf{x}^t, t) = M(\mathbf{x}^t, t)$$

$$\mathbf{g}(\mathbf{x}^t, t) = \sqrt{2}\mathbf{Q}^{1/2}$$



Truth
Vortex 1
Vortex 2
Drifter
1.5
1
0.5
0
−0.5
−1
−1.5
y
−1
−0.5
0
0.5
1
1.5
2
x



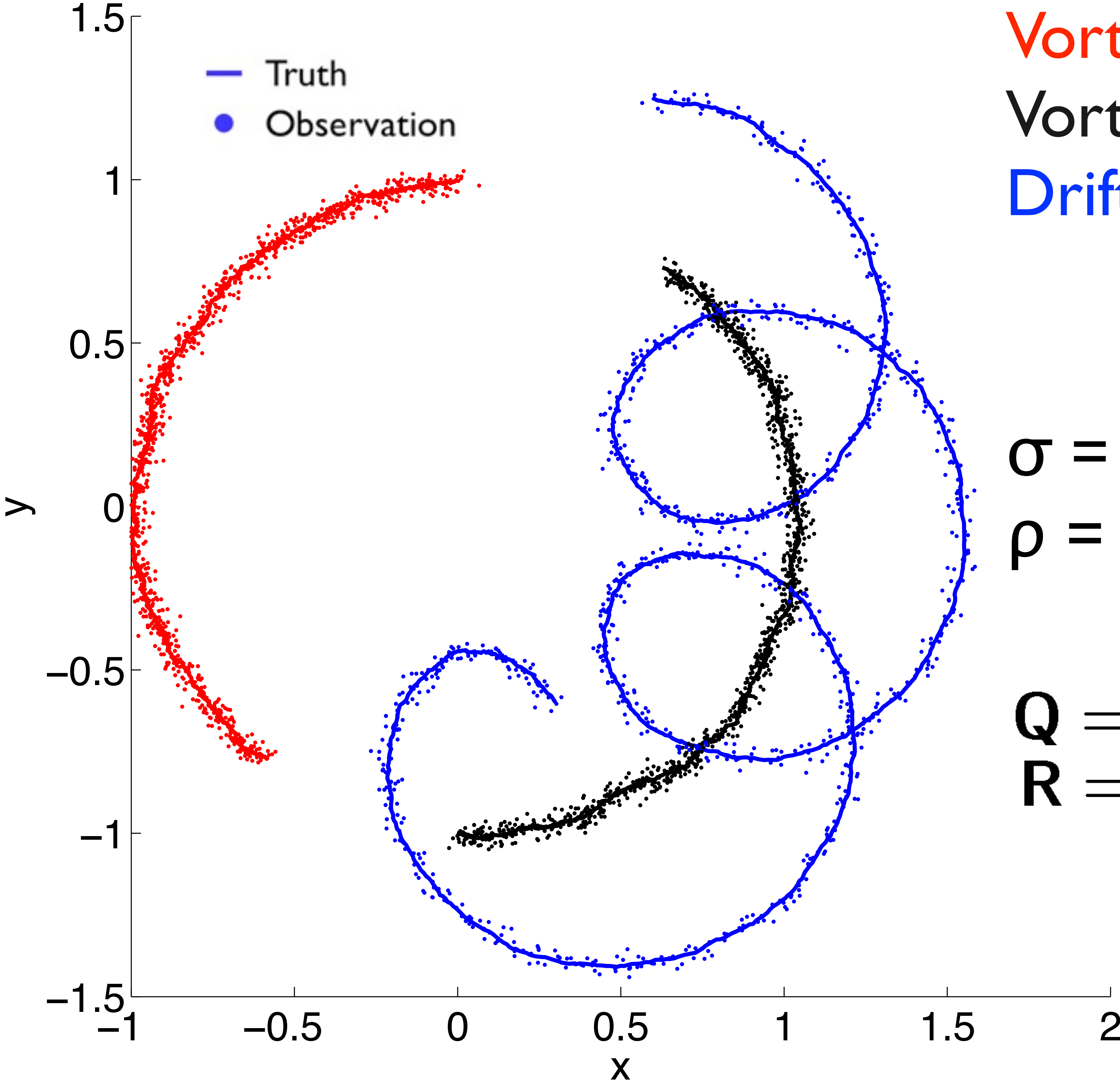
Vortex 1

Vortex 2

Drifter

$\sigma = 0.02$

$$\mathbf{Q} = 2\sigma^2 \mathbf{I}$$

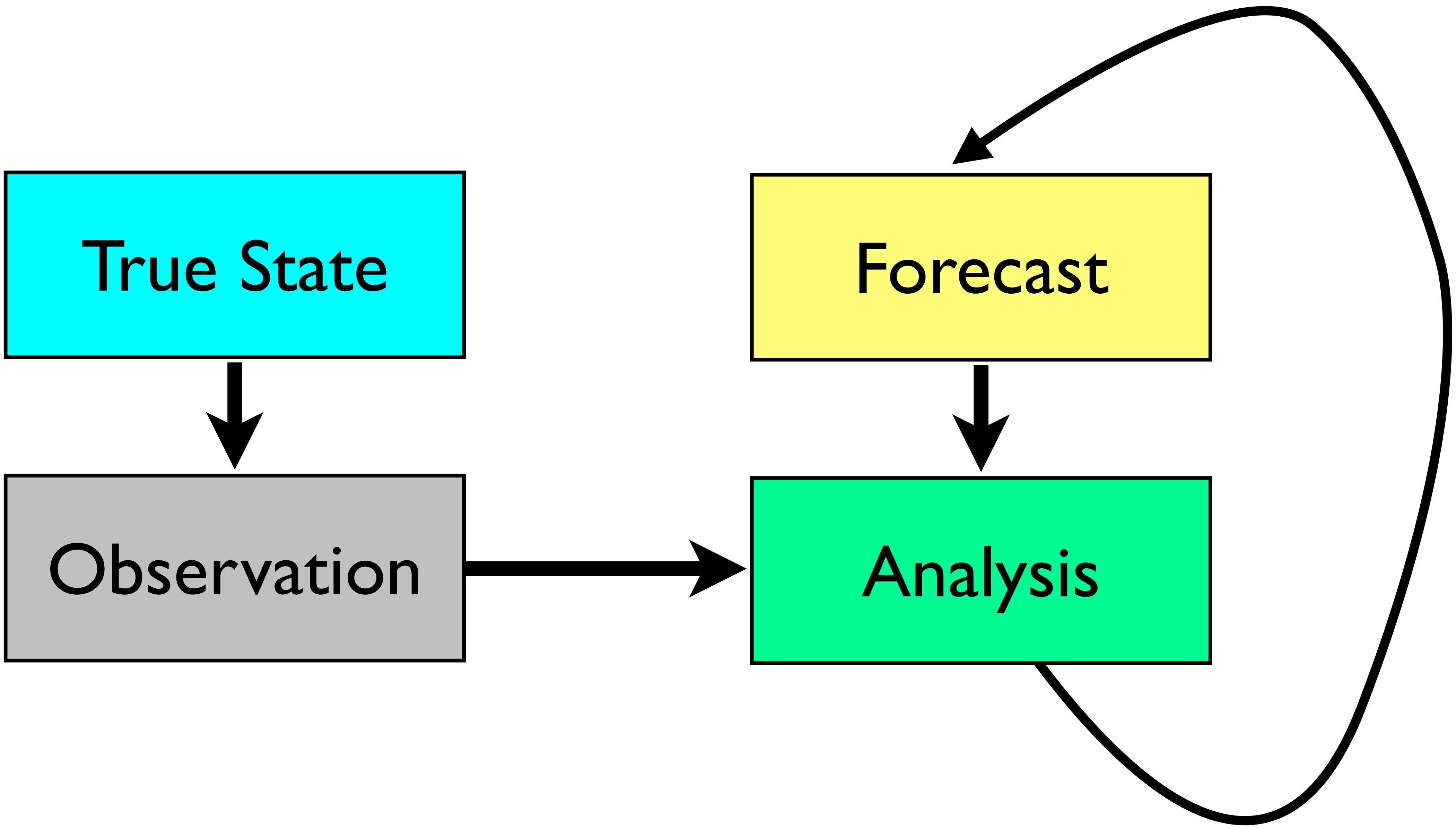


Vortex 1
Vortex 2
Drifter

σ = 0.02
ρ = 0.02

$$\mathbf{Q} = 2\sigma^2\mathbf{I}$$
$$\mathbf{R} = \rho^2\mathbf{I}$$

Data Assimilation



Data Assimilation

Approach 1:
EKF

Approach 1

Extended Kalman Filter (EKF), Forecast

$$\frac{d}{dt}\mathbf{x}^f = M(\mathbf{x}^f, t)$$

$$\frac{d}{dt}\mathbf{P}^f = \mathbf{M}(t)\mathbf{P}^f + \mathbf{P}^f\mathbf{M}^T(t) + \mathbf{Q}$$

$\mathbf{Q}$ – covariance matrix from SDE

$\mathbf{M}(t) = J[M(\mathbf{x}, t)]\big|_{x=x^f}$ - Jacobian of M

Approach 1

Extended Kalman Filter (EKF)

Validation - Jacobian via Tangent Linear Model

$\mathbf{x}_1$ - Reference Trajectory

$\mathbf{x}_2$ - Perturbed Trajectory

Approach 1

Extended Kalman Filter (EKF)

Validation - Jacobian via Tangent Linear Model

$\mathbf{x}_1$ - Reference Trajectory

$\mathbf{x}_2$ - Perturbed Trajectory

$$\mathbf{x}_1(0) = \mathbf{x}^0$$
$$\mathbf{x}_2(0) = \mathbf{x}^0 + \mathbf{y}^0$$

Approach 1

Extended Kalman Filter (EKF)

Validation - Jacobian via Tangent Linear Model

$\mathbf{x}_1$ - Reference Trajectory

$\mathbf{x}_2$ - Perturbed Trajectory

$$\mathbf{x}_1(0) = \mathbf{x}^0$$
$$\mathbf{x}_2(0) = \mathbf{x}^0 + \mathbf{y}^0$$

↑

Tangent Vector (small)

Approach 1

Extended Kalman Filter (EKF)

Validation - Jacobian via Tangent Linear Model

$$\frac{d\mathbf{y}}{dt} = \left.\frac{\partial M(\mathbf{x})}{\partial \mathbf{x}}\right|_{\mathrm{x}=\mathrm{x}(t)} \mathbf{y}$$

