Displacement Data Assimilation

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Abstract

We show that modifying a Bayesian data assimilation scheme by incorporating kinematically-consistent displacement corrections produces a scheme that is demonstrably better at estimating partially observed state vectors in a setting where feature information is important. While the displacement transformation is generic, here we implement it within an ensemble Kalman Filter framework and demonstrate its effectiveness in tracking stochastically perturbed vortices.

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1. Bayesian Estimation and Displacement Assimilation

Most sequential estimation strategies are Bayesian. They seek to find estimates of moments of the posterior probability density function of the random, time-dependent, state variable $X(t)$, subject to noisy observations of the state, $Y(t)$. The posterior probability is thus

$$P(X|Y) \propto P(Y|X)P(X),$$

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where the first term on the right hand side is the likelihood, and is informed by observations. $P(X)$ is the prior, which is informed by the model. The model is usually an evolution equation for X . The model “error” might be an explicit
5 stochastic term representing uncertainties in the evolution equation or its initial or boundary data. The observations are usually stochastic because there are inherent errors in the measurements. When the prior and the likelihood are Gaussian (or a product of Gaussians), minimizing the sum of thee quadratic arguments of $P(Y|X)$ and $P(X)$ (equivalently $\log P(Y|X) + \log P(X)$) maximizes
10 $P(X|Y)$. Moreover, it does so by taking into account the relative certainties in the model and in the measurements. The most familiar sequential estimation technique is the Kalman Filter (see [1]). It seeks a minimizer of the trace of the posterior covariance. It yields an optimal estimate of the time dependent posterior mean and covariance of $X(t)$, over some interval in t when the stochasticity
15 is normally distributed, the dynamics are linear, and relationship between the observations and the state is a linear transformation.

The extended Kalman Filter (see [1]) and the ensemble Kalman Filter (enKF) [2] are frequently-used in mildly non-linear problems with inherently modal statistical distributions. They are not guaranteed to converge without exceptions.
20 The enKF is very popular since it is relatively easy to implement. It will be employed in this study, as it provides a useful and familiar framework for developing more targeted assimilation methods. The enKF strategy is, like the Kalman Filter approach, a two-stage sequential estimation process. There is a forecast, wherein the model is advanced from $t - \delta t$ to t . An ensemble forecast is
25 computed (the model is usually not linearized) by perturbing slightly the state at $t - \delta t$. This is then followed by an analysis stage, which is the Gaussian update from the Kalman scheme. In the absence of measurements, the best estimate is the sample mean and covariance of the ensemble forecast. (This presumes very critically that the mean of forecast errors remains close to zero).
30 If observations are available at that time t , these are individually assimilated into each ensemble member. Rather than solving the update of the covariance matrix, one uses a sample covariance based on the ensemble of forecasts. More

details on the enKF filtering scheme appear in Appendix B.

Most data assimilation schemes are variance-minimizing; they give an appropriately weighted average of the predictions of the model and the noisy observations [3]. These methods thus tend to decrease sharp gradients, consequently smearing or obliterating “features” (vortices, shock-fronts, etc.) in the state variable being estimated. If tracking the features are critical, a purely variance-minimizing methodology will produce estimates that might not be accurate enough for prediction, particularly in problems where capturing characteristics is critical, as in wave propagation problems. In this paper we propose a modification to sequential state estimation that can improve estimates where features are important. We denote this two-state data assimilation strategy *displacement assimilation*. Many of the sequential data assimilation procedures yield an estimate of $X(t)$ that may not be in the solution space of the model; for that matter, it might not even be physical. Constraints may be added to the Bayesian statement to promote physically reasonable properties in the analysis estimate, which motivates inserting an extra step into the data assimilation process. The method developed here applies this strategy to improve the estimates of a variance minimizing strategy when morphological features in the state variable are important. For example, suppose we want to estimate characteristic paths for a wave process. These paths are both space and time dependent (phase dependent). If designed properly, an assimilation method that makes a phase correction in addition to a blending of observations and model outcomes might deliver better estimates of such things, as the space-time information of what generated a wave, or the space-time information that better tracks the wave characteristics. This two-stage process is what we call *displacement assimilation*.

If the displacement correction and the estimation process are kept separate, it is possible to develop a displacement correction scheme that could then be applied to a variety of different estimation strategies. The development we present here is in that spirit. In this study we will be contrasting the standard enKF and something we call displacement enKF, wherein the difference is that

in the latter we add a phase correction.

65 Adding phase corrections within the context of data assimilation is not a new idea. Among other works, we can mention [4], who argued how this procedure might improve predictions in meteorology (see also [5], [6]). Ravella and collaborators [7] applied variational techniques (3DVAR) to jointly optimize displacement and amplitude corrections, and improve alignment of vortex-like
70 features. Recently, displacement assimilation has been incorporated into the spatio-temporal data assimilation capabilities (4DVAR) of the weather forecasting tool WRF DAS for short-term hurricane prediction. [8]

Percival used ideas from control theory to find coordinate transformations that could improve predictions. [9] He applied area preserving flows whose limit
75 in a pseudo-time variable defines a phase correcting map that locally minimizes a Bayesian-type penalty functional. In contrast, we will use area preserving maps to do the position correction “in one shot” every time new data is assimilated into the model.

An additional criterion in our methodology is to ensure that the phase corrections are kinematically consistent with the underlying physics of the system.
80 This is not always necessary for making phase corrections. Frazin [10], for example, makes phase corrections that have no physical basis – the aim of his work is to improve the optical data using a data assimilation system. In our context however, it is critical that the corrections be consistent with the underlying physics, *because we are using the phase corrections to capture the effects of unresolved/unmodeled (but physically constrained) effects in the system.*
85

The key in regularizing (or imposing) convexity in the space of displacement maps is to invoke physics or some ad-hoc constraint. We suggest the use of a physically-motivated constraint. When compared to an ad-hoc constraint, a
90 physics-motivated constraint leads to estimates whose optimality can be understood on physical grounds. Intuitive approaches to displacement corrections can be found in early works by Brewster [5, 6]. This strategy is formalized mathematically by Ravela [7, 11], who proposes that the optimal map be constructed so as to minimize the wave number of the displacement. The present work pro-

95 poses an alternative form and implementation of these constraints, pursuing the same motivation.

2. Displacement Assimilation, Defined

Consider the problem of determining the state y which best explains a set of noisy observations $d = h(y^t) + \epsilon$ of an unknown true state y^t , where the nonlinear observation operator can be modeled by $h(y)$ and the observation noise $\epsilon \sim \mathcal{N}(0, R)$. We want to solve the ill-posed problem $d = h(y)$, and resort to minimizing the likelihood functional,

$$\mathcal{J}_L[y] = \|d - h(y)\|_{R^{-1}}^2 \quad (1)$$

where the so-called maximum likelihood estimator is the maximizer of $\exp^{-\mathcal{J}_L[y]}$. Next, presume we have prior information that $y^t \sim \mathcal{N}(y^f, P^f)$, where y^f is a forecast mean, and P^f the forecast covariance. The maximum-a-posteriori estimator is the maximizer of $\exp^{-\mathcal{J}[y]}$, where

$$\mathcal{J}[y] = \mathcal{J}_L[y] + \|y - y^f\|_{(P^f)^{-1}}^2 \quad (2)$$

We are penalizing the distance from the forecast y^f in the matrix-weighted norm defined by the inverse of the forecast covariance, $(P^f)^{-1}$. The covariance matrices in real applications are often singular, by design or to machine precision.
100 This is equivalent to the so-called Bayesian formulation of the inverse problem; conditioning on a prior probability distribution is equivalent to the addition of a regularizing term.

While the distribution of a dependent variable such as vorticity depends
105 on the underlying distribution of spatial displacements of the vortices, typically displacement assimilation is rendered explicit by correcting for displacement, and then correcting the dependent variables. In general, our algorithm applies a regularized (Bayesian) optimization procedure to both steps. If y_a is a displacement-corrected model field, and a the parameters identifying the

displacement vectors, then the general algorithm attempts to minimize sequentially/iteratively the two penalty functionals,

$$\mathcal{J}_p[a] = \|d - h_a(a)\|_{R^{-1}}^2 + \|a - a^f\|_{(P_a^f)^{-1}}^2 \quad (3)$$

$$\mathcal{J}_a[y] = \|d - h_y(y_a)\|_{R^{-1}}^2 + \|y_a - y_a^f\|_{(P_{y_a}^f)^{-1}}^2 \quad (4)$$

We are taking advantage of the fact that we can use a given set of observations d and likelihood covariance R more than once: both for the displacement parameters and the corrected model fields. Remaining undefined are the observation operators h_a and h_y which convert the displacement parameters and model fields into measureable data, and the forecast statistics of the displacement parameters, a^f and P_a^f . An advantage of this methodology is that these can be tailored to a particular problem, and we define them specifically when we pose the vortex tracking problem and our data assimilation implementation.

