

Nonlinear Estimation and Control of Particle Trajectories in the Ocean

PI: Toshio Michael Chin

CoPI: Ashwanth Srinivasan

Division of Meteorology and Physical Oceanography
Rosenstiel School of Marine and Atmospheric Science
4600 Rickenbacker Causeway, Miami, Florida 33149

phone: 305-421-4057 fax: 305-421-4696 email: tchin@rsmas.miami.edu

Award Number: N000140710175

<http://www.rsmas.miami.edu/divs/mpo/People/Faculty/Chin/>

LONG-TERM GOALS

Our long-range goal is to develop optimization methods: 1) to estimate the physical state of the ocean in order to understand the present and future conditions and associated variability/uncertainty, and 2) to utilize such forecast information for control-decisions such as optimal drifter deployment strategy. This is being accomplished through the use of data assimilation methods for ocean circulation models and the study of extending the assimilation formulation to an optimal control problem.

OBJECTIVES

In this effort, we study application of the Monte Carlo numerical techniques to problems of ocean data assimilation and optimal drifter deployment. This report focuses on our efforts on application of the *particle filter* to the inverse Lagrangian prediction problem relevant to drifter deployment.

APPROACH

An *inverse Lagrangian prediction* (ILP) problem addresses retrospective estimation of drifter trajectories through a turbulent flow given their final positions. In a typical ILP scenario, the launch location of a single or a set of drifters in the past is sought given the present location(s) of these drifter(s). Due to chaotic nature of the forward Lagrangian problem and limitations in accuracy and resolution of current and wind data, it is usually difficult to expect a unique and deterministic answer to an ILP problem. It may, however, be possible to estimate the launch site and time statistically so that the drifters deployed in the estimated region and time would have the largest probability of arriving at the desired final location. For most practical problems it is desirable to minimize the optimal deployment region while maximizing the probability of successful delivery.

One approach to solving the ILP problem is to simulate an ensemble of Lagrangian trajectories backwards in time using the known final locations and a stochastic model of the flow field. Due to

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14. ABSTRACT Our long-range goal is to develop optimization methods: 1) to estimate the physical state of the ocean in order to understand the present and future conditions and associated variability/uncertainty, and 2) to utilize such forecast information for control-decisions such as optimal drifter deployment strategy. This is being accomplished through the use of data assimilation methods for ocean circulation models and the study of extending the assimilation formulation to an optimal control problem.					
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the typically fast rate (exponential or geometrical functions of time) dispersion of the trajectories, however, the distribution of the drifter locations tends to be too diffuse to be able to locate the launch site.

We have investigated a numerical method that employs the particle filter to control the spread of the drifter location (Chin and Mariano, 2008). The particle filter is a general sequential estimation method, is highly flexible, and is based on Monte Carlo simulations of the state trajectory (Doucet et al, 2001). Application of the particle filter to general data assimilation problems has been under consideration (van Leeuwen, 2003). Only a special case, known as the *ensemble Kalman filter* (Evensen, 1994) which is based on formulas optimal only under the assumption that the state (prognostic) variables have a jointly Gaussian distribution, has so far been found to be practical, because the particle filter otherwise demands a prohibitive number of samples of ocean state to be effective. However, since simulation of Lagrangian trajectories can be repeated easily without a prohibitive demand on computational resources, an unrestricted particle filter (that allows non-Gaussian distributions) would be applicable to ILP problem.

For ILP, we assume knowledge of an empirical time characteristics of *ensemble spread*, quantified here by the standard deviation

$$D_{\mathbf{r}}(t) = \sqrt{\frac{1}{N-1} \sum_{n=1}^N \|\mathbf{r}_n(t) - \bar{\mathbf{r}}(t)\|^2} \quad (1)$$

where $\mathbf{r}(t)$ is the unknown drifter trajectory, $\mathbf{r}_n(t)$ is the n^{th} sample of such trajectory by simulation, and $\bar{\mathbf{r}}(t) \equiv \sum_{n=1}^N \mathbf{r}_n(t)/N$ is the ensemble-mean of such samples. In ILP, the drifter trajectories simulated backward in time are expected to converge towards each other due to causality. For example, in our test cases, we have derived $D_{\mathbf{r}}(t) \propto t^c$ for $c \approx 4/3$ by forward simulations. To formally express the information with which to constrain the backward trajectory ensemble, we let $\mathbf{s}(t)$ be a fictitious “noisy observation” of the unknown trajectory $\mathbf{r}(t)$