$$= \mathbf{M}(\mathbf{x}(t))\mathbf{y}$$

Approach 1

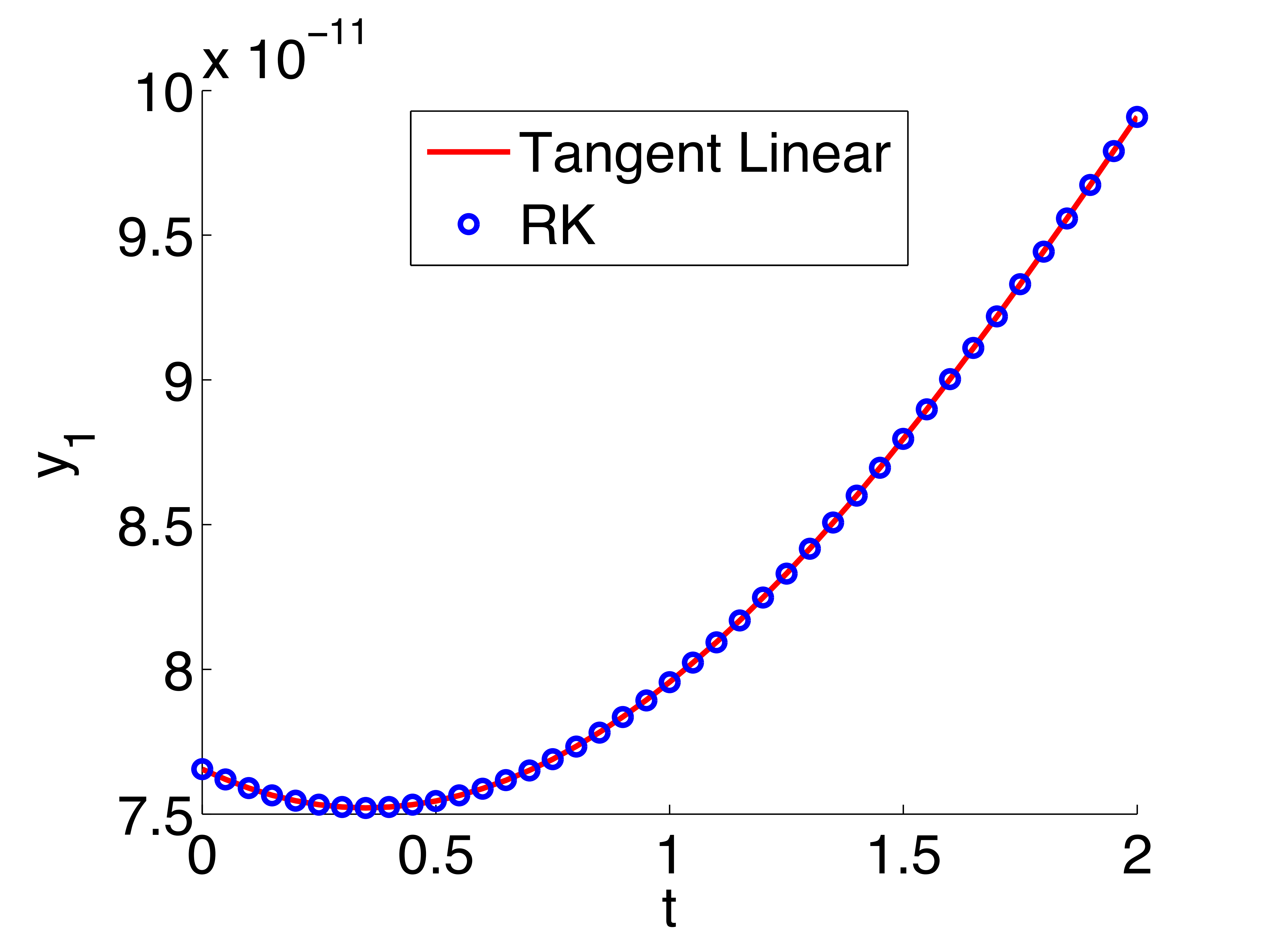
Extended Kalman Filter (EKF)

Validation - Jacobian via Tangent Linear Model

Evolve reference and perturbed trajectories forward using deterministic ODE

Evolve tangent vector forward using Tangent Linear Model

Compare $\mathbf{y}_{\text{perturbed}}$ and $\mathbf{y}_{\text{TL}}$


x 10^−11
10
9.5
9
8.5
8
7.5
y_1
Tangent Linear
RK
0
0.5
1
1.5
2
t

Approach 1

Extended Kalman Filter (EKF), Analysis

$$\mathbf{x}_k^a = \mathbf{x}^f(t_k) + \mathbf{K}_k(\mathbf{y}_k^o - h_k(\mathbf{x}^f(t_k)))$$

$$\mathbf{P}_k^a = (\mathbf{I} - \mathbf{K}_k\mathbf{H}_k)\mathbf{P}^f(t_k)$$

$$\mathbf{K}_k = \mathbf{P}^f(t_k)\mathbf{H}_k^T(\mathbf{H}_k\mathbf{P}^f(t_k)\mathbf{H}_k^T + \mathbf{R}_k^o)^{-1}$$

$\mathbf{R}^o$ – covariance matrix from observation

$\mathbf{H}_k = J[h(\mathbf{x}, t_k)]\Big|_{x=x^f}$ - Jacobian of h_k

Approach 1

Extended Kalman Filter (EKF)

Validation - No Noise

$$\mathbf{x}_k^a = \mathbf{x}^f(t_k) + \mathbf{K}_k(\mathbf{y}_k^o - h_k(\mathbf{x}^f(t_k)))$$

$$\mathbf{P}_k^a = (\mathbf{I} - \mathbf{K}_k\mathbf{H}_k)\mathbf{P}^f(t_k)$$

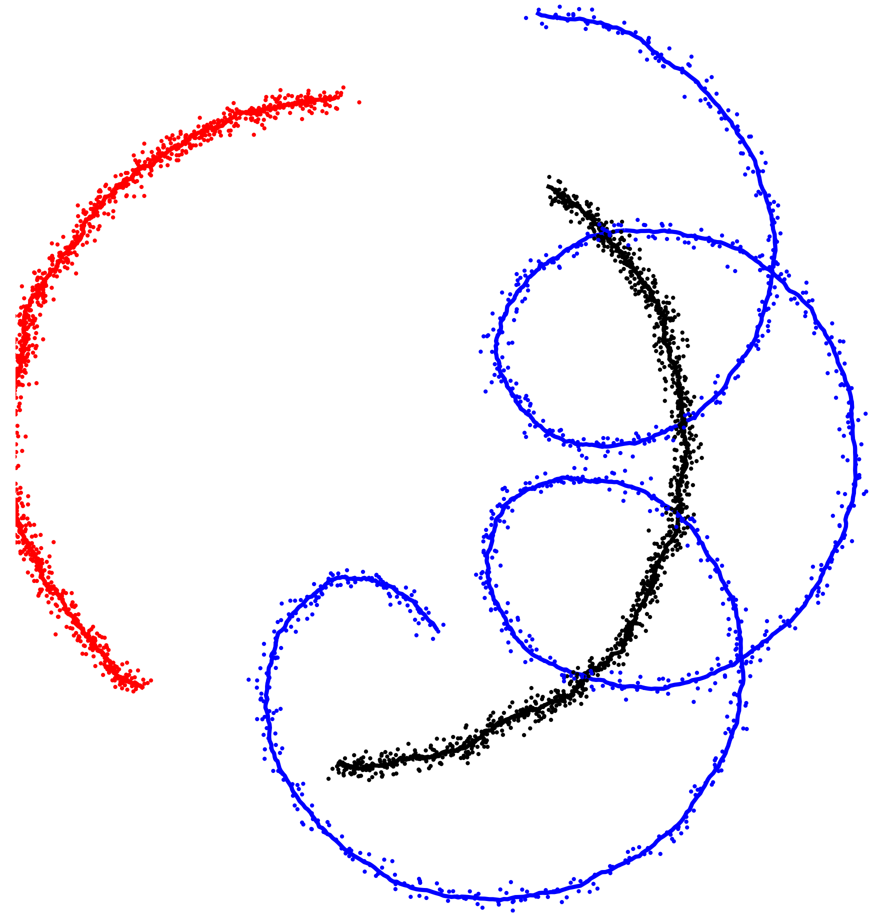
$$\mathbf{K}_k = \mathbf{P}^f(t_k)\mathbf{H}_k^T(\mathbf{H}_k\mathbf{P}^f(t_k)\mathbf{H}_k^T + \mathbf{R}_k^o)^{-1}$$

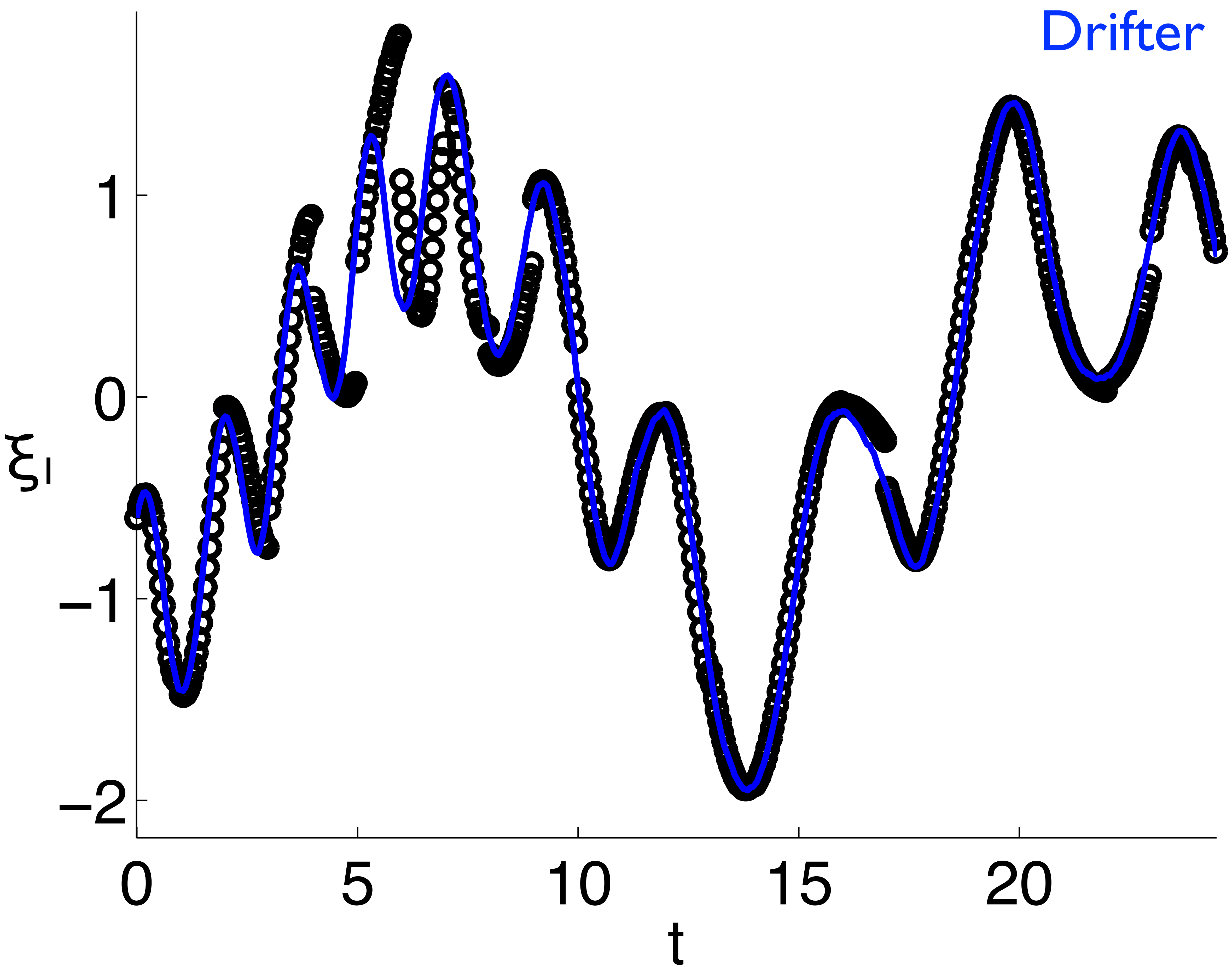
Approach 1

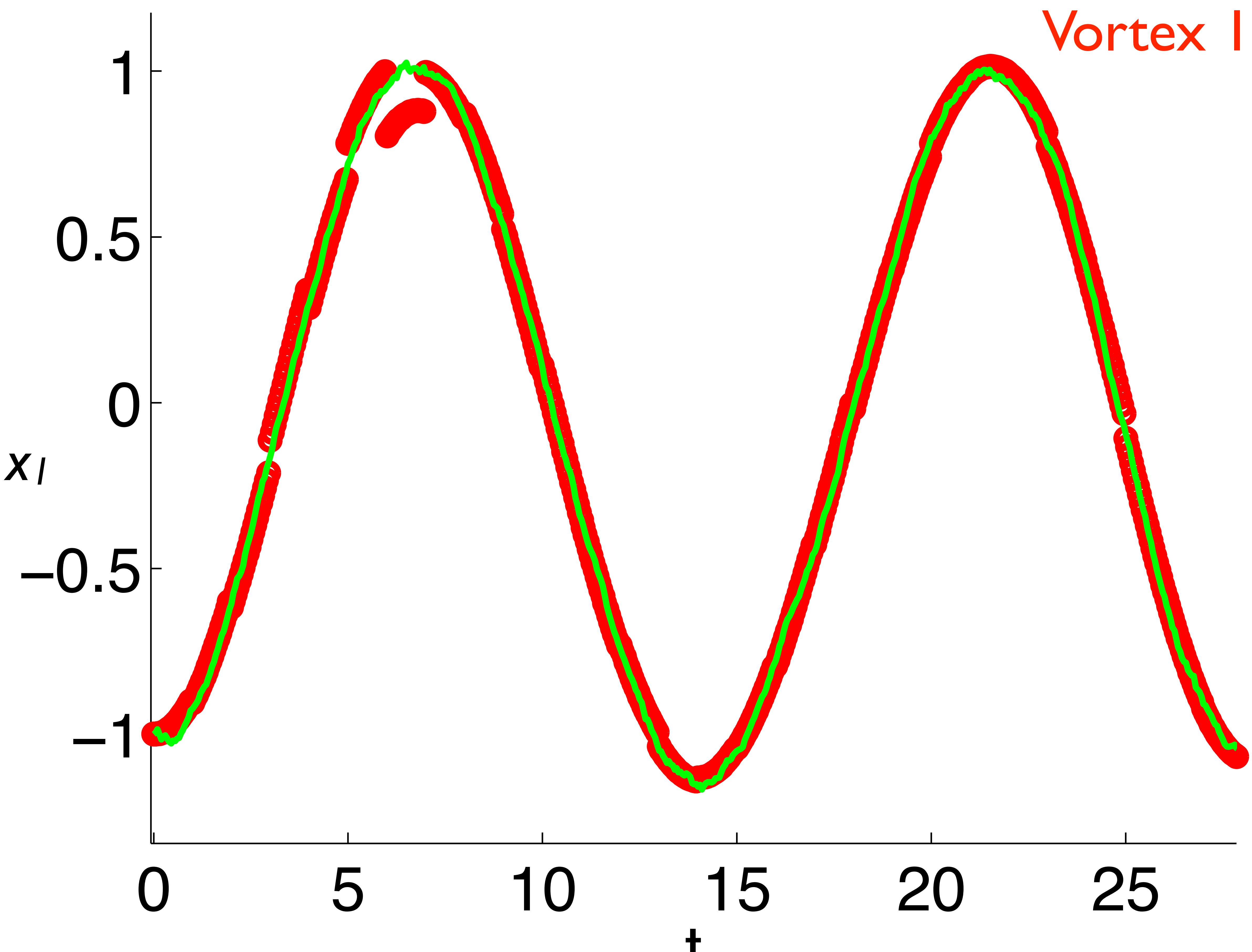
Extended Kalman Filter (EKF)