3. Displacement Assimilation in Ensemble Vortex Tracking

The net effect of large-scale forcing on a system of interacting coherent vortices is two-fold. The dominant effect is in modifying the trajectories of the vortex centers. A much smaller effect is changing the shape/structure of individual vortices [12]. This naturally suggests the use of statistically derived filtering algorithms to track the trajectories of the vortices for data assimilation. The trajectories of interacting vortices are highly sensitive to changes in their relative displacement and amplitude, and thus present a useful “toy model” for developing and testing our displacement assimilation methodology. We will use a stochastic barotropic vorticity equation to compare the enKF estimates with and without displacement adjustments. Our model is noisy; we do not use the ideal vorticity equation. The added noise accounts for unresolved or ignored physical processes in the actual physical system. Furthermore, there can also be uncertainties in initial and boundary conditions. The *stochastic vorticity model* solutions are therefore realizations of the stochastic process, drawn from a probability distribution.

Consider an ideal incompressible fluid in a two-dimensional domain $D \subset \mathbb{R}^2$. Denote the velocity vector field $V = (u, v)$. Assume this velocity is incompressible, $\nabla \cdot V = 0$. The vorticity associated with the velocity field is $\omega = \nabla \times V$. Let the stream function be $\psi = \left(-\frac{\partial \psi}{\partial y}, \frac{\partial \psi}{\partial x}\right)$. The stochastic model for the vorticity

140 is

$$\partial_t \omega + V \cdot \nabla \omega = \delta f, \quad \omega : D \times [0, \infty) \rightarrow \mathbb{R}, \quad (5)$$

$$\omega(z, 0) = \omega_0(z) + \delta \omega_0(z),$$

$$\nabla^2 \psi = \omega, \quad \psi : D \rightarrow \mathbb{R}, \quad (6)$$

$$\nabla \psi \cdot \partial D = \delta b,$$

where δf , $\delta \omega_0$, and δb are perturbations in the forcing, initial condition, and boundary condition with known probability distributions. Perturbations in initial condition and boundary conditions will not be invoked in this study. The value of the stream function, along the boundary of the domain, ∂D is prescribed. Note that (6) couples the the vorticity and stream functions, and consequently couples a set of vorticity features to their Lagrangian paths. The Poisson equation (6) is linear, so it maps perturbations in vorticity features directly into perturbations in their trajectory. Accumulated noise in nearby features mutually affects the trajectories of the vortices. Conversely, in systems constrained by diagnostic relationships such as (6), studying spatial displacements in features provides a way to correct the accumulated errors in their amplitude, which improves the subsequent prediction of their future path. Hence, the importance of the forcing error term δf which can generate random local changes in the intensity of features, as well as nudge the positions of nearby features.

Appendix C gives details on the parameter values for the calculations that follow. They were chosen to provide a system of spatially continuous features which experience significant position errors while retaining enough structure to persist throughout the simulation. The initial condition defines a system of co-rotating vortices. In Figure 1 two known ($\delta \omega_0 = 0$) and initially identical

vorticity pulses are mutually advected in a bounded rectangular domain. The boundary conditions enforce a zero-outflow condition ($\delta b = 0$) that serves two purposes. The first is to ensure features cannot leave the domain, so that the complexity of the tracking problem remains consistent over time and between
165 independent realizations of the model. The second is that it ensures the energy from the forcing errors cannot leave the system, and increases the variance in vorticity over time. The forcing δf is driven by independent Gaussian random functions in the velocity variables with spatial decorrelation on the scale of the vortex features (≈ 0.25). This results in low frequency perturbations that
170 modulate the amplitude of each vortex while preserving its geometry so that it can remain coherent throughout the simulation. The amplitude perturbations in the vortices disrupt the stream function governing their oscillation and alter their spatial trajectories, which introduces position errors. Hence the forcing noise places the system in a regime where position variance is the dominant
175 form of model error, and the noise correlation is on a scale that maintains the feature geometry while allowing each vortex to have independent amplitude perturbations.

The performance of the standard and displacement-corrected enKF will be compared. In particular, the decay of forecast and analysis bias with ensemble
180 size is confirmed and compared between both filters. A reduction in forecast and analysis variance with respect to the standard method is observed. Moreover, the displacement filter preserves the vortex structure evident in the true vortex system, while the standard enKF introduces spurious deformations. We present an argument explaining this improvement by relating it to the correction of
185 forecast statistics that is a result of the preconditioned filter.

3.1. Model Setup and Observations

In the stochastic vorticity dynamics we assume a (deterministic) initial vorticity condition $\omega(z, 0) = \omega_0(z)$ for $z \in D = [x_L, x_U] \times [y_L, y_U]$. The vorticity trajectory $\omega : D \times [0, \infty) \rightarrow \mathbb{R}$ is given by

$$\frac{\partial \omega}{\partial t} = -V \cdot \nabla \omega + B_\omega(z) \cdot \xi \quad (7)$$

Figure 1: **The noise regime of the model.** A sample of 35 realizations of the vorticity model, with equal-height ($\omega = .5$) contours displayed.

Equation (7) is subject to zero-outflow boundary condition $\nabla\Psi \cdot \partial D = 0$, where $\Psi : D \rightarrow \mathbb{R}$ is the stream function corresponding to ω . The model error forcing term δf is defined by a Gaussian random function with spatial covariance factor $B_\omega(z)$, and white noise process $\xi \sim \mathcal{N}(0, I_r)$. Equation (7) is approximated on a uniform rectangular grid on D with N_x and N_y subintervals in the $\{x, u\}$ and $\{y, v\}$ dimensions, respectively, and the vorticity, velocity, and stream function grids are aligned. Then the total dimensionality of the problem is $N = (N_x + 1)(N_y + 1)$. This stochastic differential equation (SDE) is integrated in time using the stochastic Heun method [13]. Each time the right-hand side of Equation (7) is evaluated, the stream function is obtained by solving the Poisson equation $\Delta\Psi = \omega$ via a second-order central difference discretization of the Laplacian. The velocity components are computed using second-order centered difference approximations of the derivatives.

The structure of B_ω and dimension r of the Gaussian random function driving the model noise are inferred from assumptions on the variability of the velocity components. Since vorticity is a derived state parameter, we make an

effort to define a (reasonable) model uncertainty based only on the (given) covariance statistics of the observable state variables, i.e. the velocity vector field components. The noise in the two velocity components is assumed mutually independent and spatially distributed with a squared-exponential correlation structure,

$$k_u(z_1, z_2) = k_v(z_1, z_2) = \sigma_V^2 \exp\left(-r_V^{-2} \|z_2 - z_1\|_2^2\right) \quad (8)$$

where σ_V^2 and r_V are the scale and shape parameters, respectively, setting the pointwise variance and decorrelation length of the model error kernels k_u and k_v . Let Q_V denote the Gramian matrix corresponding to the evaluation of the kernels on the discretized domain D , and compute its factorization $Q_V = B_V B_V^T$, where $\text{rank}(B_V)$ is sufficient to represent all numerically significant modes of the original covariance matrix. Each spatial mode of each velocity component is then dampened to zero at the boundaries in the outflow directions, so that the model perturbations are guaranteed consistent with the boundary conditions. Specifically, another shape parameter r_b is introduced to scale the width of the transition region. Then the following bump function is defined,

$$\left[1 - \exp\left(-\frac{|x - x_L|}{r_b}\right)\right] \cdot \left[1 - \exp\left(-\frac{|x - x_U|}{r_b}\right)\right] \quad (9)$$

which is unity in $[x_L + r_b, x_U - r_b]$, and scales the u model noise modes. A similar bump function in the y dimension is defined and applied to the v modes. With consistent velocity perturbations, the vorticity perturbation modes can be computed from the definition $\omega = \partial_x v - \partial_y u$,

$$\delta\omega = B_\omega \cdot \xi = \left[\frac{\partial B_v}{\partial x} \quad -\frac{\partial B_u}{\partial y} \right]^T \cdot \begin{pmatrix} \xi_u & \xi_v \end{pmatrix} \quad (10)$$

200 where the derivatives are approximated by centered differences. The vorticity model perturbations driving the SDE in Equation (7) follow a Gaussian random function with spatial covariance $Q_\omega = B_\omega B_\omega^T$. We should keep in mind that this covariance actually measures noise from velocity perturbations in a $r = 2 \cdot \text{rank}(B_V)$ -dimensional (observation) space expressed in $r/2$ -dimensional
205 vorticity model space.

