EnKF-C user guide

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Contents

License

Introduction

EnKF-C aims to provide a compact generic framework for off-line data assimilation (DA) into large-scale layered geophysical models with the ensemble Kalman filter (EnKF). Here "light-weight" has higher priority than "generic"; that is, the code is not designed to cover every virtual possibility for the sake of it, but rather to be expandable in practical (from the author's point of view) situations. Following are its other main features:

- coded in C for GNU/Linux platform;
- model-agnostic;
- can conduct DA either in EnKF or ensemble optimal interpolation (EnOI) mode;
- permits multiple model grids;
- can handle rectangular or curvilinear horizontal grids, z, sigma or hybrid vertical grids.

EnKF-C is available from `https://github.com/sakov/enkf-c`. This user guide is a part of the EnKF-C package. It is also available from `http://arxiv.org/abs/1410.1233`.

The user guide has two main sections. Section 1 overviews the basics of the EnKF; section 2 provides technical description of EnKF-C.

Chapter 1

EnKF

1.1 Kalman filter

The Kalman filter (KF) is the underlying concept behind the EnKF. It is rather simple if formulated as the recursive least squares.

Consider the global (in time) nonlinear minimisation problem

$$\{\mathbf{x}_i^a\}_{i=1}^k = \arg\min_{\{\mathbf{x}_i\}_{i=1}^k} J_k(\mathbf{x}_1, \ldots, \mathbf{x}_k), \tag{1.1}$$

$$\begin{aligned} J_k(\mathbf{x}_1, \ldots, \mathbf{x}_k) = {} & (\mathbf{x}_1 - \mathbf{x}_1^f)^{\mathrm{T}} (\mathbf{P}_1^f)^{-1} (\mathbf{x}_1 - \mathbf{x}_1^f) \\ & + \sum_{i=1}^{k} \left[\mathbf{y}_i - \mathcal{H}_i(\mathbf{x}_i)\right]^{\mathrm{T}} (\mathbf{R}_i)^{-1} \left[\mathbf{y}_i - \mathcal{H}_i(\mathbf{x}_i)\right] \\ & + \sum_{i=2}^{k} \left[\mathbf{x}_i - \mathcal{M}_i(\mathbf{x}_{i-1})\right]^{\mathrm{T}} (\mathbf{Q}_i)^{-1} \left[\mathbf{x}_i - \mathcal{M}_i(\mathbf{x}_{i-1})\right]. \end{aligned} \tag{1.2}$$

Here $\{\mathbf{x}_i^a\}_{i=1}^k$ is a set of k state vectors that minimise the cost function (1.2); indices $i = 1, \ldots, k$ correspond to a sequence of DA cycles, so that $\mathbf{x}_1$ is the estimated model state at the first cycle and $\mathbf{x}_k$ is the estimated model state at the last cycle; $\mathbf{y}_i$ are observation vectors related to the model state by nonlinear observation operators $\mathcal{H}_i(\mathbf{x})$; $\mathcal{M}_i(\mathbf{x})$ are nonlinear model functions that map the model states $\mathbf{x}_{i-1}$ to $\mathbf{x}_i$; $\mathbf{P}_1^f$ is the initial state error covariance; $\mathbf{R}_i$ are observation error covariances; and $\mathbf{Q}_i$ are model error covariances; and $(\cdot)^{\mathrm{T}}$ denotes matrix transposition.

The minimisation problem (1.1, 1.2) is, generally, very complicated, but, luckily, has an exact solution in the *linear* case; moreover, this solution is recursive. Namely, assume that $\mathcal{M}$ and $\mathcal{H}$ are affine:

$$\mathcal{M}_i(\mathbf{x}^{(1)}) - \mathcal{M}_i(\mathbf{x}^{(2)}) = \mathbf{M}_i\,(\mathbf{x}^{(1)} - \mathbf{x}^{(2)}), \tag{1.3a}$$

$$\mathcal{H}_i(\mathbf{x}^{(1)}) - \mathcal{H}_i(\mathbf{x}^{(2)}) = \mathbf{H}_i\,(\mathbf{x}^{(1)} - \mathbf{x}^{(2)}), \tag{1.3b}$$

where $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}$ are arbitrary model states, and $\mathbf{M}_i$, $\mathbf{H}_i$ = Const. Then the cost function (1.2)

becomes quadratic and can be written in canonical form in regard to $\mathbf{x}_k$ as follows:

$$J_k(\mathbf{x}_1, \ldots, \mathbf{x}_k) = (\mathbf{x}_k - \mathbf{x}_k^a)^{\mathrm{T}} (\mathbf{P}_k^a)^{-1} (\mathbf{x}_k - \mathbf{x}_k^a) + \tilde{J}_{k-1}(\mathbf{x}_1, \ldots, \mathbf{x}_{k-1}),$$

so that

$$\min_{\{\mathbf{x}_i\}_{i=1}^{k-1}} J_k(\mathbf{x}_1, \ldots, \mathbf{x}_k) = (\mathbf{x}_k - \mathbf{x}_k^a)^{\mathrm{T}} (\mathbf{P}_k^a)^{-1} (\mathbf{x}_k - \mathbf{x}_k^a) + \text{Const.} \tag{1.4}$$

(*Proposition*) Then

$$\min_{\{\mathbf{x}_i\}_{i=1}^{k}} J_{k+1}(\mathbf{x}_1, \ldots, \mathbf{x}_k, \mathbf{x}_{k+1}) = (\mathbf{x}_{k+1} - \mathbf{x}_{k+1}^a)^{\mathrm{T}} (\mathbf{P}_{k+1}^a)^{-1} (\mathbf{x}_{k+1} - \mathbf{x}_{k+1}^a) + \text{Const}, \tag{1.5}$$

where

$$\mathbf{x}_{k+1}^a = \mathbf{x}_{k+1}^f + \mathbf{K}_{k+1} \left[\mathbf{y}_{k+1} - \mathcal{H}_{k+1}(\mathbf{x}_{k+1}^f) \right], \tag{1.6a}$$

$$\mathbf{P}_{k+1}^a = (\mathbf{I} - \mathbf{K}_{k+1} \mathbf{H}_{k+1}) \mathbf{P}_{k+1}^f, \tag{1.6b}$$

where

$$\mathbf{K}_{k+1} \equiv \mathbf{P}_{k+1}^f (\mathbf{H}_{k+1})^{\mathrm{T}} \left[\mathbf{H}_{k+1} \mathbf{P}_{k+1}^f (\mathbf{H}_{k+1})^{\mathrm{T}} + \mathbf{R}_{k+1} \right]^{-1} \tag{1.6c}$$

and

$$\mathbf{x}_{k+1}^f = \mathcal{M}_{k+1}(\mathbf{x}_k^a), \tag{1.7a}$$

$$\mathbf{P}_{k+1}^f = \mathbf{M}_{k+1} \mathbf{P}_k^a (\mathbf{M}_{k+1})^{\mathrm{T}} + \mathbf{Q}_{k+1}. \tag{1.7b}$$

This solution is known as the Kalman filter (KF, Kalman, 1960). Equations (1.7) describe advancing the system in time and represent the stage commonly called "forecast", while equations (1.6) describe assimilation of observations and represent the stage called "analysis". The superscripts f and a are used hereafter to refer to the forecast and analysis variables, correspondingly. The forecast and analysis model state estimates $\mathbf{x}^f$ and $\mathbf{x}^a$ are commonly called (simply) forecast and analysis. Matrix $\mathbf{K}$ is called Kalman gain.

There are a few things to be noted about the KF:

1. It follows from the Kalman filter (equations 1.4-1.7) that the state of the DA system (SDAS) $\mathbf{X}$ is carried by the estimated model state vector and model state error covariance:

$$\mathbf{X}_k = \{\mathbf{x}_k, \mathbf{P}_k\}. \tag{1.8}$$

2. The KF provides solution for the *last* analysis, corresponding to $\mathbf{x}_k^a$ in (1.1) (or, with a minor re-formulation, to the last forecast); finding the full (global in time) solution requires application of the Kalman *smoother* (KS). Both the KF and KS can be derived by decomposition of the positive (semi)definite quadratic function (1.2).

3. Because the SDAS represents a (part of a) solution of the global least squares problem, it does not depend on the order in which observations are assimilated or on their grouping.

4. Ditto, the SDAS does not depend on a linear non-singular transform of the model state in the sense that the forward and inverse transforms commute with the evolution of the DA system.

5. Solution (1.7, 1.6) can be *used* in a nonlinear case by approximating

$$\mathbf{M}_i \leftarrow \nabla \mathcal{M}_i(\mathbf{x}_{i-1}^a),$$
$$\mathbf{H}_i \leftarrow \nabla \mathcal{H}_i(\mathbf{x}_i^f),$$

in which case it is called the extended Kalman filter (EKF).