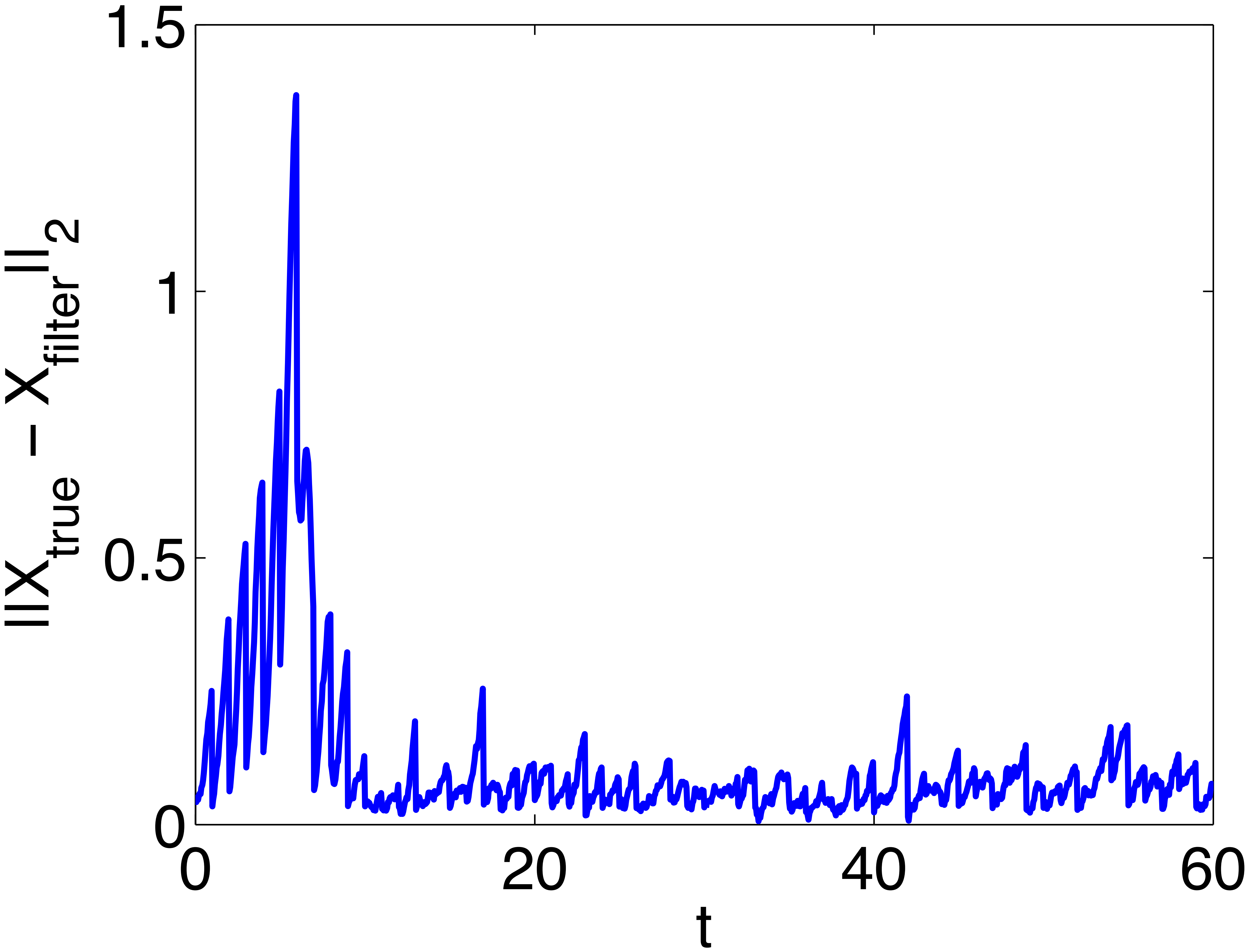
Validation - Full Observation, Imperfect Data

Observe vortices and drifter under observational noise




Drifter
1
0
−1
−2
0
5
10
15
20
t
ξ


Vortex 1
1
0.5
0
−0.5
−1
x_I
0
5
10
15
20
25
t



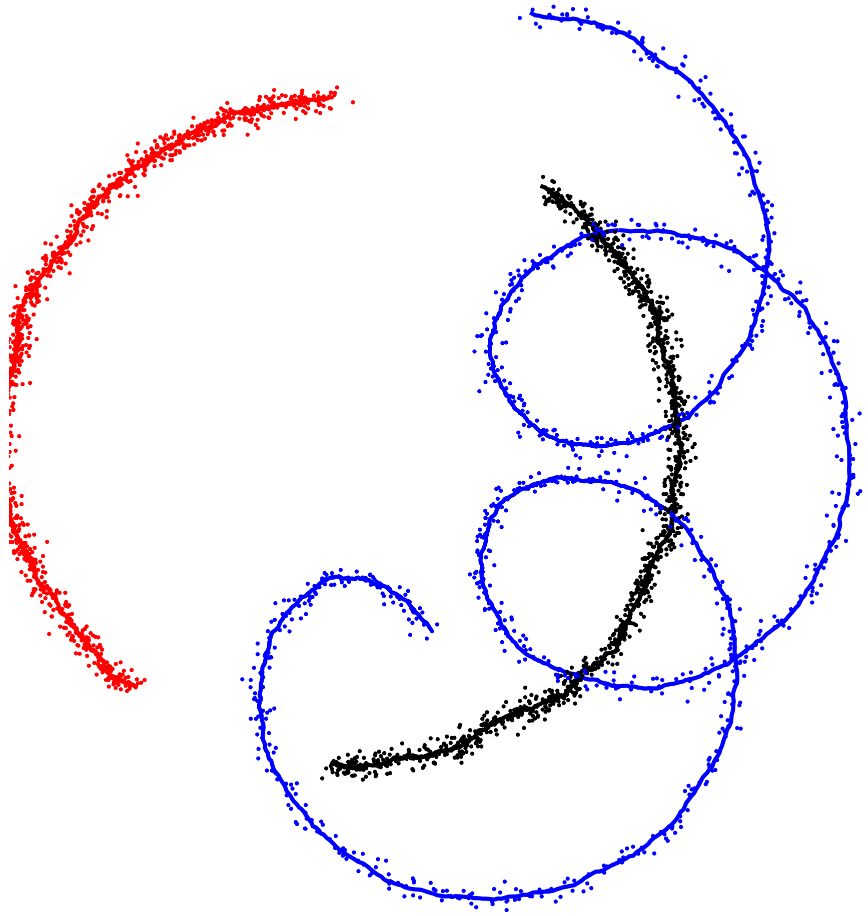
1.5
1
0.5
0
0
20
40
60
t
$||X_{true} - X_{filter}||_2$

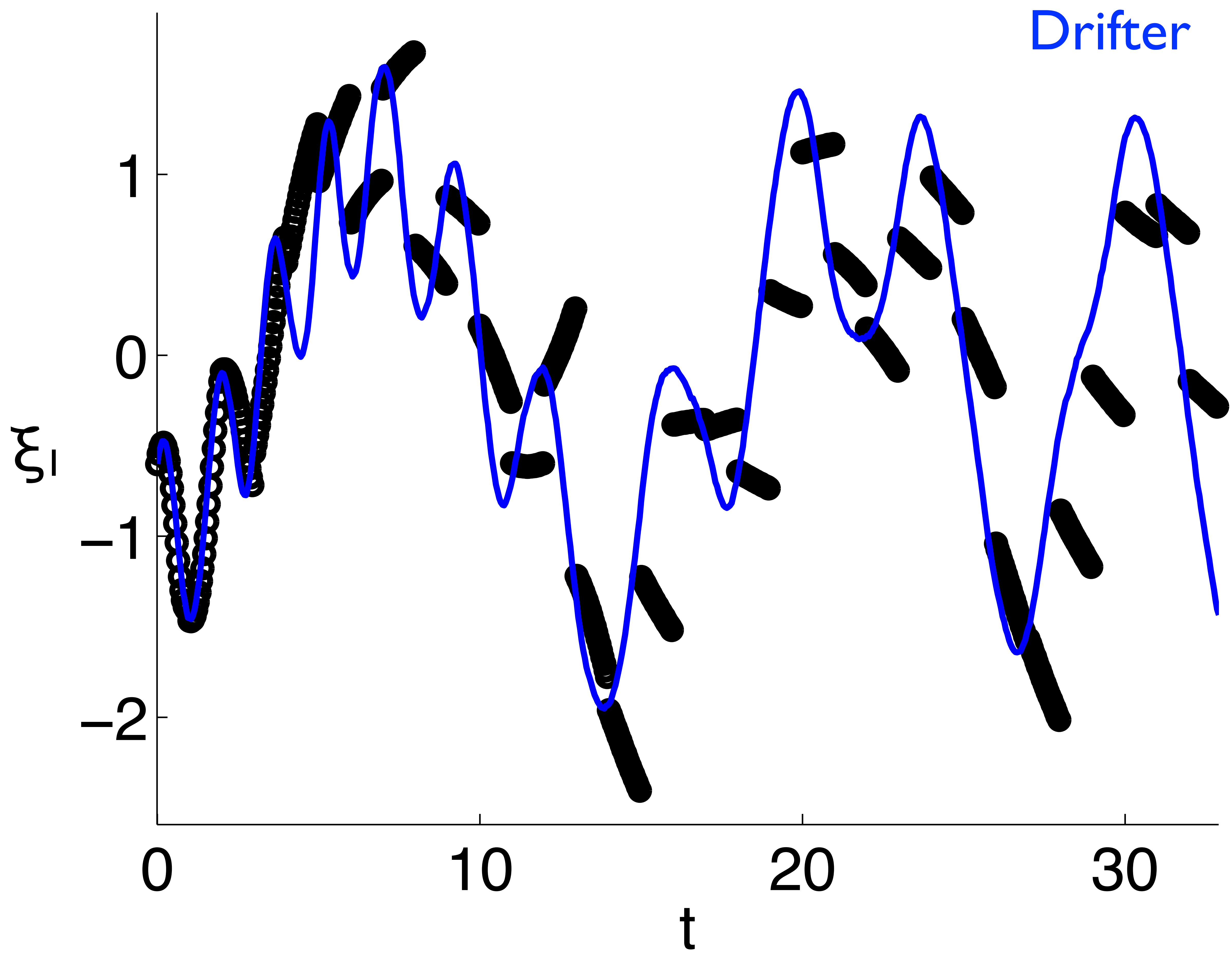
Approach 1

Extended Kalman Filter (EKF)