In our simulations, the initial condition was deterministic and consisted of two co-rotating vortices,

$$\omega_0(z) = a_1 \cos^2 \left[\frac{\pi}{2} r_1(z) \right] + a_2 \cos^2 \left[\frac{\pi}{2} r_2(z) \right] \quad (11)$$

where the rescaled radius $r_j(z)$ defines the support of each vortex, and is given by

$$r_j(z) = \frac{d_j(z)}{r_{s,j}} \chi_{\{d_j(z) \leq r_{s,j}\}}(z) \quad (12)$$

and $d_j(z) = \left[(x - x_{c,j})^2 + (y - y_{c,j})^2 \right]^{1/2}$, the squared distance from the vortex, center, and $\chi_A(z)$ is the indicator function for all $z \in A$. The trajectory of one realization of the generalized model, including the initial condition, is provided in Figure 4, with one frame for each assimilation time.

210 The observations of the state variables in the present example will be a sparse array of noisy Eulerian measurements of the velocity components. The observation operator is a map from the state variables to the measured quantities. In particular, let $h_a(\omega, \{x_{d,j}, y_{d,j}\})$ estimate the velocity components at each $(x_{d,j}, y_{d,j})$ from the continuous model vorticity field ω . As is standard practice
215 in twin simulation experiments, synthetic observations are generated given a true vorticity field ω^t . Then, the velocity components measured are given by $d_V := (d_u, d_v)^T = h_a(\omega^t) + \epsilon_d$, where $\epsilon_d \sim \mathcal{N}(0, R)$ are the assumed independent and identically distributed normal observation errors, and $R = \tau I_{2N_d}$ is the observation covariance matrix. Note that the locations where velocity is measured
220 will be a rectangular array and a subset of the discretization of the spatial domain D , though in principle the observed locations can be any scattered points in D .

3.2. Displacement Correction Via Area-Preserving Maps

The stochastic vorticity equation produces a distribution of vorticity functions whose features have perturbed amplitudes; this introduces noise in the Lagrangian path of these features. The generalized inverse problem for position errors is to identify which of the possible Lagrangian perturbations would produce a realization of the stochastic vorticity function that most closely matches

the true state of the system. Consider a quadratic penalty functional that measures the Eulerian distance between the true vorticity function ω^t and various candidate analyses ω with respect to a specific norm $\|\cdot\|$,

$$\mathcal{J}_a[\omega] = \frac{1}{2} \|\omega^t(Z) - \omega(Z)\|^2 \quad (13)$$

In order to relate the forecast prediction to candidate analyses through corrections in the position of features, we define a family of smooth, invertible maps $Z = \Phi(z; a)$. Throughout the following discussion we will consistently refer to the coordinates native to the true and observed vorticity function by Z , and the coordinates on which the forecast model ω^f is defined by z . Then we can write $\omega(Z) = \omega^f(z) = \omega^f \circ \Phi^{-1}(Z; a)$. Now we can recast (13) in terms of the map parameters,

$$\mathcal{J}_p[a] = \frac{1}{2} \|\omega^t(Z) - \omega^f \circ \Phi^{-1}(Z; a)\|^2, \quad (14)$$

which allows us to ask which position corrections provide the best agreement
 225 (minimum $\mathcal{J}_p$) with measurements of the true vorticity function. If the maps Φ are to model stream function perturbations, they also must be divergence-free, in the sense that they preserve the total vorticity on any subset as it is mapped from one position to another. These subsets include any closed contour of the vorticity function, including the concentric and parallel contours that
 230 describe the geometry of features. Hence, preserving the total vorticity and area on contours is akin to preserving the geometry of features, i.e quantities like volume and intensity.

3.2.1. Symmetric Parameterization of Displacement Maps

A standard method from classical mechanics to define area preserving maps
 235 is by canonical transformation of the spatial coordinates. However, the transformed coordinates must be implicitly solved. Furthermore, the maps are difficult to parameterize symmetrically, in the sense that spatial symmetries in the map parameters are not necessarily reflected in the transformed coordinates. Instead, under a small-displacement assumption, we can show an approximate

240 equivalence to following a divergence-free flow along stream functions for a fixed time. Details and references are provided in Appendix A.

We define area preserving maps $(X, Y) = \Phi(x, y; a)$ by integrating stream functions over a fixed time interval,

$$\Phi(x, y; a) = (x, y) + \int_0^1 (-\Psi_y[x(t), y(t); a], \Psi_x[x(t), y(t); a]) dt \quad (15)$$

The parameterization of the stream function Ψ is linear in a , i.e. taking
 245 $\Psi(x, y; a) = \sum_j^N a_j B_j(x, y)$, then the inverse map $(x, y) = \Phi^{-1}(X, Y; a)$ is obtained simply by making the substitutions $(x, y, a) \rightarrow (X, Y, -a)$. Unlike the usual formulations of canonical transformations, the approach of integrating a flow gives an explicit, rather than an implicit function, and is un-constrained, unlike the constraints on the mixed partial derivatives of a generating function
 250 to guarantee the invertibility of a canonical transformation [14]. For a given position correction problem, a sequence of maps can be defined through iterative optimization of functionals like Equation (14). In this context, the small displacement assumption is reasonable, and we can proceed to take advantage of the theoretical simplicity of the canonical map structure to develop additional tools. Moreover, to generate the maps we take advantage of the practical
 255 convenience of integrating divergence-free flows. Hereafter we identify the map function and stream function, $\Psi(x, y; a) \leftrightarrow \zeta(X, y; a)$, and the particular usage will be clear from context. In fact, these two approaches are identical in applications which require the map to be linearized, such as when we project the
 260 statistics of amplitude perturbations in vorticity onto the space of displacement map parameters. In the next section we apply both points of view in order to derive regularization terms that help provide smooth displacements where feature information is present, based on an application of continuum mechanics.

3.2.2. Transformation Regularization

265 In the set of possible feature displacement maps, we want to avoid coordinate transformations which excessively deform the geometry of strong features in the

model function. In fact, excessive deformations in general should be avoided. Since the likelihood functional will penalize only coordinate transformations where there is significant feature information, then an otherwise unfettered optimization routine can significantly distort regions where there are no features in either the observed or modeled functions. Perturbations in lightly-constrained regions can generate enough of a change in the penalty functional to create local decreases in the objective function that have nothing to do with the displacement of significant features—precisely the non-convexity that regularization schemes, such as Tikhonov regularization, are designed to eliminate.

Suppose the displacement map complexity is kept well below that of the original problem,

$$\dim(a) \ll \dim(\omega) = \dim(\zeta) = \dim(\Phi) \quad (16)$$

Denote the linear map from the displacement parameters to vorticity values as $T_{\omega a}$, and denote its pseudoinverse $T_{a\omega}$, the map projecting a vorticity function into displacement parameter space. These maps can be used to estimate a prior model covariance of map parameters from a given prior vorticity covariance. For vorticity perturbations $\delta\omega$ and map parameter perturbations δa , we can write

$$\begin{aligned} P_\omega &= \text{Cov}(\delta\omega) = \mathbb{E}(\delta\omega\delta\omega^T) \\ &= \mathbb{E}(T_{\omega a}\delta a\delta a^T T_{\omega a}^T) \\ &= T_{\omega a}\mathbb{E}(\delta a\delta a^T)T_{\omega a}^T \\ &= T_{\omega a}\text{Cov}(\delta a)T_{\omega a}^T = T_{\omega a}P_aT_{\omega a}^T \end{aligned} \quad (17)$$

and

$$P_a = T_{a\omega}T_{\omega a}P_\omega T_{\omega a}^T T_{a\omega}^T = T_{a\omega}P_\omega T_{a\omega}^T \quad (18)$$

Then we can consider regularization terms defined directly in the space of displacement parameters. In particular, we write

$$J_p[a] = \frac{1}{2} \|d_\omega - \omega^f \circ \Phi^{-1}(Z_d, a)\|_{R^{-1}}^2 + S[a; \alpha] \quad (19)$$

where we could take the regularization term $S[a] = \|a - a^f\|_{C_a^{-1}}^2$, the usual quadratic form for the model prior, with the forecast $a^f = 0$, and the co-

variance penalty factor C_a . Note that in practice the functional will not be expressed in terms of direct vorticity observations, d_ω , but rather with velocity measurements, d_V .
285

There is one impediment to using this regularization – it requires knowledge of P_ω , the covariance of the vorticity (or velocity) fluctuations. In a situation where we have knowledge of the vorticity covariance P_ω , it is optimal to minimize the functional in eq. (19). However, P_ω is often not known in practice,
290 because vorticity fluctuations are driven by unresolved/unmodeled physical processes, e.g. sub-grid processes. As an alternative, especially in a situation where we do not have information on the covariance of the vorticity fluctuations, we can choose an ad hoc regularization term which includes more information than just the weighted distance from the forecast, such as a preference for smoothly
295 varying transformation maps. Below, we present one such procedure – *strain regularization*. We use this ad hoc regularization method, instead of the expression in eq. (19), to demonstrate the applicability of the method, even in situations where we do not have access to the vorticity covariance P_ω .