$$\mathbf{s}(t) = \mathbf{r}(t) + \mathbf{e}(t) \quad (2)$$

where $\mathbf{e}(t)$ is vector of random observation errors each with a known variance E^2 . Assuming that $\mathbf{r}(t)$ and $\mathbf{e}(t)$ are uncorrelated, the variance of $\mathbf{s}(t)$ would become $D_{\mathbf{r}}(t)^2 + E^2$. Since the mean of $\mathbf{s}(t)$, or an observation of the mean trajectory, is not available, we estimate it in a bootstrapping fashion using the ensemble mean $\bar{\mathbf{r}}(t)$ of the on-going simulation. The probability density function (PDF) $p_{\mathbf{s}|\mathbf{r}}$ of the observation \mathbf{s} conditioned on the unknown \mathbf{r} is used by the particle filter algorithm to constrain the state trajectory; the specific algorithm is called the *resampled particle filter* (RPF; Chin et al 2007). By experimentation, we have found that an alternative, non-Gaussian PDF is effective in imposing the constraint onto the ensemble of backward trajectories:

$$p_{\mathbf{s}|\mathbf{r}}(\mathbf{x}|\bar{\mathbf{r}}, t) = \frac{1}{c} \exp \left[-\frac{1}{2} \left(\frac{\|\mathbf{x} - \bar{\mathbf{r}}\|^2}{D_{\mathbf{r}}^2 + E^2} \right)^F \right] \quad (3)$$

where c is a normalization constant and F is a constant parameter to control “flatness” of the PDF. For $F = 1$, $p_{\mathbf{s}|\mathbf{r}}$ would become a Gaussian PDF. We use $F = 3$ so that the PDF would have a relatively flat peak near its maximum. Choosing the larger value of F would give more equal

importance (probability) to the ensemble members within a certain distance from the maximum, rather than favoring those in the immediate vicinity of the maximum. More complete details of the numerical procedure can be found in (Chin and Mariano, 2008).

WORK COMPLETED

1) Performance of particle filter-based ILP solution method has been evaluated using test experiments of “source estimation” and “array deployment” (see Result below).

2) Inter-comparison study involving the EnROIF assimilation system, a Monte-Carlo (or ensemble-based) enhancements to the existing ROIF method (Chin et al 2002), is complete for the 1/12-degree resolution Gulf of Mexico circulation model using HYCOM, and a report (Srinivasan et al, 2008) is being finalized.

RESULTS

To examine performance of the particle filter-based ILP solution method, two types of controlled experiments have been conducted. In *source estimation experiment*, the final locations, called *targets* and denoted as \mathbf{X}_m , are given by forward trajectory simulations using a single launch site (for five different cases shown in Fig. 1). The goal is to estimate the launch-site probability distribution given the target locations using the filtered backward trajectory ensemble. In *array deployment experiment*, the target locations are arbitrarily chosen and there is no guarantee that a single launch site is sufficient to reliably deliver drifters to all targets.

We evaluate benefit of the particle filter (or more specifically RPF) by comparing two ensembles of trajectories. One is an ensemble produced with the RPF procedure denoted as $\mathbf{r}_n^{\text{RPF}}$, $n = 1, \dots, N$; the other is an ensemble of trajectories without any constraint and denoted as $\mathbf{r}_n^{\text{Ens}}$. To compare the two ensembles, the launch site distribution estimated by each ensemble is used to initialize some *test drifters* for *forward* trajectory simulations. The target locations estimated by the test drifters can then be used to evaluate statistical accuracy in reproducing the known target locations \mathbf{X}_m , $m = 1, \dots, M$.

Two skill scores are computed to compare the ensembles $\mathbf{r}_n^{\text{RPF}}$ and $\mathbf{r}_n^{\text{Ens}}$. By letting $G(\mathbf{X}_m)$ be the chance (in %) of the m^{th} target being reached by any of test drifters, we define the *coverage score* to be $\gamma \equiv \min_m G(\mathbf{X}_m)$. We also define the μ to be average chance (in %) of a test drifter to reach any of the targets. A higher μ value indicates that a drifter from the ensemble is less likely to miss a target and that the drifter destination is more likely to be focused near a target location. We hence call μ the *resolution score*.