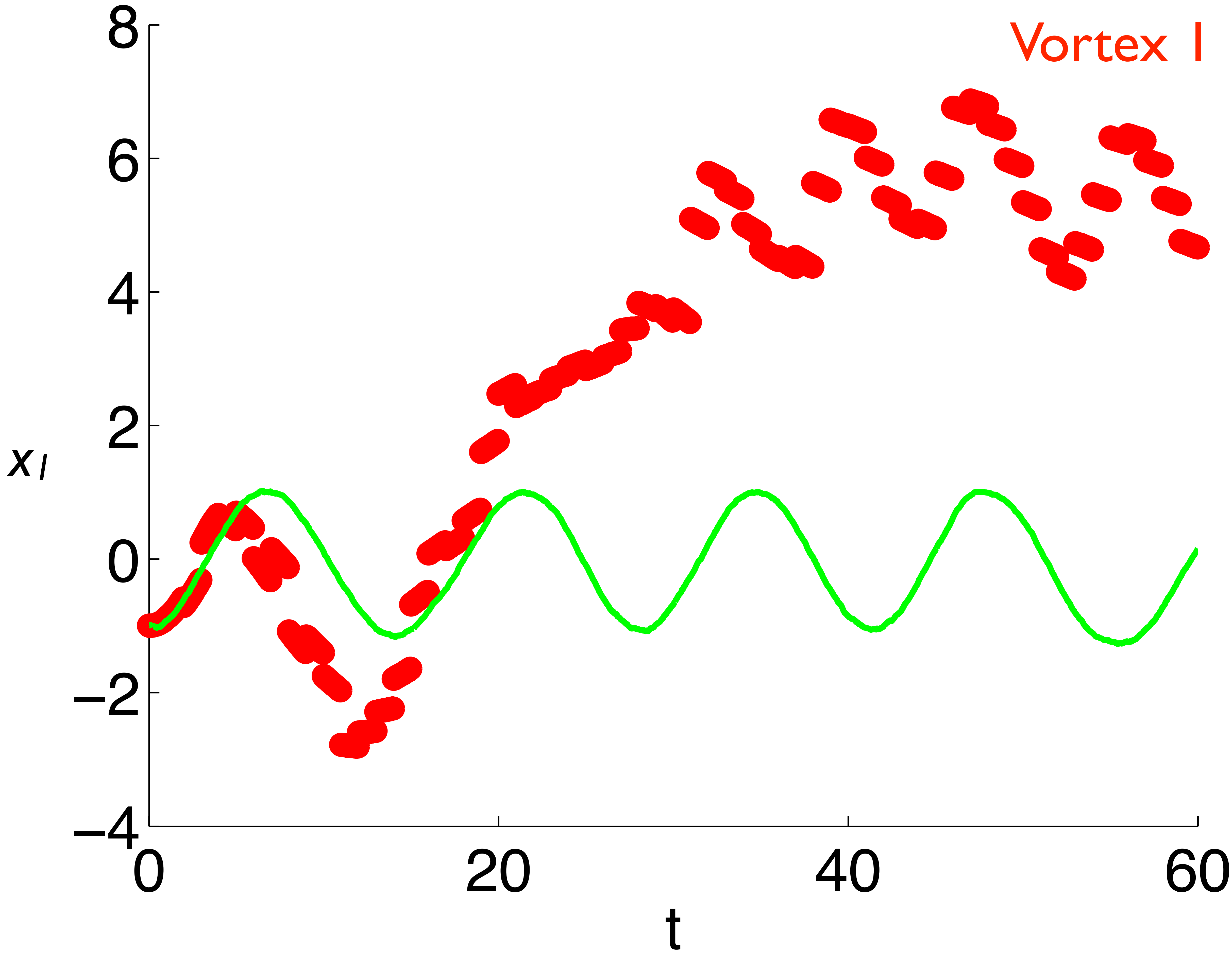
Results - Partial Observation, Imperfect Data

Observe only drifter under observational noise

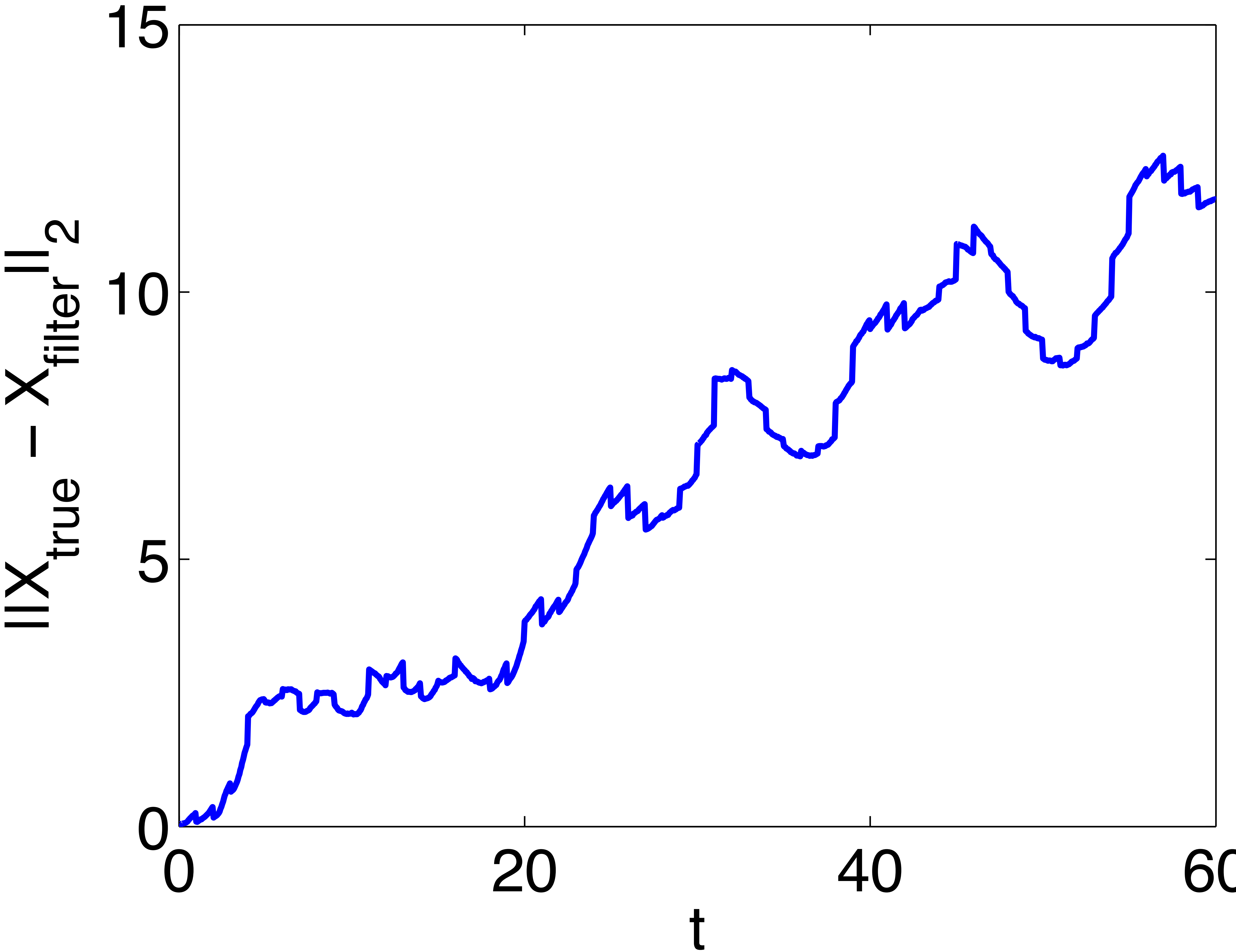




Drifter
1
0
−1
−2
ξ
0
10
20
30
t



Vortex 1
8
6
4
2
0
−2
−4
x_1
0
20
40
60
t



15
10
5
0
0
20
40
60
t
||X_true − X_filter||_2

Data Assimilation

Approach 1:
EnKF

Approach 2

Ensemble Kalman Filter (EnKF)

Approximate pdf by an ensemble of particles:

$$\{\mathbf{x}_i^f\}_{i=1}^N$$

Forecast: Evolve particles forward using SDE

Analysis: Perform Kalman-like analysis

Approach 2

Ensemble Kalman Filter (EnKF)

Approximate pdf by an ensemble of particles:

$$\{\mathbf{x}_i^f\}_{i=1}^N$$

Forecast: Evolve particles forward using ~~SDE~~ ODE

Analysis: Perform Kalman-like analysis

Approach 2

Ensemble Kalman Filter (EnKF)

Approximate pdf by an ensemble of particles:

$$\{\mathbf{x}_i^f\}_{i=1}^N$$

Forecast: Evolve particles forward using ODE

Analysis: Perform Kalman-like analysis

Approach 2a

EnKF with Observational Perturbations

$$\mathbf{y}^o_{k,i} = \mathbf{y}^o_k + \epsilon_i, \qquad i = 1, \dots, n$$

$$\epsilon_i \sim N(\mathbf{0}, \mathbf{R}^o)$$

Approach 2a

EnKF with Observational Perturbations

$$\mathbf{y}^o_{k,i} = \mathbf{y}^o_k + \epsilon_i, \qquad i = 1, \ldots, n$$

$$\epsilon_i \sim N(\mathbf{0}, \mathbf{R}^o)$$

$\{\mathbf{x}^f_i\}_{i=1}^N$ Forecast ensemble

$\{\mathbf{y}^o_{k,i}\}_{i=1}^N$ Observation ensemble

Approach 2a

EnKF with Observational Perturbations

Kalman-like update

$$\mathbf{x}^a_{k,i} = \mathbf{x}^f_i(t_k) + \mathbf{K}_k(\mathbf{y}^o_{k,i} - h_k(\mathbf{x}^f_i(t_k)))$$

$$\mathbf{K}_k = \mathbf{P}^f_e(t_k)\mathbf{H}^T_k(\mathbf{H}_k\mathbf{P}^f_e(t_k)\mathbf{H}^T_k + \mathbf{R}^o_k)^{-1}$$

Approach 2a

EnKF with Observational Perturbations

Kalman-like update

$$\mathbf{x}^a_{k,i} = \mathbf{x}^f_i(t_k) + \mathbf{K}_k(\mathbf{y}^o_{k,i} - h_k(\mathbf{x}^f_i(t_k)))$$

$$\mathbf{K}_k = \mathbf{P}^f_e(t_k)\mathbf{H}^T_k(\mathbf{H}_k\mathbf{P}^f_e(t_k)\mathbf{H}^T_k + \mathbf{R}^o_k)^{-1}$$

Sample Covariance Matrix

$$\mathbf{P}^f_e(t_k) = \frac{1}{N-1}\sum_{i=1}^{N}(\mathbf{x}^f_i - \bar{\mathbf{x}}^f)(\mathbf{x}^f_i - \bar{\mathbf{x}}^f)^T$$

Approach 2

Ensemble Kalman Filter (EnKF)

Approximate pdf by an ensemble of particles:

$$\{\mathbf{x}_i^f\}_{i=1}^N$$

Forecast: Evolve particles forward using ~~SDE~~ ODE

Analysis: Perform Kalman-like analysis

Approach 2b

Ensemble Transform Kalman Filter (ETKF)

$$\mathbf{x}_k^a = \mathbf{x}^f(t_k) + \mathbf{K}_k(\mathbf{y}_k^o - h_k(\mathbf{x}^f(t_k)))$$

$$\mathbf{P}_k^a = (\mathbf{I} - \mathbf{K}_k\mathbf{H}_k)\mathbf{P}^f(t_k)$$

$$\mathbf{K}_k = \mathbf{P}^f(t_k)\mathbf{H}_k^T(\mathbf{H}_k\mathbf{P}^f(t_k)\mathbf{H}_k^T + \mathbf{R}_k^o)^{-1}$$

Approach 2b

Ensemble Transform Kalman Filter (ETKF)

$$\mathbf{x}_k^a = \mathbf{x}^f(t_k) + \mathbf{K}_k(\mathbf{y}_k^o - h_k(\mathbf{x}^f(t_k)))$$

$$\mathbf{P}_k^a = (\mathbf{I} - \mathbf{K}_k\mathbf{H}_k)\mathbf{P}^f(t_k)$$

$$\mathbf{K}_k = \mathbf{P}^f(t_k)\mathbf{H}_k^T(\mathbf{H}_k\mathbf{P}^f(t_k)\mathbf{H}_k^T + \mathbf{R}_k^o)^{-1}$$