3.2.3. Strain regularization

Since we can write down the formula for a coordinate transformation $z = \Phi^{-1}(Z)$, then we can write down the local displacement induced by the transformation, $U(Z) = Z - z(Z) = Z - \Phi^{-1}(Z)$. This is the amount the original coordinate system was deformed to arrive at the current coordinates Z . We also can write down how differential length elements in the former system dz are deformed in the new system dZ . For sufficiently smooth displacements, and $|\zeta| \ll 1$,

$$\epsilon := \frac{1}{2} [\nabla_Z U + (\nabla_Z U)^T] \quad (20)$$

300 or in terms of the map function, ζ , the displacement gradient and strain tensor simplify to

$$\begin{aligned}\epsilon[\zeta] &= \begin{bmatrix} \epsilon_{XX}[\zeta] & \epsilon_{XY}[\zeta] \\ \epsilon_{YX}[\zeta] & \epsilon_{YY}[\zeta] \end{bmatrix} \\ &\approx \begin{bmatrix} -\zeta_{yX} & \frac{1}{2}(\zeta_{XX} - \zeta_{yy}) \\ \frac{1}{2}(\zeta_{XX} - \zeta_{yy}) & \zeta_{yX} \end{bmatrix}. \end{aligned} \quad (21)$$

For the strain regularization treatment, we augmented (14) with a weighted Frobenius norm of the engineering strain tensor in (21) at each model point,

$$\begin{aligned}\|\epsilon[\zeta]\|_{F,\alpha}^2 &= \frac{\alpha_n}{2} (\epsilon_{XX}^2[\zeta] + \epsilon_{YY}^2[\zeta]) \\ &+ \frac{\alpha_s}{2} (\epsilon_{XY}^2[\zeta] + \epsilon_{YX}^2[\zeta]) \\ &= \alpha_n \|\zeta_{yX}\|^2 + \frac{\alpha_s}{4} \|\zeta_{XX} - \zeta_{yy}\|^2 \\ &\sim \alpha_n \|\Psi_{yx}\|^2 + \frac{\alpha_s}{4} \|\Psi_{xx} - \Psi_{yy}\|^2\end{aligned} \quad (22)$$

where α_n and α_s calibrate the size of the normal and shear strain penalties, respectively. Since there is no prior model distribution limiting the displacement, the optimization algorithm is free to find the true bulk position shift. However, without a calibrated regularization term, the algorithm also is free to suggest local deformations wherever there is not significant feature information. This situation can result from not having any background error at all, as is the case here, or whenever observation uncertainty or scarcity effectively places observation uncertainty on the same or greater scale as the background signal noise.

310 Provided a linear parameterization of the stream function $\Psi(z) = \sum_j^N a_j B_j(z) = B(z) \cdot a$, the strain regularization term can be written as a matrix-weighted norm,

$$\begin{aligned}\|\epsilon[\Psi]\|_{F,\alpha}^2 &= \alpha_n (B_{yx} \cdot a)^T (B_{yx} \cdot a) \\ &+ \frac{\alpha_s}{4} (B_{xx} \cdot a - B_{yy} \cdot a)^T (B_{xx} \cdot a - B_{yy} \cdot a) \\ &= \|a\|_{C_{\epsilon,\alpha}^{-1}}^2\end{aligned} \quad (23)$$

where

$$C_{\epsilon,\alpha} = \left[\alpha_n B_{yx}^T \cdot B_{yx} + \frac{\alpha_s}{4} (B_{xx} - B_{yy})^T (B_{xx} - B_{yy}) \right]^{-1} \quad (24)$$

If this constraint is simply added to the penalty functional in (19), the standard least-squares minimizer requires the sum $C_a^{-1} + C_{\epsilon,\alpha}^{-1}$, forcing us to explicitly calculate the model prior covariance inverse. Alternatively, we directly regularize the model covariance

$$C_{a,\alpha} = C_a + C_{\epsilon,\alpha} \quad (25)$$

315 so that only the deformation gradient information in (24) need be inverted. This is no problem provided the complexity condition in (16) is maintained, which depends on the manner in which the displacement maps are discretized.

To confirm the efficacy of strain regularization for penalizing excessive deformations while permitting bulk feature position realignment, a numerical optimization experiment was designed and performed with and without a regularization term (See Figures 2, 3). A simple feature modeled after two coalescing vortices was generated with no background error, and a truth feature was generated by a combination of a rigid transformation and amplitude perturbation. The L^2 -norm penalty functional from (13) was used to quantify the residual
320 after realignment by a displacement map $\Phi(z)$.
325

3.2.4. Displacement Algorithm Implementation Details

No basis has yet been prescribed for representing the displacement function ζ . Typical decorrelation lengths for the amplitude perturbations that generate position errors are not global in scale. It is reasonable to assume noise length
330 scales are no greater than the dominant features in the model. For this reason, historically, local parameterizations of displacement functions have been proposed. Mariano [15] decomposed individual contours into angular sections and analyzed displacement along these directions, while Brewster [6] considered a hierarchical model of discretizations, where first three and then one grid step
335 corrections would be sought. Ravela [7] proposed a bicubic spline representation. Frazin [10], like Brewster, combined approximation with regularization by considering a hierarchical spline model similar to multigrid techniques, where the displacement function estimate is refined on a sequence of increasingly fine scales.

Figure 2: **Position realignment** (a) a forecast of a prominent feature with no background noise (upper-left), the true feature with amplitude perturbations (upper-right), an optimal realignment obtained by a standard constrained numerical optimization code (lower-left), and the residual between the optimization and the true feature (lower-right); (b) the displacement maps generated for the realignment as a mesh overlaying the corresponding map function ζ , no regularization.

Figure 3: **Position realignment, with strain regularization.** Same panels as Figure 2, except that displacement maps have been regularized by the inclusion of the strain regularization term with $\alpha_s = 10$ and $\alpha_n = 0.1$.

340 There is an issue here regarding how hidden regularizations imposed by the
 displacement map parameterization affect the model statistics. For any ap-
 proximation method, the number of discretization points used determines the
 maximum roughness in the functions which can be modeled. For global meth-
 ods, this is determined by the highest rank polynomial allowed, while for local
 345 methods like splines with fixed rank, the roughness is determined directly by
 the dimension of the subdomains. The variability of a function can be strongly
 determined by that of a random displacement map, and local spline interpolants
 provide a natural way to set the decorrelation length scale of its perturbations.
 Clearly, a calibration must be performed here to ensure that the map coefficients
 350 have the proper statistics for a given amplitude model error, though the details
 of such calculations do not appear in the published literature. We partially
 addressed this issue explicitly in Equation (18), and will take it up again after
 introducing the particular displacement map parameterization we will use.

We will adopt the bicubic spline representation, which has a convenient
 representation as a linear combination of B-splines [16]. With the B-spline
 formulation rectangular approximations of complex boundaries are easily carried
 out. For any $p \in C^2(D)$, define a uniform rectangular partition of the domain
 with grid line intersections at nodes $\{(x_j, y_j)\}$ and spacings $\ell = \Delta x = \Delta y$, and
 extend this partition one layer of nodes into the exterior of the boundary. For
 example, a 3×3 array of sub-rectangles will have $4 \times 4 = 16$ nodes in D , and a
 ring of 20 nodes immediately outside the domain boundary, spaced exactly one
 grid spacing away. Then p is exactly represented by the linear combination of
 tensor products of B-splines,

$$p(x, y) = \sum_j a_j B_j(x, y) = \sum_j a_j b(x; x_j) b(y; y_j) \quad (26)$$

where the B-spline kernel $b(z; z_j)$ is the piecewise-cubic polynomial

$$b(z; z_j) = \begin{cases} \frac{1}{6}s^3 & 0 \leq s < 1 \\ \frac{1}{6}(-3s^3 + 12s^2 - 12s + 4) & 1 \leq s < 2 \\ \frac{1}{6}(3s^3 - 24s^2 + 60s - 44) & 2 \leq s < 3 \\ \frac{1}{6}(-s^3 + 12s^2 - 48s + 64) & 3 \leq s \leq 4 \\ 0 & \text{otherwise} \end{cases}$$

and $s = 2 + (z - z_j)/\ell$ is the local normalized coordinate parameterizing the support of the kernel. The extra ring of B-splines around the exterior provides the extra polynomial basis support on each sub-domain along the boundary to make the computation of polynomial coefficients there well-determined.