For the source estimation experiment, the area bounded by the 95-percentile density contours (thick lines, Fig. 2) of $\mathbf{r}_n^{\text{Ens}}$ expands as the simulation progresses as expected, while the analogous area for $\mathbf{r}_n^{\text{RPF}}$ contracts in accordance with $D_r(t)$. By the launch time, $\mathbf{r}_n^{\text{RPF}}$ has surrounded the launch site (star, lower-right panel) tightly with the 10-percentile contour, while the $\mathbf{r}_n^{\text{Ens}}$ could surround the

launch site only loosely with the 50-percentile contour (lower-left panel). This observation, that the launch site estimate is significantly tighter for the filtered ensemble $\mathbf{r}_n^{\text{RPF}}$ than unconstrained ensemble $\mathbf{r}_n^{\text{Ens}}$, is generally true for each of five launches that we tested (Fig. 3). The area A_{95}^{RPF} enclosed by the 95-percentile contours of $\mathbf{r}_n^{\text{RPF}}$ was 19 \sim 32% of the unconstrained counterpart A_{95}^{Ens} (Table 1). The coverage scores were perfect ($\gamma = 100$) for both $\mathbf{r}_n^{\text{Ens}}$ and $\mathbf{r}_n^{\text{RPF}}$ in all five cases, implying that the filtered solutions are just as effective in delivering drifters to all target sites. The resolution scores are 1.6 to 1.9 times higher for the filtered results than their unconstrained counterparts, indicating that 1.6 to 1.9 times more drifters launched according to the filtered solution would reach a target than those prescribed by the unconstrained solution.

In the array deployment experiment, the launch site for each of four arrays of 5×5 targets (Fig. 4) is estimated. Again, the filtered ensemble $\mathbf{r}_n^{\text{RPF}}$ has yielded more compact estimate of the launch site than the unconstrained ensemble $\mathbf{r}_n^{\text{Ens}}$, as indicated by the ratio $A_{95}^{\text{RPF}}/A_{95}^{\text{Ens}}$ ranging 11 \sim 23% in four cases (Table 2). However, while the unconstrained solution has perfect coverage scores, the filtered solution has missed perfect coverage in all but one cases (γ^{RPF} , Table 2). In particular, there were one target site each in the ‘‘NW’’ and ‘‘SC’’ array cases and two target sites in the ‘‘SW’’ case that had less than perfect ($G(\mathbf{X}_m) < 100$) coverage. To remedy the coverage issue, we have performed the *supplemented RPF* (SPF) procedure, where extra simulations of backward drifters are initialized only at the target site(s) \mathbf{X}_m with imperfect coverage $G(\mathbf{X}_m) < 100$. The resulting, enhanced solution still is nearly as compact (Fig. 5) as before ($A_{95}^{\text{SPF}}/A_{95}^{\text{Ens}}$, Table 2), yet now with perfect coverage (γ^{SPF} , Table 2).

IMPACT/APPLICATIONS

We have explored a particle filter approach to solve the inverse Lagrangian prediction problem by an ensemble simulation of backward trajectories. The numerical experiments demonstrate that ensemble spread can be controlled using a constraint derived empirically and that the constrained solution leads to a spatially more compact estimate of the launch site. The constrained solution is thus more efficient than the unconstrained counterpart, while not compromising much effectiveness in delivery to the intended target sites. Due to high demands for shipping resources in drifter deployment, adopting the technique to actual operations and evaluating its benefits would be potential topics of future investigation.

The particle filter, more specifically the resampled particle filter, is well suited for realization of the constrained trajectory simulation due to flexibility of the method. While the particle filter methods are known generally to require a large number of samples to perform well (Chin et al 2007), this issue should not become a limiting factor in Lagrangian applications due to relatively low computational cost of simulating a trajectory given a background flow field.

Systematic errors in the background flow would pose the main challenge in application of the method studied. The main issue is not that these errors can affect the mean trajectory of a drifter ensemble (and hence the estimate of the launch site) but that there is general lack of viable models, statistical or otherwise, of such errors. Use of basis functions such as empirical orthogonal functions may be among the few available techniques to characterize systematic flow errors. Efforts are

under way to enhance the presented techniques to incorporate some assumed mathematical forms for systematic errors in the background flow field.