Use sample estimates:

$$\bar{\mathbf{x}}_k^a = \bar{\mathbf{x}}^f(t_k) + \mathbf{K}_{e,k}(\mathbf{y}_k^o - h_k(\bar{\mathbf{x}}^f(t_k)))$$

$$\mathbf{P}_{e,k}^a = (\mathbf{I} - \mathbf{K}_{e,k}\mathbf{H}_k)\mathbf{P}_e^f(t_k)$$

$$\mathbf{K}_{e,k} = \mathbf{P}_e^f(t_k)\mathbf{H}_k^T(\mathbf{H}_k\mathbf{P}_e^f(t_k)\mathbf{H}_k^T + \mathbf{R}_k^o)^{-1}$$

Approach 2b

Ensemble Transform Kalman Filter (ETKF)

Define

$$\mathbf{X}^f = \left[\begin{array}{cccc} \mathbf{x}_1^f - \bar{\mathbf{x}} & \mathbf{x}_2^f - \bar{\mathbf{x}} & \ldots & \mathbf{x}_n^f - \bar{\mathbf{x}} \end{array} \right]$$

Approach 2b

Ensemble Transform Kalman Filter (ETKF)

Define

$$\mathbf{X}^f = \left[\begin{array}{cccc} \mathbf{x}_1^f - \bar{\mathbf{x}} & \mathbf{x}_2^f - \bar{\mathbf{x}} & \dots & \mathbf{x}_n^f - \bar{\mathbf{x}} \end{array}\right]$$

$$\frac{1}{N-1}\mathbf{X}^f (\mathbf{X}^f)^T = \mathbf{P}_e^f$$

Approach 2b

Ensemble Transform Kalman Filter (ETKF)

Define

$$\mathbf{X}^f = \left[\begin{array}{cccc} \mathbf{x}_1^f - \bar{\mathbf{x}} & \mathbf{x}_2^f - \bar{\mathbf{x}} & \ldots & \mathbf{x}_n^f - \bar{\mathbf{x}} \end{array} \right]$$

$$\frac{1}{N-1}\mathbf{X}^f(\mathbf{X}^f)^T = \mathbf{P}_e^f$$

$$\boxed{\mathbf{X}^a = \mathbf{X}^f \mathbf{W}}$$

Approach 2b

Ensemble Transform Kalman Filter (ETKF)

Define

$$\mathbf{D} = \mathbf{W}\mathbf{W}^T$$

$\mathbf{W}$ is the *matrix square root* of $\mathbf{D}$

Choose

$$\mathbf{D} = (\mathbf{I} + (\mathbf{X}^f)^T \mathbf{H}^T (\mathbf{R}^o)^{-1} \mathbf{H}\mathbf{X}^f)^{-1}$$

Approach 2b

Ensemble Transform Kalman Filter (ETKF)

Analysis Ensemble

$$\mathbf{X}^a = \mathbf{X}^f \mathbf{W}$$

$$\bar{\mathbf{x}}^a = \bar{\mathbf{x}}^f + \mathbf{X}^f \mathbf{D} (\mathbf{X}^f)^T \mathbf{H}^T (\mathbf{R}^\circ)^{-1} (\mathbf{y}^o - \mathbf{H}\bar{\mathbf{x}}^f)$$

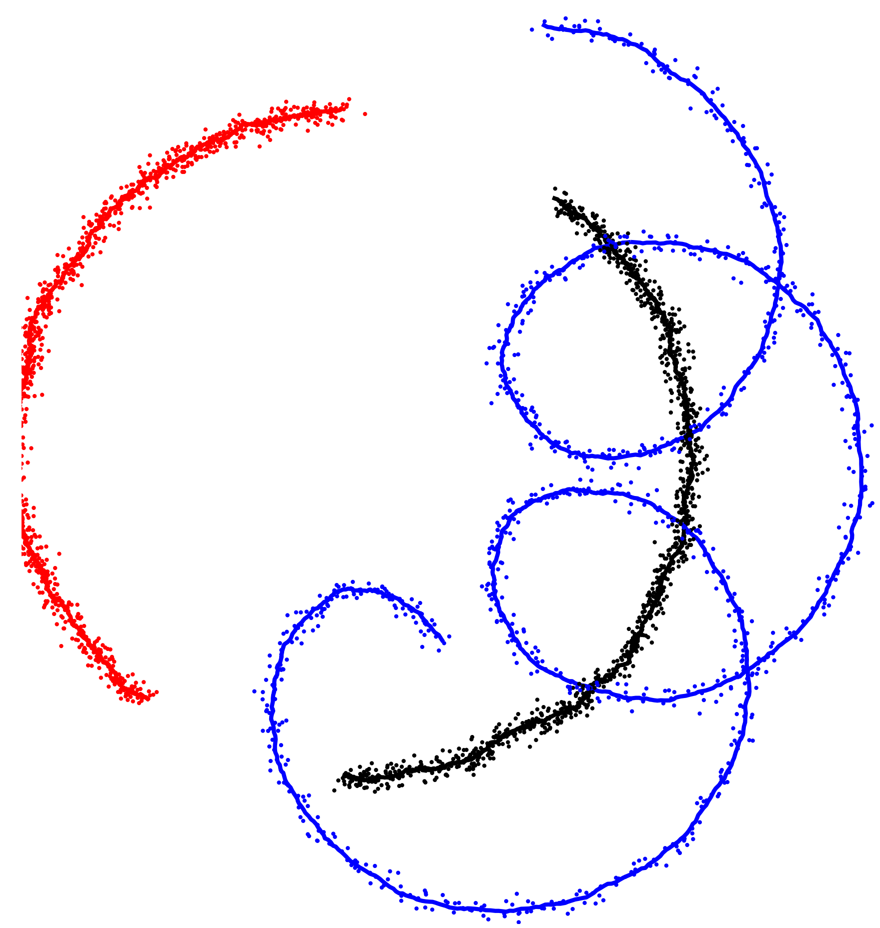
Approach 2

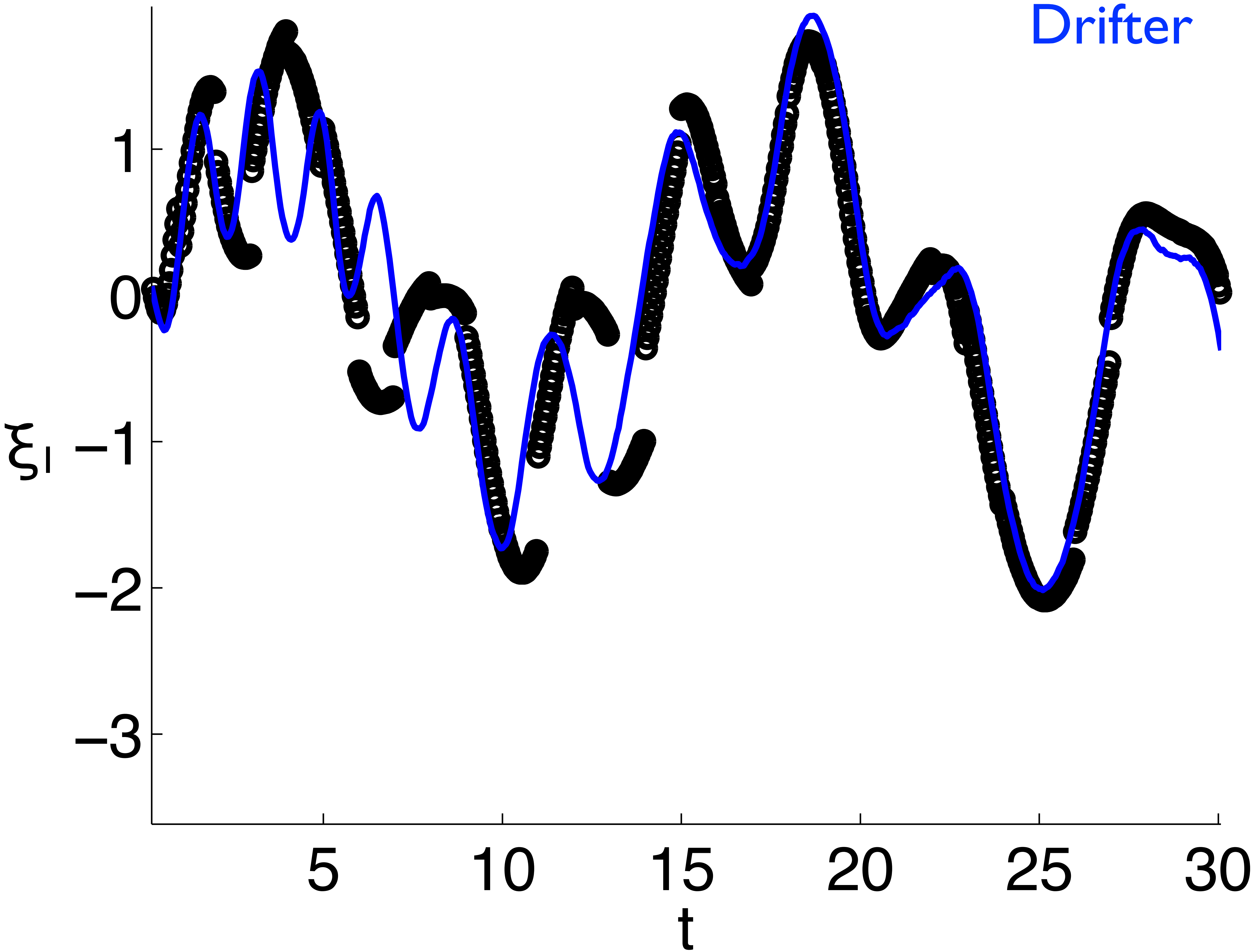
Ensemble Kalman Filter (EnKF)

Validation - Full Observation, Imperfect Data

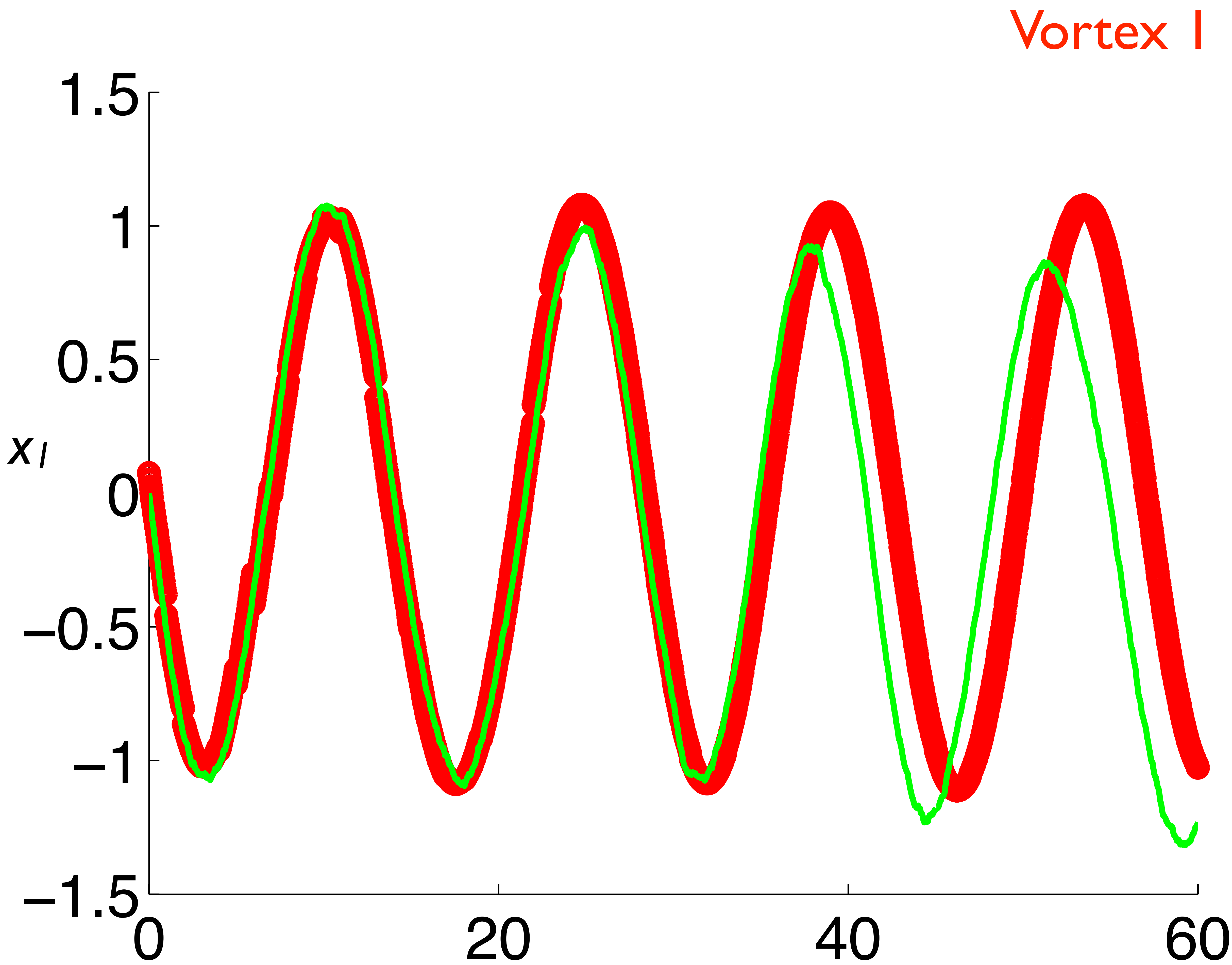
Observe vortices and drifter under observational noise