As a parameterization for the map function Ψ , bicubic B-splines like other linear approximation schemes allow us to conveniently represent the map function as a linear operation on the spline coefficients, $\Psi = B \cdot a$, as well as any linear operation on Ψ , such as the displacement map in Equation (15), or the local strains induced by the map in Equation (21). The position error penalty function in Equation (23) can be represented directly in terms of the spline basis, and amplitude covariance information is mapped onto position perturbation coordinates using the diagnostic relationship between the vorticity and stream functions, Equation (6). This resolves the issue of the degree of regularization imposed by the displacement function parameterization, since the position coefficient statistics will be computed directly from the amplitude covariance. For example, if $\delta\omega \sim \mathcal{N}(0, C_\omega)$, and we want to approximate position uncertainty by a Gaussian distribution, $\delta\Psi \sim \mathcal{N}(0, C_a)$, then we can estimate $C_a = T_{a\omega}C_\omega T_{a\omega}^T$.

For the remainder of this Section, we address a common issue encountered when computing statistical covariances in theoretical, numerical, and observational contexts. Techniques that estimate, propagate, or regularize statistical data often destroy the structure that distinguishes a valid covariance matrix from a generic square matrix. In these cases, one needs to (re)project the information back into the space of covariance matrices, i.e. symmetric positive semi-definite (SPSD) matrices. The sense in which a candidate projection is

closest to the given matrix also must be determined. Consider a small perturbation to a SPSD matrix A that contributes a negative eigenvalue: take any u in its nullspace and add the rank-1 perturbation $-\epsilon uu^T$ for some $0 < \epsilon \ll 1$. Then A is no longer positive semi-definiteness. Then subsequent covariance operations, such as the Kalman filter covariance update, can yield unexpected results. While there are methods of finding the closest SPSD matrix in the 2-norm, they are much more theoretically and computationally complex than in the Frobenius norm. A polar factorization of the symmetric matrix component of A , given by $B = (A + A^T)/2$, can be accomplished through a singular value decomposition. If $B = U_B \Sigma_B V_B^T$, where U_B and V_B are unitary and Σ_B is diagonal and positive semi-definite, then

$$B = QH = (U_B V_B^T) (V_B \Sigma_B V_B^T) \quad (27)$$

Observe that the first factor on the right-hand side is unitary, and since the second factor is a similarity transformation of Σ_B , then the result is SPSD.

Anticipating the needs of the two-stage statistical model, we also need an observation operator for the kind of displacement maps posed in (15), or rather
 375 the map parameters which index them. These are of course the components, at the observed locations, of the image of the velocity function under the coordinate transformation $Z = \Phi(z; a)$, for which we can write

$$\begin{aligned} h_p(a; \omega; \{x_{d,j}, y_{d,j}\}) = \\ h_a [\omega \circ \Phi^{-1}(\cdot; a); \{x_{d,j}, y_{d,j}\}] \end{aligned}$$

Note that a continuous interpolation for the vorticity function ω must be used to estimate the velocity at mapped observation locations, for which the most
 380 accessible choice is the current forecast ω^f , although other choices may be possible.

At this point, the only detail left to be addressed before an analysis scheme can be presented relates to the projection of forecast vorticity amplitude information into position coordinates. Such a method already has been introduced in Equation (18). The new wrinkle here is the imposition of boundary con-

ditions, without which the transformation operator from map parameters to vorticity values, $T_{\omega a}$, will not have full rank. This would preclude the definition of its pseudoinverse $T_{a\omega} = T_{\omega a}^\dagger$, which is the desired projection operator. In other words, the space of displacement map parameters must be restricted to a dimension equal to the degrees of freedom unconstrained by the boundary conditions. There are three sets of conditions to be imposed on the coefficients of the map function $\Psi(z; a) = \sum_{j=1}^{N_c} a_j B_j(z)$, where $N_c = (N_{c,x} + 3) \cdot (N_{c,y} + 3)$ is the number of B-spline coefficients: The Laplacian of the map function must be a fixed constant on ∂D , so we set $\Delta \Psi = 0$ on these nodes. The tangent gradient of the map function must be zero on ∂D , so we set $\Psi_y = 0$ for $x \in \{x_L, x_U\}$, and $\Psi_x = 0$ for $y \in \{y_L, y_U\}$. The height of the map function must be fixed on ∂D , so we set $\Psi(x_L, y_L) = 0$. The tangent condition prevents the map from moving vorticity mass out of the domain D where it is lost to the model. Since the displacement map is defined by derivatives of the map function, any constant term disappears. Constants typically are the first term of any basis for L^2 function representations on a compact domain, including bicubic splines, and the height condition removes this degree of freedom. These linear conditions on the map parameters can be expressed by the linear system

$$0 = W \cdot a = (U_W \Sigma_W V_W^T) \cdot a \quad (28)$$

where the last equality factors the constraint matrix into its singular value decomposition. If r_W is the rank of the constraint matrix, then the columns of V_b , defined to be the last $N_c - r_W$ columns of V_W , are a basis for the null space of W . Now any set of boundary-constrained map parameters can be represented by $a = V_b \cdot a_b$, and $T_{\omega a_b} = T_{\omega a} V_b$ will have full rank. Then the transformation operator from vorticity model space to boundary-constrained map parameter space is given by

$$T_{a\omega} = V_b T_{\omega a_b}^\dagger \quad (29)$$

Given a forecast covariance for the vorticity amplitude perturbations, P_ω^f , then a forecast displacement map parameter covariance, for perturbations subject to

zero-outflow boundary conditions, can be estimated from the projection $P_a =$
 385 $T_{a\omega} P_{\omega}^f T_{a\omega}^T$.

3.3. Two-stage Analysis Scheme

At each assimilation time t_k for $1 \leq k \leq N_a$ we seek a model (vorticity) state analysis $\omega = \omega^a$ which minimizes a likelihood functional that has been conditioned (or regularized) by a forecast penalty term,

$$\begin{aligned} \mathcal{J}_a[\omega] &= \frac{1}{2} \|d_V - h_a(\omega; \{z_{d,j}\})\|_{R^{-1}}^2 \\ &+ \frac{1}{2} \|\omega - \omega^f\|_{(P_{\omega}^f)^{-1}}^2, \end{aligned} \quad (30)$$

where d_V are observations of the velocity field at discrete points in D . Denote the time series of analysis ensembles in enKF by $\mathcal{E}_k^a = \{\omega_j^a(z, t_k)\}$, for $1 \leq j \leq N_{ens}$ and $0 \leq k \leq N_a$, initialized with the exact initial condition, $\omega_j(z, t_0) = \omega_0(z)$, for each ensemble member. See Appendix B. The goal of the enKF is to compute these analysis ensembles by statistical interpolation of forecast and observation ensembles at each analysis step. Denote this the *amplitude analysis step*, which specifically consists of the following: each forecast ensemble $\mathcal{E}_k^f$ is produced by integrating the generalized model over $t \in (t_{k-1}, t_k]$, using the previous analysis ensemble $\mathcal{E}_{k-1}^a$ as an initial condition. Each forecast member becomes the estimate of the forecast mean, $\omega^f \rightarrow \omega_j^f(\cdot, t_k)$, in their own copy of (30), with synthetic observations perturbed from original measurements, $d_{V,k,j} = d_{V,k} + \epsilon_{d,j,k}$, with $\epsilon_{d,j,k} \sim \mathcal{N}(0, R)$, simulating the spread of the same likelihood distribution. The members of each analysis ensemble are correlated by taking the corresponding forecast covariance to be the sample covariance from the forecast ensemble,

$$P_{\omega,k}^f = \frac{1}{N_{ens} - 1} \mathcal{E}_k^f \left(\mathcal{E}_k^f \right)^T \quad (31)$$

The enKF estimates a Kalman gain matrix, K_k , for the entire ensemble such that the linear combination of the simulated forecast and observation ensembles,

$$\mathcal{E}_k^a = \mathcal{E}_k^f + K_k \cdot \left[d_{V,k} - h_a \left(\mathcal{E}_k^f; \{z_{d,j}\} \right) \right] \quad (32)$$

has minimal analysis variance when h_a is linear and $N_{ens} \rightarrow \infty$. This Kalman gain follows the standard formula, replacing the forecast covariance with the sample covariance of the forecast ensemble,

$$K_k = P_{\omega,k}^f H_{a,k}^T (R + H_{a,k} P_{\omega,k} H_{a,k}^T)^{-1} \quad (33)$$

390 where $H_{a,k} = \nabla_{\omega} h_a(\omega; \{z_{d,j}\})$ at $\omega = \mathcal{E}_k^f$, the concatenation of linearizations of the vorticity observation operator about each forecast ensemble member.