RELATED PROJECTS

The data assimilation (EnROIF) component of this project has been associated with the U.S. GODAE: Global Ocean Prediction with the Hybrid Coordinate Ocean Model (HYCOM), in collaboration with the HYCOM Consortium (<http://hycom.rsmas.miami.edu>).

The ILP solution methodology developed in this project may see applications in larval dispersal study (Cowen et al, 2008) using HYCOM simulated velocity fields over the Intra-America Seas region.

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Table 1. Skill scores from the source estimation experiment.

launch point	$A_{95}^{\text{RPF}}/A_{95}^{\text{Ens}}$	γ^{Ens}	γ^{RPF}	μ^{Ens}	μ^{RPF}	$\mu^{\text{RPF}}/\mu^{\text{Ens}}$
NW Saddle	0.186	100	100	29.1	48.4	1.66
Jet	0.210	100	100	30.1	52.8	1.76
Cold Core	0.278	100	100	38.5	66.4	1.72
Far East	0.316	100	100	49.4	80.9	1.64
Center Saddle	0.240	100	100	33.1	64.2	1.94

Table 2. Skill scores from the array deployment experiment.
“SPF” denotes supplemented RPF runs.

array	$A_{95}^{\text{RPF}}/A_{95}^{\text{Ens}}$	$A_{95}^{\text{SPF}}/A_{95}^{\text{Ens}}$	γ^{Ens}	γ^{RPF}	γ^{SPF}	μ^{Ens}	μ^{RPF}	μ^{SPF}
NW	0.232	0.279	100	39.5	100	57.4	79.3	76.4
NE	0.148	0.148	100	100.0	100	52.4	74.5	74.5
SC	0.111	0.135	100	21.4	100	55.2	73.5	73.2
SW	0.156	0.271	100	1.2	100	56.4	76.9	73.5

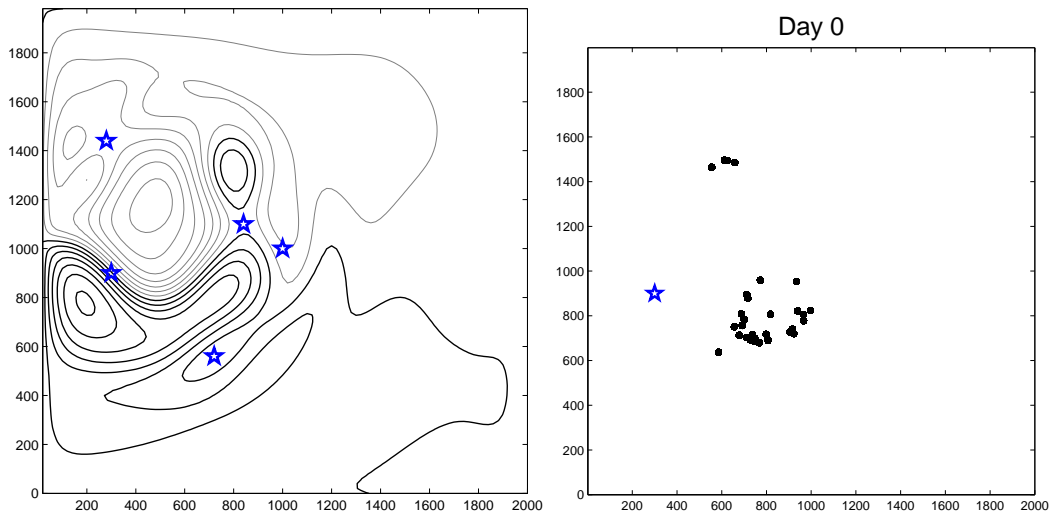


Figure 1. Left: The five launch sites (stars) and the background flow at the launch time (dark contours are anti-cyclonic; light contours are cyclonic) for the source estimation experiment. The launch sites are named, counter-clockwise from upper-left, “NW Saddle”, “Jet”, “Cold Core”, “Far East”, and “Center Saddle”. Right: The 30 target sites (dots) corresponding to the “Jet” launch site (star).