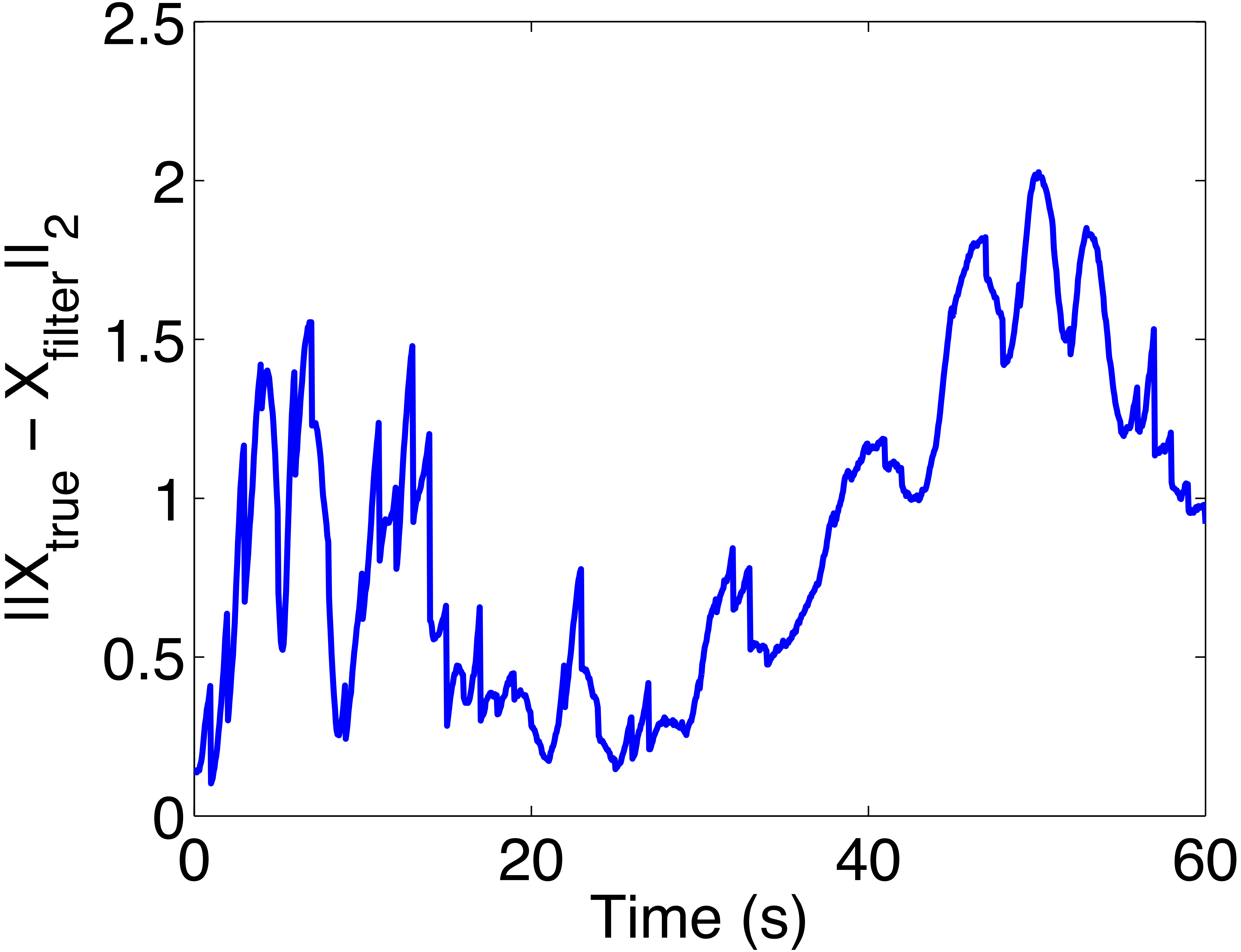
N = 6 ensemble members





Drifter
1
0
−1
−2
−3
ξ_1
5
10
15
20
25
30
t


Vortex 1
1.5
1
0.5
x_l
0
−0.5
−1
−1.5
0
20
40
60



2.5
2
1.5
1
0.5
0
0
20
40
60
Time (s)
||X_true - X_filter||_2

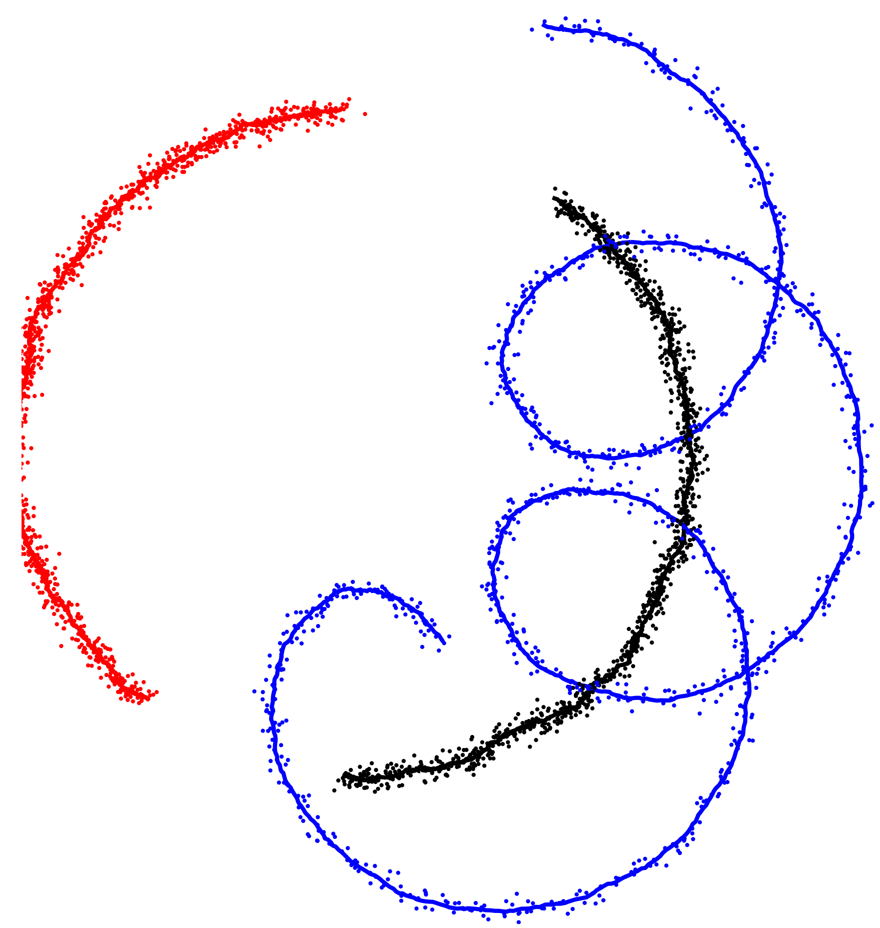
Approach 2

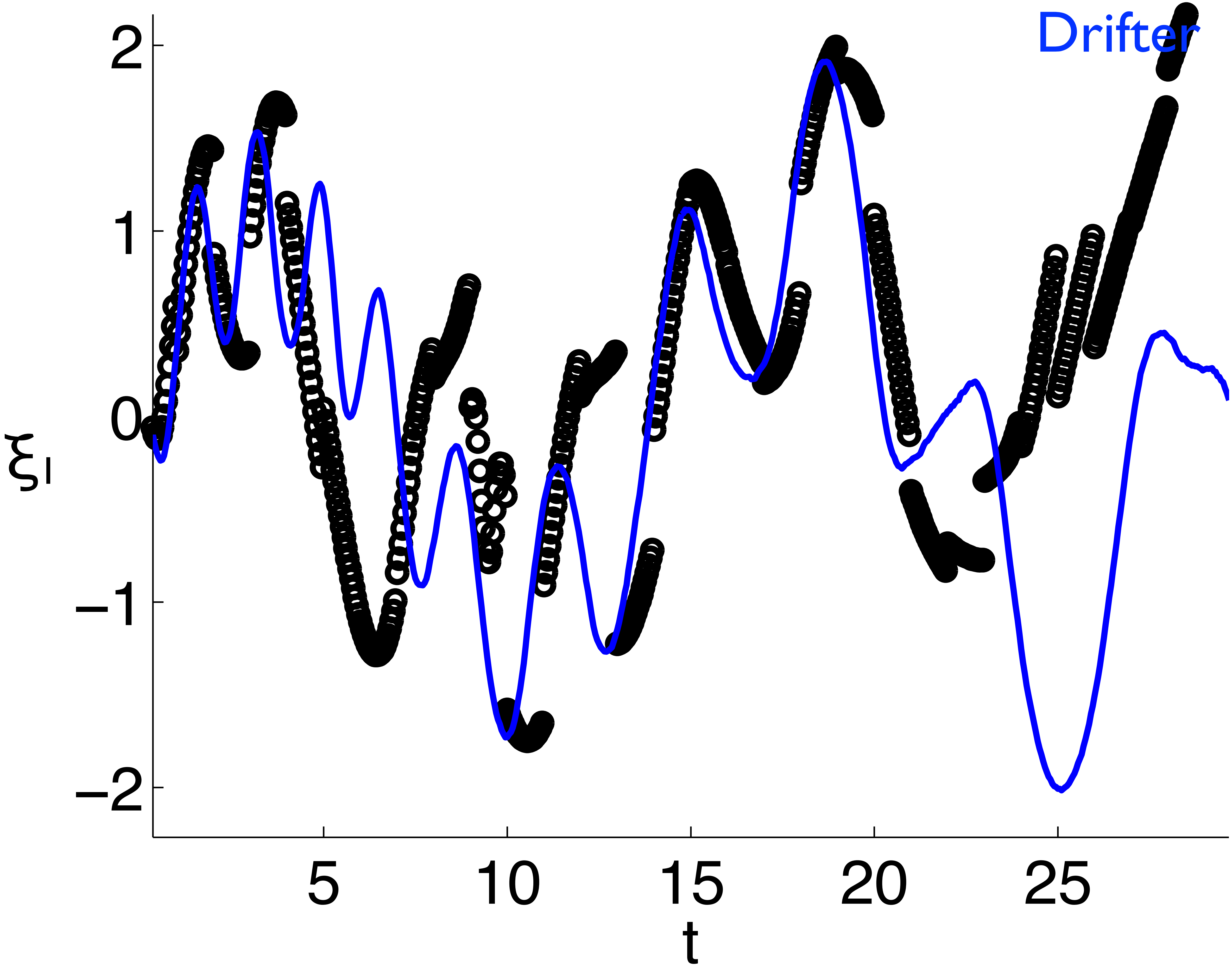
Ensemble Kalman Filter (EnKF)