The *displacement assimilation* strategy prefaces the amplitude analysis step by a position analysis that preconditions the forecast ensemble. The position statistical model follows the amplitude model in (30) in form, although the
395 statistics of the displacement map parameter distribution are regularized following (24) and (25). At each analysis step, between the generation of a new forecast ensemble and the assimilation of new observations, we seek a set of displacement parameters $a = a^a$ which optimize the cost functional

$$\begin{aligned} \mathcal{J}_p[a] &= \frac{1}{2} \|d_V - h_p(a; \omega^f, \{z_{d,j}\})\|_{R^{-1}}^2 \\ &+ \frac{1}{2} \|a - a^f\|_{(P_{d,\alpha}^f)^{-1}}^2 \end{aligned} \quad (34)$$

We note here a few key deviations from the usual enKF definitions: There is
400 no premise for a forecast displacement map, so we take $a^f = 0$ for all ensemble members and at all assimilation times. Consequently, the forecast map ensemble is collapsed, so we must obtain a forecast map parameter covariance some other way. Fortunately, we defined in the previous section the mapping $T_{a\omega}$ with which to project the forecast vorticity amplitude covariance. This information is
405 contained in the forecast vorticity ensemble, and as with the amplitude analysis, to avoid explicitly constructing the forecast vorticity covariance, the forecast increments are first projected into the much lower dimensional map parameter space. Forming the mean vorticity forecast ensemble $\hat{\mathcal{E}}^f$ from concatenated copies of the ensemble sample mean, then the forecast map parameter covariance

410 can be written as

$$P_{a,k}^f = \frac{1}{N_{ens} - 1} \left[T_{a\omega} \left(\mathcal{E}_{k,m}^f - \hat{\mathcal{E}}_{k,m}^f \right) \right] \cdot \left[T_{a\omega} \left(\mathcal{E}_{k,m}^f - \hat{\mathcal{E}}_{k,m}^f \right) \right]^T,$$

and of course still is subject to regularization before it can be used in (34). The new index m is defined below. There is no need to define a forecast map parameter ensemble, since it is 0 by construction. Let the analysis map parameter ensemble be denoted by $\mathcal{A}_{k,m} = \{a_{j,m}(t_k)\}$. Since the initial vorticity condition
 415 is known exactly, $\mathcal{A}_0 = 0$. At each subsequent analysis time t_k , the linear enKF position analysis update can be expressed as

$$\begin{aligned} \mathcal{A}_{k,m} &= 0 + L_{k,\alpha} \cdot \left[d_{V,k} - h_p \left(0; \mathcal{E}_{k,m}^f, \{z_{d,j}\} \right) \right] \\ &= L_k \cdot \left[d_{V,k} - h_a \left(\mathcal{E}_{k,m}^f; \{z_{d,j}\} \right) \right] \end{aligned} \quad (35)$$

where the Kalman gain matrix $L_{k,\alpha}$ for the map parameter estimator depends on the strain regularization parameters α , and is given by

$$L_{k,\alpha} = P_{a,\alpha,k} H_{p,k}^T (R + H_{p,k} P_{a,\alpha,k} H_{p,k}^T)^{-1} \quad (36)$$

where the linearization of the map parameter observation operator, $H_{p,k}$, must be taken with respect to a and not ω . From the chain rule, the linearization about $\mathcal{A}_{k,m} = 0$ is

$$\begin{aligned} H_{p,k} &= \nabla_a h_p \left(\mathcal{A}_{k,m}; \mathcal{E}_{k,m}^f, \{z_{d,j}\} \right) \\ &= \nabla_a \left[\mathcal{E}_{k,m}^f \circ \Phi^{-1}(\cdot; \mathcal{A}_{k,m}) \right] \\ &= \nabla_z \mathcal{E}_{k,m}^f \cdot \nabla_a \Phi^{-1}(\cdot; \mathcal{A}_{k,m}) \end{aligned} \quad (37)$$

420 Given the linearity and skew-symmetry of the stream function displacement map Φ defined in (15), then the gradient of the map about $\mathcal{A} = 0$ is

$$\begin{aligned} &\nabla_a \Phi^{-1}(\cdot; \mathcal{A})|_{(\mathcal{A}=0)} \\ &= \nabla_a \Phi(\cdot; -\mathcal{A})|_{(\mathcal{A}=0)} \\ &= \begin{bmatrix} B_y(\cdot) \\ -B_x(\cdot) \end{bmatrix} \end{aligned} \quad (38)$$

regardless of the map parameters $\mathcal{A}$, where we recall that $B(\cdot)$ are the basis functions of the map function Ψ . The resulting map parameter analysis ensemble defines a new forecast ensemble, presumably with less position error near observed features,

$$\mathcal{E}_{k,m+1}^f = \mathcal{E}_{k,m}^f \circ \Phi^{-1}(\cdot; \mathcal{A}_{k,m}) \quad (39)$$

where now can be seen that m counts the number of times this position correction process is repeated, $1 \leq m \leq M$.

4. Vortex Tracking Twin Experiment

425 A twin experiment was used to measure forecast and analysis errors by comparing the vorticity trajectory predicted by the standard and the displacement enKF to a truth which, like the forecast ensembles, is a simulation of the stochastic vorticity model. Observations of the entire truth are not permitted to be used with the filter, only a grid of noisy velocity measurements that have been
430 synthetically generated from the true vorticity trajectory. The analysis times were spaced far enough apart to begin to see performance differences between the standard and the displacement enKF. Constant-height contours at assimilation times are provided in Figures 5 and 6 to illustrate the effectiveness of each enKF in forecasting and tracking the truth. The number of ensemble members
435 was $N_{ens} = 5$. A more general argument comparing the efficiency and accuracy of each filter is made in Section 4.1. The contours show that the strain regularized displacement maps appear to generate tighter forecasts. The contours of the two-stage analyses preserve the circular feature geometry of the truth with much higher fidelity than the analyses provided by the standard filter. The loss
440 of structure may be due to the bias in forecast mean and inflation of forecast uncertainty that can arise from a spatially dispersed set of predictions of the same strong feature, such as an ensemble of realizations of the same vortex. Details supporting this claim will be presented in Section 4.1. That most of the forecast displacement is corrected without these distortions in the two-stage

445 analyses is evidence that strain regularization is penalizing excessively tortuous displacement maps.

In addition to the preservation of features, the performance of the standard and displacement enKF will be evaluated and compared by quantifying the resulting distributions of forecast error, $\epsilon^f := \omega^t - \omega^f$, and analysis error, $\epsilon^a :=$
450 $\omega^t - \omega^a$. The error bias, $\mathbb{E}(\epsilon)$, in the forecast and analysis of each filter is measured by comparing these to the true vorticity function at each analysis time in the L_2 -norm. The error variance, $\text{Var}(\epsilon)$, is measured by computing the sample variance of these errors over several repetitions of the twin experiment, and measuring this variance in the L_1 -norm. These are taken to be functions on
455 the entire model domain, D , and not just the observed subset, $D_d \subset D$; since the model interpolates the data, it is expected that the most accurate predictions will occur at observed locations. When the domain is only sparsely observed, the errors measured on D_d are not indicative of the accuracy of predictions made on all of D . Figure 7 gives the time sequences of forecast and analysis error biases
460 and variances for the standard and two-stage filters. More specifically, these are the average error bias and variance statistics for the 16 repetitions of the twin experiment with $N_{ens} = 5$. The consistently increasing error statistics are due to the fact that the boundary conditions do not permit energy to leave the system, as the stochastic forcing in the vorticity model continually increases the
465 model variance over time. It was shown in Figure 1 that the model uncertainty is dominated by position perturbations in the vortex positions, as opposed to amplitude perturbations. Likewise, the majority of forecast error removal is done through the position analysis. The standard filter does not define position error directly, so it cannot remove as much of the forecast variance with each
470 analysis step. This is why the error bias and variance is consistently higher with the standard enKF than for the displacement enKF.

4.1. Performance Comparison

The twin experiment of the previous section was repeated several times for several different ensemble sizes, N_{ens} (Table 1). Only the true vortex trajectory

Figure 4: **The common vorticity truth trajectory used in all twin experiments.** The array of observation locations for each twin experiment is displaced as black “+s.” Underlaid is a vorticity intensity map of one of the truth realizations, ω^t .

Figure 5: **Standard enKF analysis of the true vortex positions in Figure 4, with $N_{\text{ens}} = 5$.** The forecast (gray), analysis (black), and truth (blue/green) vortices are depicted by equal-height contours at $\omega = .5$.

Figure 6: **Displacement enKF analysis of the true vortex positions in Figure 4, with $N_{\text{ens}} = 5$.** Same conditions as in Figure 5.

Figure 7: Forecast and analysis estimation errors in tracking co-rotating vortices with zero-outflow boundary conditions.