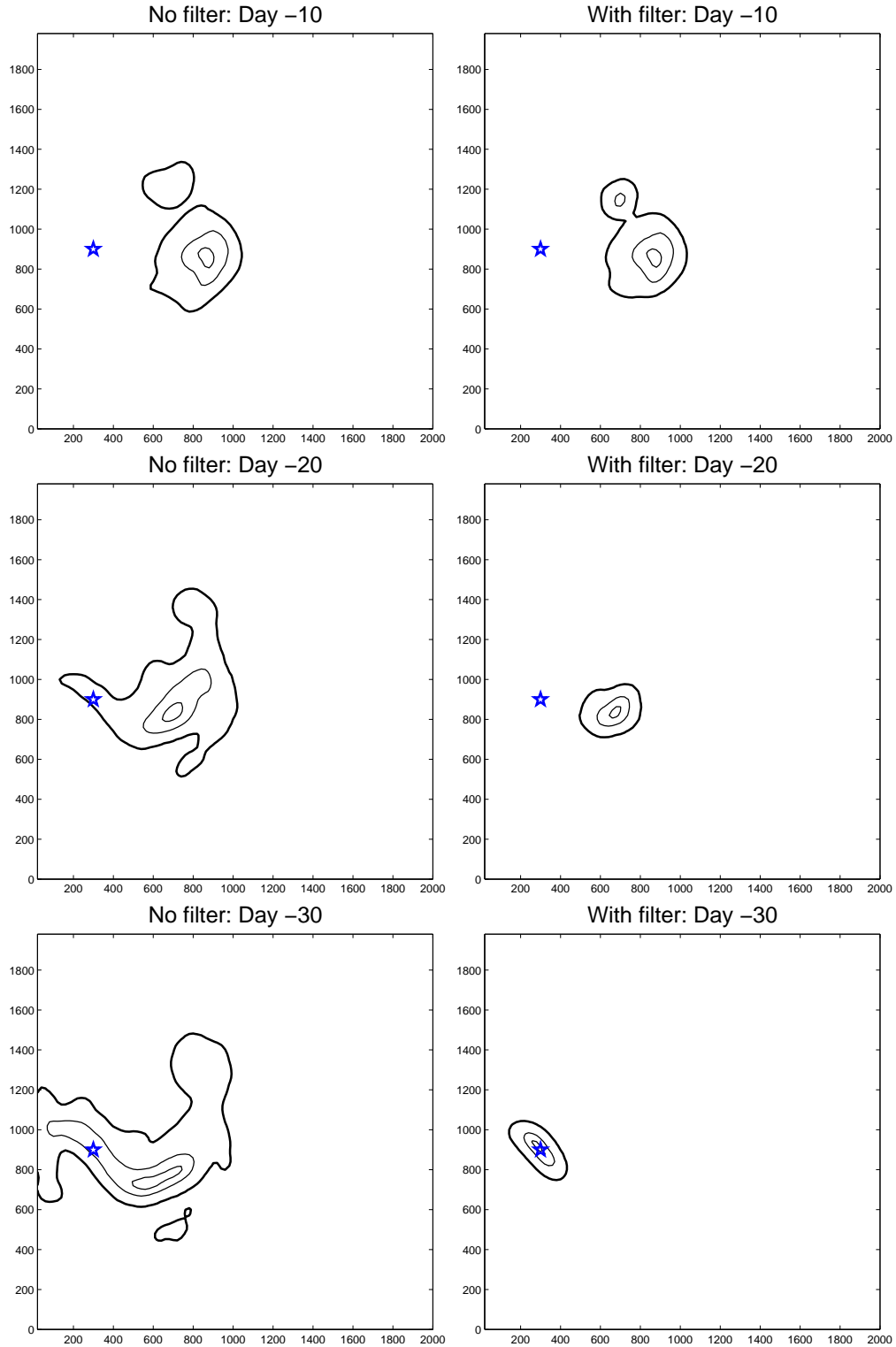


Figure 2. Progression of the density of backward drifters initialized at each of the 30 target sites shown in Fig. 1 (right panel). The 95 percentile (thick lines) as well as 50 and 10 percentile (thin lines) contours of the drifter density are shown after 10, 20, and 30 days of simulation. The left and right columns show the simulations without and with the particle filter, respectively. The source (star) is located more accurately with the particle filter after the 30-day analysis period.