Results - Partial Observation, Imperfect Data

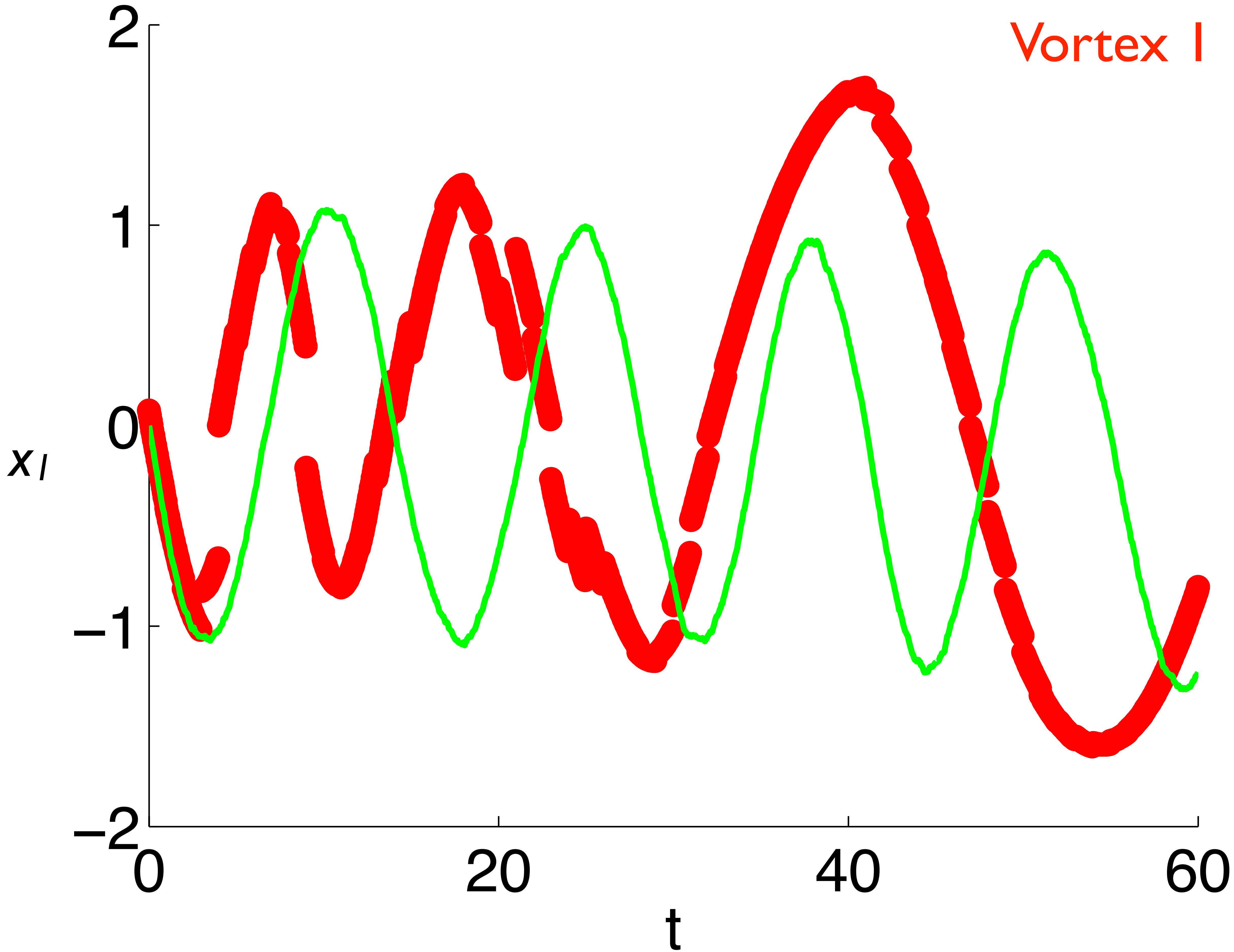
Observe only drifter under observational noise

N = 6 ensemble members

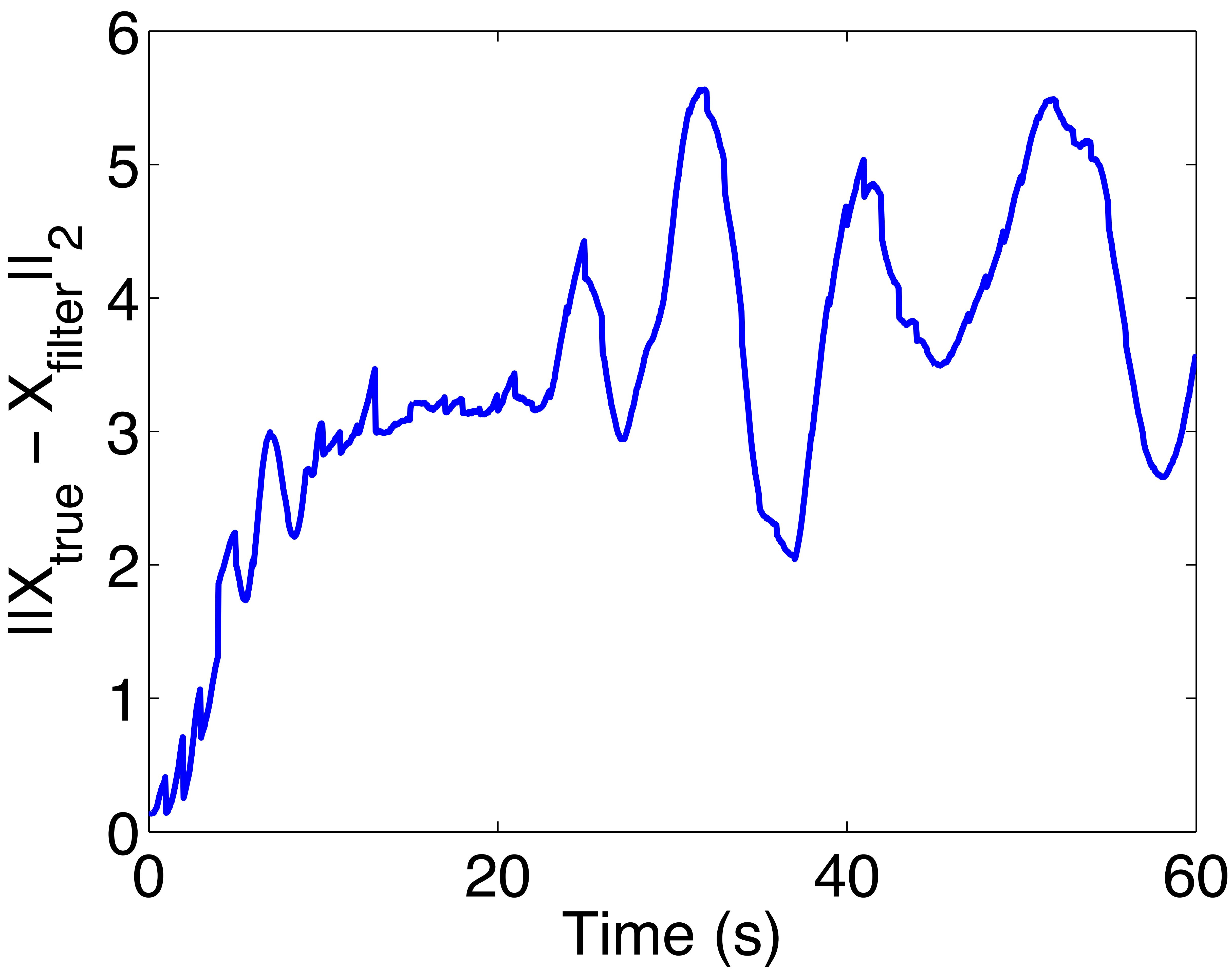




Drifter
2
1
0
−1
−2
ξ_l
5
10
15
20
25
t



Vortex I
2
1
0
−1
−2
x_I
0
20
40
60
t



6
5
4
3
2
1
0
0
20
40
60
Time (s)
$||X_{true} - X_{filter}||_2$

Data Assimilation

Testing

Testing, Phase I

Failure statistic: time to failure

Compare EKF, perturbed observations EnKF and ETKF

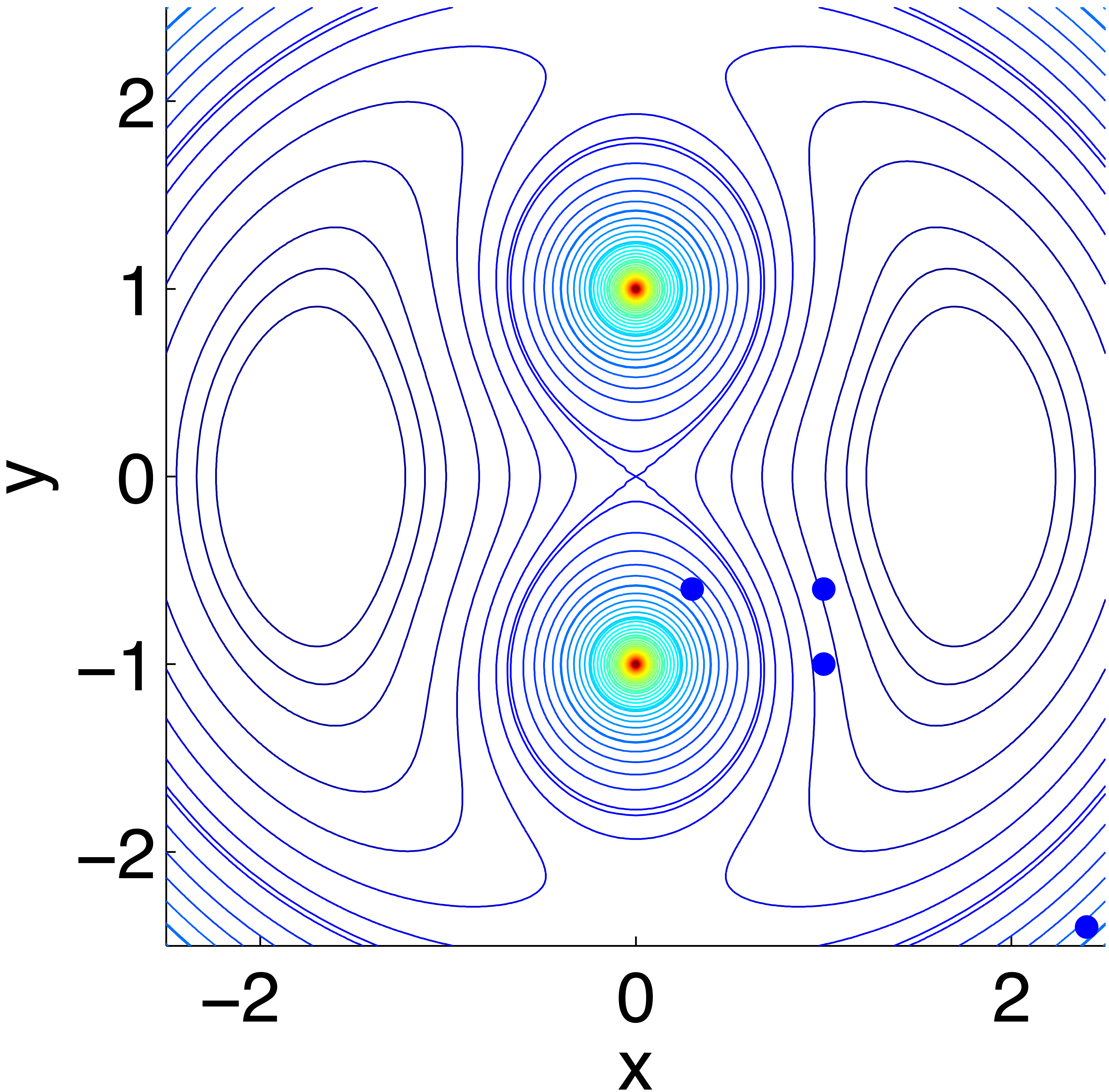
Testing, Phase 1

Failure statistic: time to failure

Generate M = 500 instances of the SDE at each of L = 4 drifter locations

Start vortex 1 at (0, 1)
Start vortex 2 at (0, -1)