Table 1: **Repetitions of twin experiment with stochastic vorticity model.**

N_{ens}	5	10	20	40
Sample size	16	12	10	8

was was reused for each repetition, which facilitates a comparison of the performance of each enKF version, while controlling for variations in observation noise and ensemble selection. For each experiment repetition, the observation errors and synthetic observations, as well as the model perturbations during ensemble integration, are driven by independent random processes. This variation is removed by averaging the error bias and variance statistics of all trials with a given ensemble size. Sensitivity to observation noise is not performed here. Rather, since the model variance naturally increases with time, then an examination of the forecast and analysis errors at different model times, $t = 150$ and 300, provides sensitivity information with respect to changes in a model variance parameter.

Figure 8 provides numerical evidence that both the standard and the displacement enKF estimates converge, although the displacement enKF does so more slowly. While the analysis bias error left by the standard enKF decays with order approximately $2/3$ and is robust to changes in model variance, the analysis bias of the displacement enKF is approximately half that, or order $1/3$, and slows by half again to order $1/6$ as model variance increases.

The forecast error bias indicates the predictive accuracy of the filter. It need not decay to zero, even if the analysis error does, since the accuracy of the prediction depends on more than the initial condition. Hence, a meaningful convergence rate is difficult to define or compute. However, a qualitative comparison of the forecast biases of the two filters shows the displacement filter is helping to improve predictive accuracy. The gains are nominal for low model variance, but as it increases, the forecast bias of the standard enKF increases for smaller ensembles ($N_{ens} < 40$), while the performance of the displacement enKF remains stable. This means the relative accuracy of the predictions of

Figure 8: **Decay of forecast and analysis error biases, $L_2\mathbb{E}(\epsilon)$, with increasing ensemble size.**

the displacement filter improves over that of the standard filter as model error increases.

The forecast and analysis error variance measures the confidence one can have in the state estimates provided by the filter, before and after, respectively, the assimilation of new data. Measurements of the uncertainty in predictions are as important as the predictions themselves, and in these terms the quantitative evidence in support of using a forecast displacement preconditioner is positive (Figure 9). The analysis error variance of the standard enKF decays at a robust order $4/3$, and again for smaller ensembles the modified enKF is slower to converge. However, for medium-sized ensembles and possibly larger, the displacement filter appears to regain the convergence of the standard method,

Table 2: **Percentage reduction in forecast variance, measured in the L_1 norm, by using displacement enKF, at $t = 150$.**

N_{ens}	5	10	20	40
L_1 (standard)	.064	.036	.023	.019
L_1 (two-stage)	.043	.029	.021	.019
% reduction	33	19	9	0

so that for all values tested, the displacement enKF provides more accurate analyses.

The displacement enKF also provides greater certainty in its state predic-
515 tions, based on an analysis of the improvements in forecast variance reduction
(Figure 9). For the small- to medium-sized ensembles tested, the forecast error
variance from the displacement filter was equal to or reduced compared to that
of the standard filter. As the ensemble size decreases, the variance reduction
increases up to 33% of the standard filter forecast error variance (Table 2). The
520 improvement in variance reduction is more pronounced as model variance in-
creases over time from $t = 150$ to $t = 300$, in which the percentage decrease
in forecast error variance ranges from 12% to 60% depending on the ensemble
size. Another way of looking at this data is in terms of the computational ef-
fort that is saved using the displacement filter to achieve a prescribed level of
525 forecast error variance (Tables 2 and 3). As the model variance increases, the
percentage reduction in the required ensemble size moves from approximately
30% to about 60%. Either measured in terms of forecast variance reduction or
computational efficiency, the evidence demonstrates that displacement filter can
improve vortex tracking.

530 5. Conclusions

We proposed a data assimilation strategy for the estimation of the mean and
the variance of the posterior distribution of a time evolution state variable sub-
ject to observations. It introduces an extra stage in the traditional sequential

Figure 9: Decay of forecast and analysis error variance, $L_1 \text{Var}(\epsilon)$, with increasing ensemble size.

Table 3: **Percentage reduction in forecast variance, measured in the L_1 norm, by using a displacement enKF, at $t = 300$.**

N_{ens}	5	10	20	40
L_1 (standard)	.133	.076	.045	.032
L_1 (two-stage)	.053	.041	.031	.028
% reduction	60	46	31	12

Table 4: **Percentage computational savings by using the displacement enKF, at $t = 150$.**

Desired L_1 forecast variance	.02	.03	.04
Required N_{ens} (standard)	35	14	9
Required N_{ens} (two-stage)	30	9	6
% reduction in computation	14	36	33

data assimilation strategy, wherein a kinematically constrained transformation
535 is applied in order to preserve geometric features of the state vector. Because the
constraint is imposed as a mapping of physical space (and in evolution problems,
by implication, on time) we denote the methodology as displacement assimila-
tion. The addition of the constraint is not intimately tied to the Kalman Filter.
However, we modified this particular estimation procedure to concretely suggest
540 how the additional constraint is used to produce a displacement assimilation.
The Kalman filter is one of the most widely used and familiar data assimilation
schemes and thus comparisons of the traditional strategy and the displacement
assimilation is instructive.

Morphing in data assimilation is not new, and in the image processing con-
545 text, the assimilation constraints can be dictated by computational constraints,
aesthetics, image processing constraints. Mariano in [15] and Frazin in [10]
use morphing to counteract the smoothing effect of sharp features produced by
assimilation procedures that minimize variance. Most Bayesian data assimila-
tion methodologies aim to minimize the posterior covariance of the state given

Table 5: **Percentage computational savings by using the displacement enKF, at $t = 300$.**

Desired L_1 forecast variance	.032	.04	.05
Required N_{ens} (standard)	40	25	18
Required N_{ens} (two-stage)	18	11	6
% reduction in computation	55	56	67

550 observations, but there is no guarantee that these estimates are even physical. For generic nonlinear/non-Gaussian dynamics problems, data assimilation methodologies that are ad-hoc when applied to nonlinear/non-Gaussian dynamics problems, this can be a very important source of concern. Adding physical constraints on the estimation process presumably produces higher fidelity in the
555 estimates. However, this is not necessarily what we are after here: the point of adding physical constraints and symmetries is to produce moments of the state that are based upon physically realizable samples or that obey essential basic laws implied by the symmetries. In evolution problems with high dimension state spaces, such as those common to geophysical fluid dynamics, the impact
560 of the constraint can be significant since it is often the case that in these settings tend to high dimension state variables and more often than not, be very sparsely sampled and poorly observed and thus the likelihood is poorly sampled.

In incompressible fluid flow a central constraint is that the velocity be divergence free. This global constraint implies mass conservation. Locally, vio-
565 lations in the incompressibility lead to errors in the velocity itself and thus in the advection and dispersion of the fluid itself or the tracers it carries. This has a bearing on applications ranging from time dependent pollution dynamics, weather/climate, fluid mechanics. For example, pinpointing pollution sources and accurately tracking the advection of pollutants, or estimating wave char-
570 acteristics, tracking large scale structures such as storm systems, etc. In two-dimensional flows, which is the setting of the dynamics in the current work, we chose for the proof of concept of the method, area-preserving maps that

automatically satisfy the conservation required by incompressibility in the flow.

The manner in which we invoke the extra constraints is not done here via a
575 hierarchical prior, since the constraints are deterministic. In order to make the
resulting optimization problem tractable, the constraint is imposed frequently
in time, so that the mapping is a small perturbation of the identity. As it turns
out, we cannot avoid invoking a weak prior when the method is implemented
numerically: we propose a regularization which is natural to the geometry of
580 the flow itself, based upon the strain field. Imposing the constraint exactly is
very computationally expensive if done frequently. Hence, in practice we find
that it is preferable to relax the exact constraint and use a regularization prior.
Nevertheless, we use it in the same spirit as in Tikhonov regularization and tune
its adjustable parameter so that the regularization has a significant effect on the
585 computation and minimal effect on the state variables being estimated.

The success of displacement assimilation, as applied to a simple system of
interacting vortices, is very encouraging. Although the dimension of the state
space is small, compared to the typical problem in the geophysical context, it
is highly nonlinear. In the numerical simulations we were able to demonstrate
590 that displacement assimilation permitted the retention of structure throughout
the data assimilation procedure, and further, reduced analysis error variance.
Within the context of ensemble data assimilation the effectiveness of displace-
ment assimilation was more dramatic for small ensembles. When model er-
ror was increased, the displacement assimilation required fewer ensemble mem-
595 bers in the estimation process than the standard enKF. These two outcomes
bode well in using the proposed scheme in data assimilation involving large
scale model simulations in which computing many ensemble members is cost-
prohibitive. The displacement correction adds computational cost but in the
vortex problem this was not an issue because local splining of the map function
600 proved effective. This type of analysis localization might prove useful in devel-
oping an efficient displacement correction in higher dimensional state spaces.