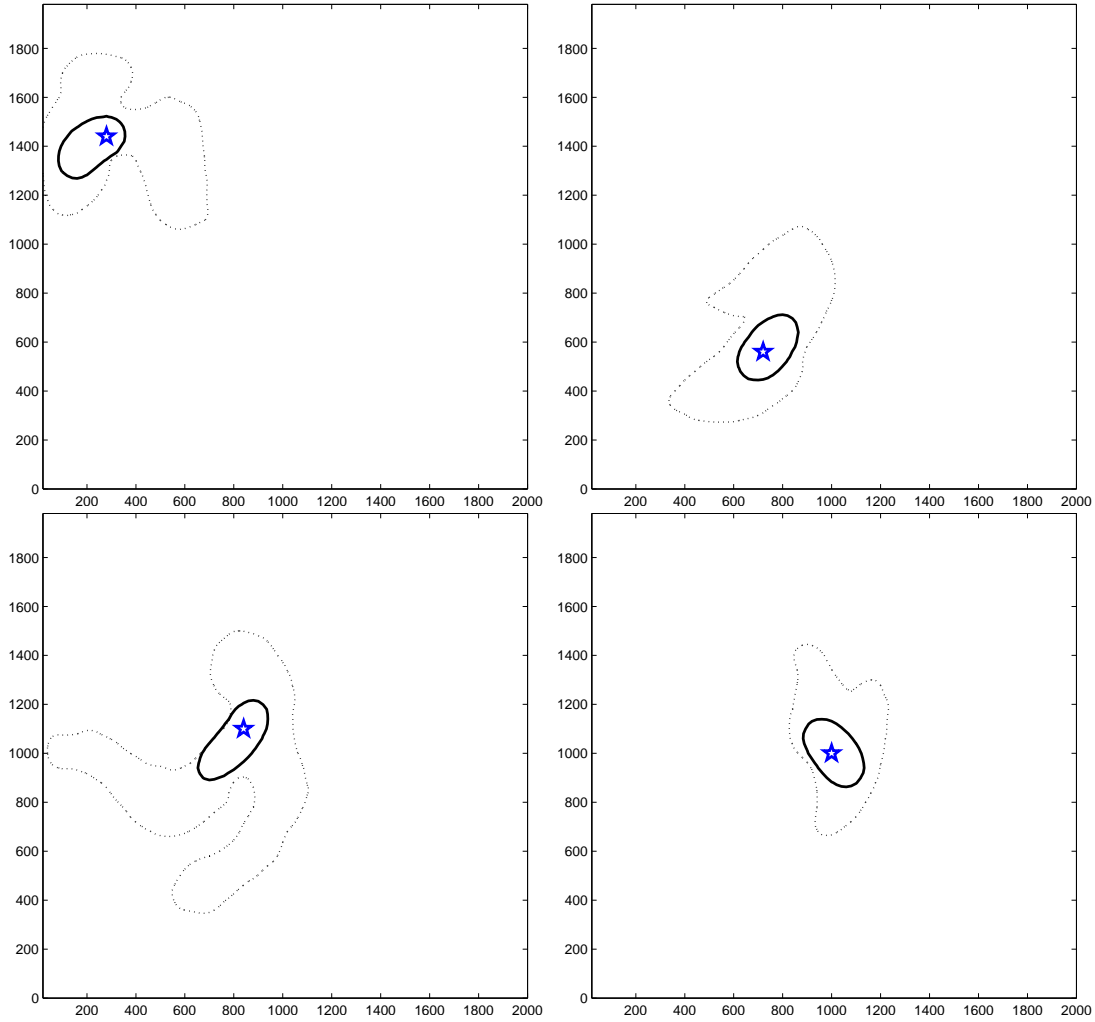


Figure 3. *The 95 percentile contours of the drifter density after 30 days of inverse simulation, estimating the four of five launch sites shown in Figure 1 (see Figure 2 for the one remaining launch site). Results obtained with (dark contour) and without (light contour) filter constraint are shown in each panel. Again, simulations with the particle filter can localize each launch site more tightly.*

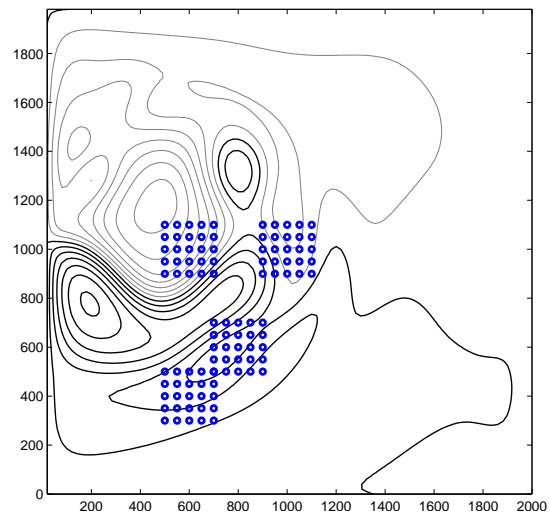


Figure 4. The four 5×5 arrays of target sites and the background flow at launch time (dark contours are anti-cyclonic; light contours are cyclonic) in the array deployment experiment. The target arrays are named, clockwise from top-left, “NW”, “NE”, “SC”, and “SW”.