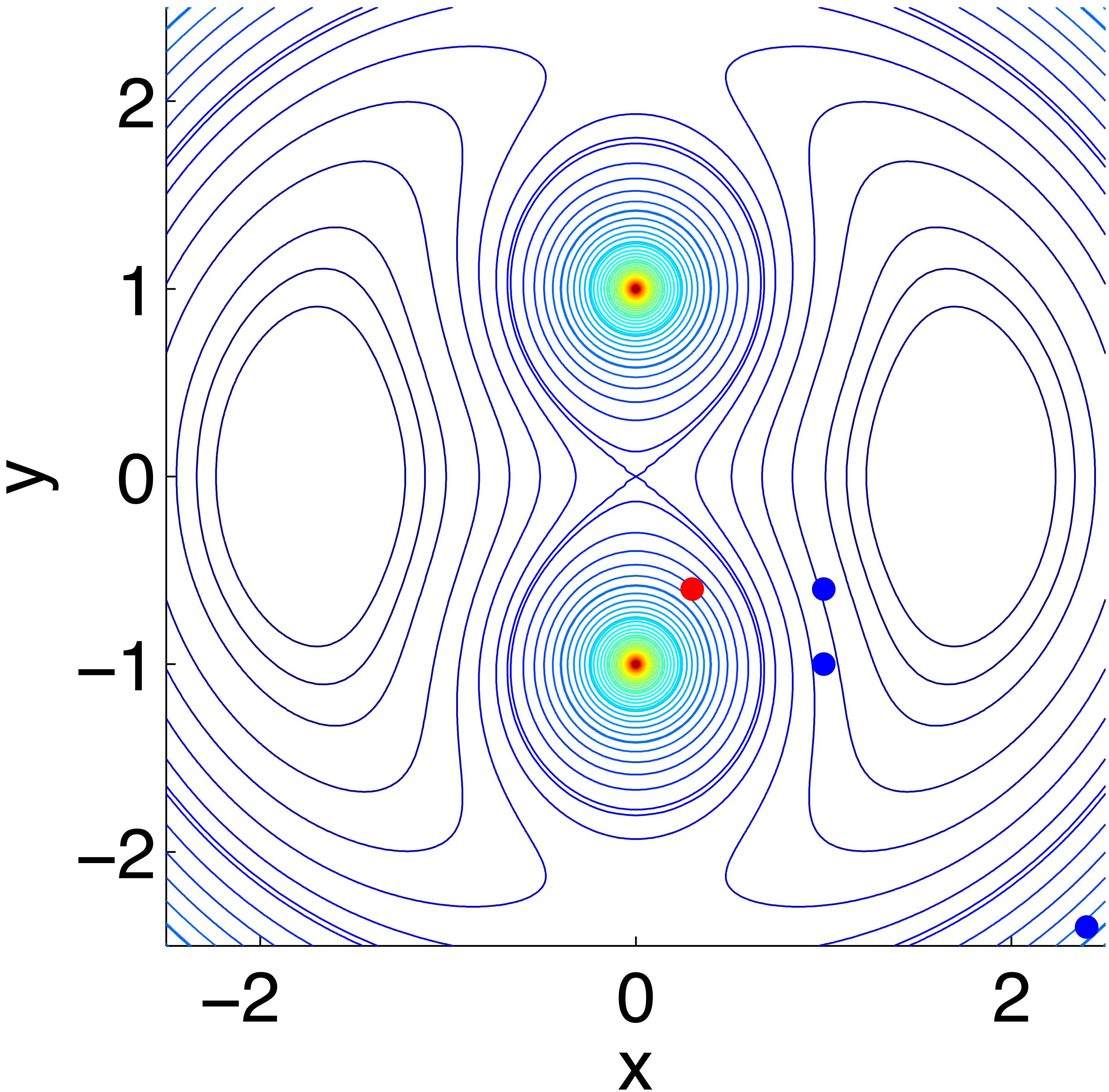
Add observational noise according to the model



2
1
0
−1
−2
y
−2
0
2
x

Testing, Phase I

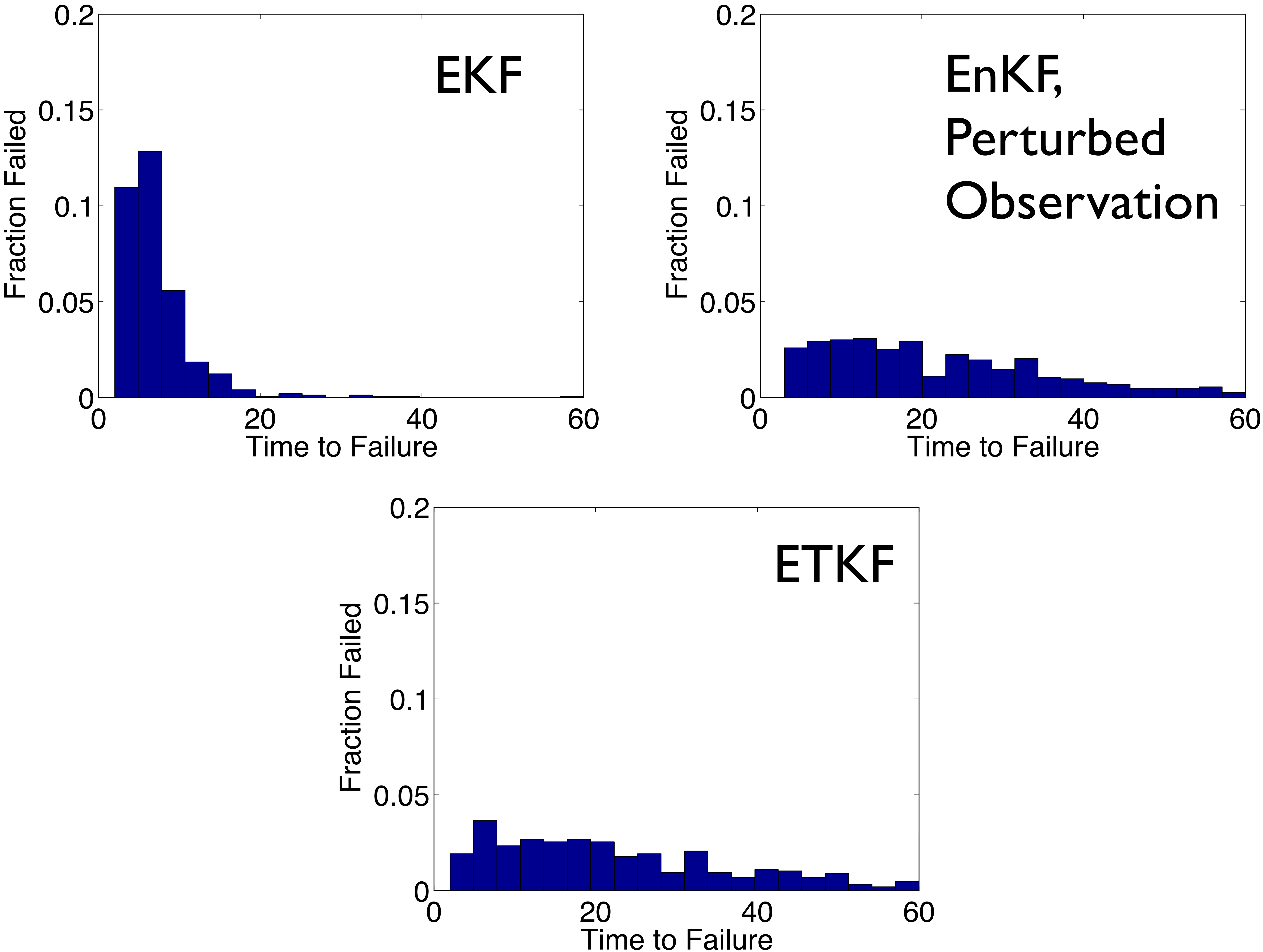
- Failure statistic: time to failure
  - Record when the distance between the analyzed state and the true state for either vortex is greater than 1


2
1
0
−1
−2
y
−2
0
2
x

Testing, Phase I

Failure statistic: time to failure

	EKF	EnKF, Pert	ETKF
Mean	8.23	25.64	25.27
Stdev	9.53	17.17	17.24
Fraction Completed	0.024	0.094	0.084



EKF
EnKF,
Perturbed
Observation
ETKF
Fraction Failed
Time to Failure
0
0.05
0.1
0.15
0.2
0
20
40
60

Moving Forward

Improvements to EnKF

- Covariance Inflation
- Localization
  - Local Ensemble Transform Kalman Filter (LETKF)

Moving Forward

Implement Particle Filter

Approximate pdf by an ensemble of *weighted* particles:

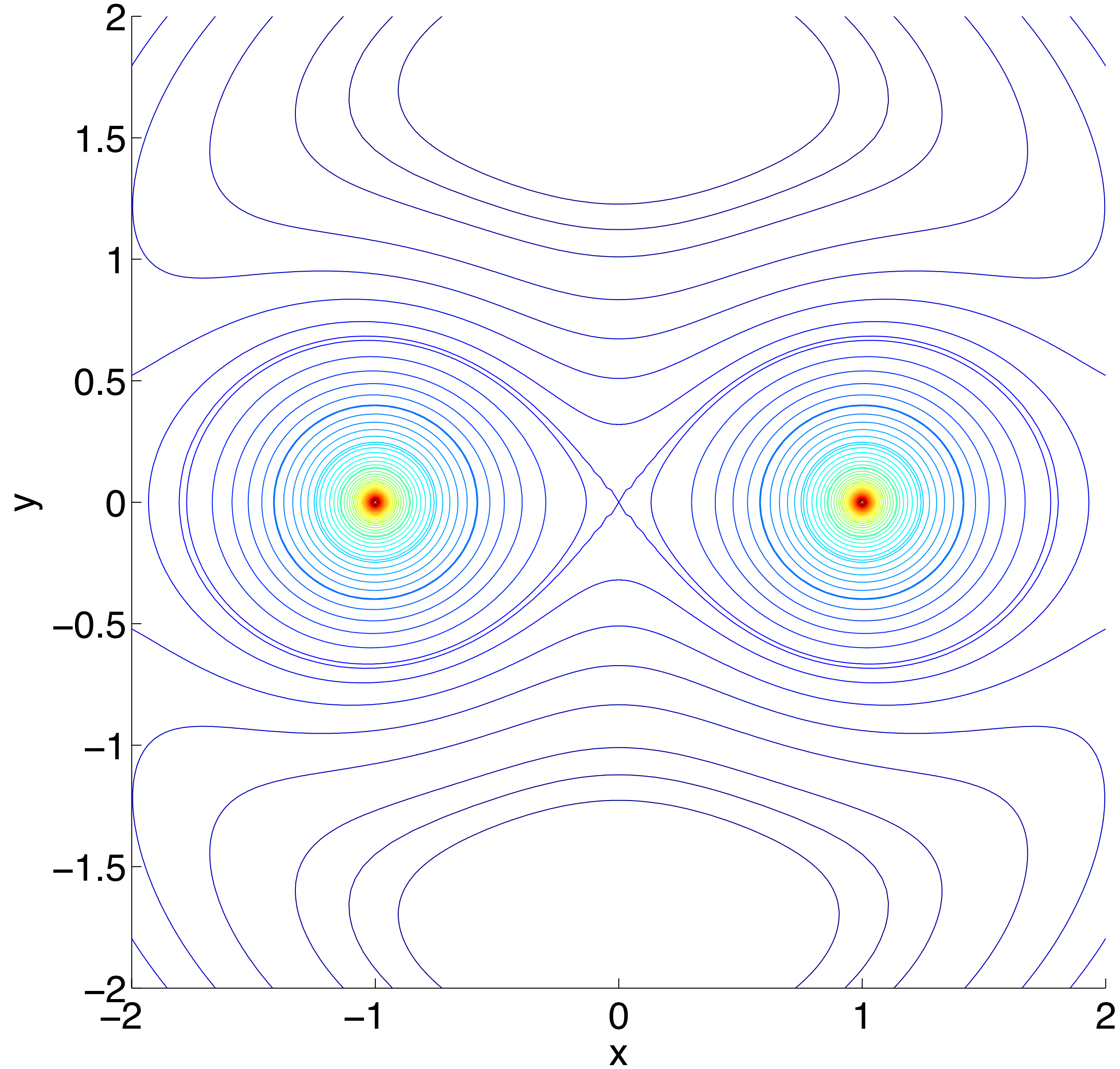
$$\{\mathbf{x}_i^f(t)\}_{i=1}^N \quad \{w_{i,k}\}_{i=1}^N$$

Forecast: Evolve particles forward using SDE

Analysis: Perform full Bayesian update at analysis

Moving Forward

Phase II - Manifold Detection for Observing System Design



Timeline

Phase I

- Produce database: now through mid-October
- Develop extended Kalman Filter: now through mid-October
- Develop ensemble Kalman Filter: mid-October through mid-November
- Develop particle filter: mid-November through end of January
- Validation and testing of three filters (serial): Beginning in mid-October, complete by February

Timeline

Phase I

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(Some) References

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Questions???