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Appendix A. Canonical Transformations in the Small-displacement Limit

Canonical transformations are coordinate transformations with the useful property that a simply-connected area remains simply-connected and has the same area after the transformation. The derivation of their form and properties is technical but well discussed standard texts on classical mechanics (e.g. [17]), so only their form is introduced here. The displacement vectors $(x, y) \rightarrow (X, Y)$ for each coordinate are determined by a twice continuously differentiable *map function* $\zeta(X, y; a)$, where a are parameters which uniquely determine each map function. Then the coordinate transformation is given by the following implicit system of differential equations:

$$\begin{aligned} x &= X + \frac{\partial}{\partial y} \zeta(X, y; a) \\ Y &= y + \frac{\partial}{\partial X} \zeta(X, y; a) \end{aligned} \tag{A.1}$$

It can be readily confirmed that the coordinate transformation defined by this system is area preserving by showing that its Jacobian and that of its inverse is unity.

If we solve for the displacements $X - x$ and $Y - y$ in Equation (A.1), we recover a system which approximately defines ζ to be a stream function for a velocity field parallel to the spatial increments. In the limit of small displacements, canonical transformations are equivalent to a particular divergence-free flow along stream function contours. The transformation equations can be rewritten so that the map Φ is an approximate cross-section of the flow. For a small time

parameter $0 < \epsilon \sim \|\nabla\zeta\| \ll 1$, define $\zeta_\epsilon(X, y) = \epsilon\Psi(x, y)$. Then,

$$\begin{aligned}\frac{\delta x}{\delta t} &= \frac{X - x}{\epsilon} = -\frac{1}{\epsilon} \frac{\partial \zeta_\epsilon}{\partial y}(X, y) \\ \frac{\delta y}{\delta t} &= \frac{Y - y}{\epsilon} = \frac{1}{\epsilon} \frac{\partial \zeta_\epsilon}{\partial X}(X, y)\end{aligned}$$

As $\epsilon \rightarrow 0$ (a formal limit) we get

$$\begin{aligned}\frac{\delta x}{\delta t} &= -\frac{\partial}{\partial y}\Psi(x, y) \\ \frac{\delta y}{\delta t} &= \frac{\partial}{\partial x}\Psi(x, y).\end{aligned}\tag{A.2}$$

620 and in the limit of small displacements, $\epsilon \rightarrow 0$, $z \rightarrow Z$, and the system converges to the stream function definition for a conservative velocity field.

Appendix B. The Ensemble Kalman Filter

The ensemble Kalman Filter (enKF) [18, 2] is an ensemble-based data assimilation technique for sequential problems. As in the standard Kalman Filter, the filter completes the assimilation process in two stages: a forecast and an analysis
625 stage. Unlike the linearized Kalman Filter, the extended Kalman Filter (EKF) (see [1] for background on the KF and EKF). The enKF uses an ensemble of model runs to compute a mean proposal at each filtering step. The analysis step is the same as in the Kalman Filter case. Namely, a Gaussian approximation is
630 made of the local posterior density, of the state vector given observations. With this assumption it is possible to write down the update on the mean, given observations, and an estimate of the posterior covariance. In the process the ensemble (model) mean, and a sample approximation of the (model) covariance are used in calculating the update and the Kalman gain. The enKF is partic-
635 ularly attractive because it is easy to code and requires minimal modifications to existing codes representing models.

At time t_0 , the random perturbations of initial conditions are $y_j^a(t_0) \sim p(y_0)$ for each $1 \leq j \leq N_{ens}$. Expressing ensembles as matrices of concatenated ensemble members, so that each analysis ensemble for $0 \leq k \leq N$ and forecast

ensemble for $1 \leq k \leq N$ can be written as the matrices

$$\mathcal{E}_k^a = [y_1^a(t_k) | \dots | y_{N_{ens}}^a(t_k)] \quad \mathcal{E}_k^f = [y_1^f(t_k) | \dots | y_{N_{ens}}^f(t_k)]$$

Then each forecast ensemble $\mathcal{E}_k^f$ at time t_k is just the column-wise integration of the model equations, using the previous analysis ensemble $\mathcal{E}_{k-1}^a$ at time t_{k-1} as initial conditions. We will also represent the sample mean of an ensemble as

$$\hat{\mathcal{E}}_k^f = [\hat{y}_k^f | \dots | \hat{y}_k^f],$$

where $\hat{y}_k = N_{ens}^{-1} \sum_{j=1}^{N_{ens}} y_j(t_k)$. The ensemble forecast covariance is

$$P_k^f = \frac{1}{N_{ens} - 1} \left(\mathcal{E}_k^f - \hat{\mathcal{E}}_k^f \right) \left(\mathcal{E}_k^f - \hat{\mathcal{E}}_k^f \right)^T.$$

Let the ensemble of synthetic observation realizations be denoted by $\mathcal{D}_k = [d_k + \epsilon_{k,1} | \dots | d_k + \epsilon_{k,N_{ens}}]$, where each normal variate $\epsilon_{k,j} \sim \mathcal{N}(t, \mathcal{R})$. The ensemble analysis and the forecast are related to each other via the standard Kalman filter estimator: The linear Kalman update for the analysis ensemble is given by

$$\mathcal{E}_k^a = \mathcal{E}_k^f + K_k \cdot [\mathcal{D}_k - h(\mathcal{E}_k^f)] \quad (\text{B.1})$$

where the observation operator $h(\cdot)$ is applied column-wise to each of the forecast ensemble members. The shared Kalman gain matrix can be expressed as

$$K_k = P_k^f H_k^T \left(H_k P_k^f H_k^T + R \right)^{-1} \quad (\text{B.2})$$

and $H_k = \nabla_y h(\mathcal{E})|(\mathcal{E} = \mathcal{E}_k^f)$ denotes the column-wise gradient of the ensemble observation operator evaluated at each forecast ensemble member.

When the observations are sparse so that $N_d \ll N$, a more efficient variant of (B.2), in terms of the observed forecast ensemble $h(\mathcal{E}_k^f) \in \Omega_d$, is used:

$$K_k = \frac{\mathcal{E}_k^f h(\mathcal{E}_k^f)^T}{N_{ens} - 1} \left[\frac{h(\mathcal{E}_k^f) h(\mathcal{E}_k^f)^T}{N_{ens} - 1} + R \right]^{-1}$$

One still can use the linearized observation matrix, $h(\mathcal{E}_k^f) \equiv H_k \mathcal{E}_k^f$, and achieve the same gain in efficiency. With this representation of the enKF analysis in (B.1), it can be written in as a weighted combination of the ensemble members,

$$\mathcal{E}_k^a = \mathcal{E}_k^f \cdot W_k \left[\mathcal{D}_k; h(\mathcal{E}_k^f), R \right].$$

Now, the weights W_k , rather than being dependent on the likelihood functional,
640 are dependent on the Gaussian parameters of the likelihood distribution.

Appendix C. Computational Parameters

Parameters of the generalized vorticity model and parameters of the two-stage filter:

- Domain geometry: $D = [-1.25, 1.25]^2$
- Domain discretization: $N_x = N_y = 64$ ($N = 4225$)
- Initial condition parameters:
- Vortex centroids x : $x_{c,1} = x_{c,2} = 0$
- Vortex centroids y : $y_{c,1} = -y_{c,2} = 2/3$
- Vortex radii: $r_{s,1} = r_{s,2} = 1/3$
- Vortex amplitudes: $a_1 = a_2 = 1$
- Time integration interval: $t \in [0, 300]$
- Integration time step: $\Delta t = 0.05$
- Model error boundary dampening width: $r_b = .1$
- Position analysis iterations: $M = 3$
- Map parameter discretization: $N_{c,x} = N_{c,y} = 20$ ($N_c = 441$)
- Regularization parameters: $\alpha_n = \alpha_s = 50$
- Observation dimensions: $N_{d,x} = N_{d,y} = 20$ ($N_d = 441$)
- Observation error standard deviation: $\tau = 10^{-3}$
- Model error pointwise standard deviation: $\sigma_V = 10^{-3}$
- Model error decorrelation length: $r_V = 0.707$
- Model error mode eigenvalue tolerance: $\lambda(Q_V) \geq 10^{-14}$
- Model error boundary dampening width: $r_b = .1$
- Assimilation time step: $\Delta t_a = 30$

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Figure 1

Figure 2a

Figure 2b

Figure 3a

Figure 3b

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Figure 4 3of6

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Figure 4 5of6

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Figure 5 1of6

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Figure 6 1of6

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Figure 6 4of6

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Figure 7 1of2

Figure 7 2of2

Figure 8 1of2

Figure 9 1of2

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