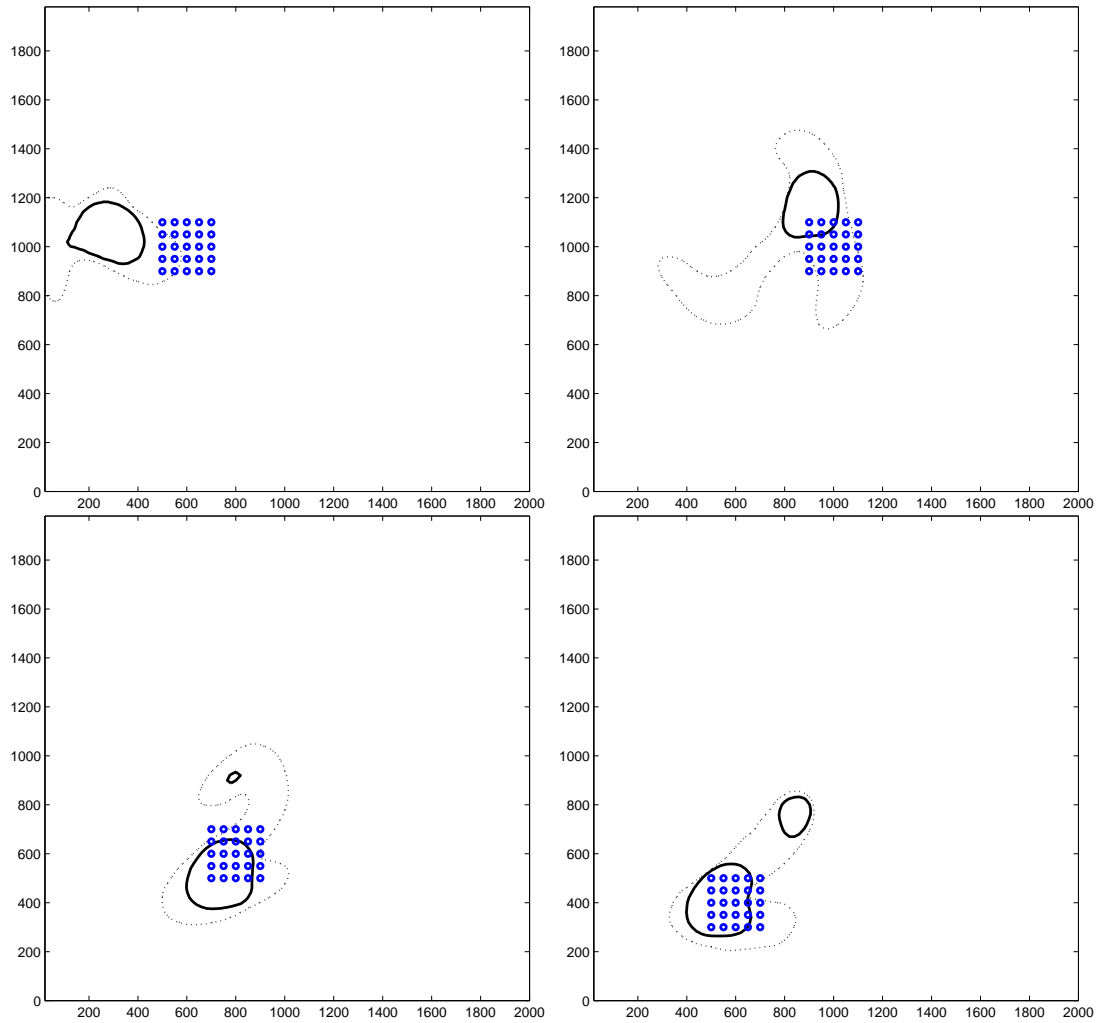


Figure 5. The 95 percentile contours of drifter density indicating the potential launch site to deploy the shown drifter array. Each panel shows results obtained with (dark contour) and without (light contour) the particle filter.