

Table 3
Filtering via ESSE at t_k : continuous-discrete problem statement

Dynamical model	$d\psi = \mathbf{f}(\psi, t)dt$, with $\hat{\psi}_0 = \Psi_0$.	(A1)
Measurement model	$d_k = C_k \psi_k + v_k$.	(A2)
Error subspace	$\{\Pi_k, \mathbf{E}_k$ with $\mathbf{P}_k^p = \mathbf{E}_k \Pi_k \mathbf{E}_k^T$ and $\text{rank}(\mathbf{E}_k) = p \min_{\Pi_k, \mathbf{E}_k} \text{tr}[\mathbf{P}_k^c]\}$.	(A3)
ES melding criterion	$\{\hat{\psi}_k \min_{\hat{\psi}_k} J_k = \text{tr}[\mathbf{P}_k^p(+)]$ using $[d_0, \dots, d_k]\}$.	(A4)

The estimation is treated in real-time as a minimum error variance filtering problem (Table 3). Using the error subspace (ES) concepts, the optimum rank- p approximation of \mathbf{P} is then the matrix \mathbf{P}^p which minimizes the trace of the complementary covariance \mathbf{P}^c , difference between \mathbf{P} and \mathbf{P}^p (Eq. (A3)). This optimum is the dominant rank- p eigendecomposition of \mathbf{P} , $\mathbf{E} \Pi \mathbf{E}^T$. The ES is characterized by the dominant rank- p error eigenvectors and eigenvalues, \mathbf{E} and Π . The filtering field estimate $\hat{\psi}_k$ (Eq. (A4)) hence minimizes the trace of the a posteriori error subspace covariance, based on past data and dynamics (Eqs. (A1), (A2), (A3) and (A4)).

The main quantities to be evolved are thus the field estimate, $\hat{\psi}$, and its principal error components and coefficients, \mathbf{E} and Π . In this study, the scheme addressing Table 3 is recursive. It requires initial conditions for the fields, Ψ_0 (Section 2.3), and for the ES, \mathbf{E}_0 and Π_0 (Section 3.1). The main ESSE computations hence consist of four steps: the initialization of the ES (Section A.1), the assimilation or data-forecast melding (Section A.2), the adaptive learning of the dominant errors (Section A.3), and the state and ES forecasts to the next assimilation time (Section A.4). All quantities are dimensional except in the SVDs so that the ordering of singular values is unit independent.³

A.1. Error subspace initial conditions

The construction of the initial ES, summarized by Table 4, uses the PE model and data available on Sept. 15. The model errors assumed null (A1) and the initial data coverage being almost uniform in space (Fig. 4a), the dominant initial error covariance is assumed proportional to the dominant covariance of the PE variability with respect to Ψ_0 . It is computed in two stages. The eigendecomposition of the covariance of the tracer variability is computed first, from data (Eqs. (A5), (A6), (A7), (A8), (A9), (A10) and (A11)). The dominant PE variability covariance is then estimated via adjustment PE integrations (Section 2.3), constructing the flow variability in accord with the dominant

³ Quantities marked with asterisks are normalized. For each field, the norm is the volume and sample averaged variance. The SVDs are carried out on normalized matrices \mathbf{M}^* such that $\mathbf{M} = \mathbf{N}\mathbf{M}^* = \mathbf{N}\mathbf{E}^* \Sigma \mathbf{V}^T$ and $\mathbf{E} = \mathbf{N}\mathbf{E}^*$, where the norm matrix $\mathbf{N} \in \mathbb{R}^{n \times n}$ is block diagonal. The notation $\text{SVD}_p(\cdot)$ denotes the operator that carries out this normalization, selects the dominant rank p SVD and renormalizes the output, to yield $\mathbf{E} \Sigma \mathbf{V}^T$.