1.2 EnKF

The standard form of the KF (1.7, 1.6) is not necessarily the most convenient or suitable one in practice. The corresponding algorithms can be prone to loosing the positive definiteness of the state error covariance $\mathbf{P}$ due to round-up errors; and more importantly, explicit use of $\mathbf{P}$ makes these algorithms non-scalable in regard to the model state dimension.

Both these immediate problems can be addressed with the ensemble Kalman filter, or the EnKF. In the EnKF the SDAS is carried by an ensemble of m model states $\mathbf{E}$, which can be split into ensemble mean and ensemble anomalies:

$$\mathbf{X} = \{\mathbf{E}\} = \{\mathbf{x}, \mathbf{A}\}. \tag{1.9}$$

It is related to the SDAS of the KF (1.8) as follows:

$$\mathbf{x} = \frac{1}{m}\mathbf{E}\,\mathbf{1}, \tag{1.10a}$$

$$\mathbf{P} = \frac{1}{m-1}\mathbf{A}\mathbf{A}^{\mathrm{T}}, \tag{1.10b}$$

$$\mathbf{A} \equiv \mathbf{E} - \mathbf{x}\mathbf{1}^{\mathrm{T}}, \tag{1.10c}$$

where $\mathbf{1}$ is a vector with all elements equal to 1. The above means that the model state estimate is given by the ensemble mean, while the model state error covariance $\mathbf{P}$ is implicitly represented by the ensemble anomalies $\mathbf{A}$ via the factorisation (1.10b).

Representing the state error covariance via ensemble anomalies yields a number of numerical benefits. In large-scale geophysical systems the state size ($\sim 10^5 - 10^9$) makes it impossible to store and manipulate the state error covariance $\mathbf{P}$ directly. At the same time it is often/typically possible to represent essential variability via an ensemble of much smaller size ($\sim 10^2$) and manipulate $\mathbf{P}$ implicitly via operations with $\mathbf{A}$. Further, using $\mathbf{A}$ ensures positive semidefiniteness of $\mathbf{P}$.

Storing the SDAS via an ensemble of model states is the first essential feature of the EnKF. In theory, one could use it in an implementation of the KF along with explicitly calculated Jacobians $\mathbf{M}$ and $\mathbf{H}$ in equations (1.7) and (1.6). The EnKF makes a further step and uses the ensemble form of the SDAS for a derivative-less formulation of the KF. Moreover, it approximates derivatives using ensemble of finite spread that characterises the estimated uncertainty in the state:

$$\mathbf{E} \quad \leftarrow \quad \mathbf{x}\mathbf{1}^{\mathrm{T}} + \mathbf{A} \tag{1.11a}$$

$$\mathcal{H}(\mathbf{x}) \quad \rightarrow \quad \mathcal{H}(\mathbf{E})\,\mathbf{1}/m \tag{1.11b}$$

$$\mathbf{HA} \quad \rightarrow \quad \mathcal{H}(\mathbf{E})\left(\mathbf{I} - \mathbf{1}\mathbf{1}^{\mathrm{T}}/m\right) \tag{1.11c}$$

$$\mathcal{M}(\mathbf{x}) \quad \rightarrow \quad \mathcal{M}(\mathbf{E})\,\mathbf{1}/m \tag{1.11d}$$

$$\mathbf{MA} \quad \rightarrow \quad \mathcal{M}(\mathbf{E})\left(\mathbf{I} - \mathbf{1}\mathbf{1}^{\mathrm{T}}/m\right) \tag{1.11e}$$

$$\mathbf{HMA} \quad \rightarrow \quad \mathcal{H} \circ \mathcal{M}(\mathbf{E})\left(\mathbf{I} - \mathbf{1}\mathbf{1}^{\mathrm{T}}/m\right). \tag{1.11f}$$

This formulation is not the only one possible; one might also use the finite difference approximations:

$$\mathbf{E} \quad \leftarrow \quad \mathbf{x}\mathbf{1}^{\mathrm{T}} + \varepsilon\mathbf{A} \tag{1.12a}$$

$$\mathbf{HA} \quad \rightarrow \quad \mathcal{H}(\mathbf{E})\left(\mathbf{I} - \mathbf{1}\mathbf{1}^{\mathrm{T}}/m\right)/\varepsilon \tag{1.12b}$$

$$\mathbf{MA} \quad \rightarrow \quad \mathcal{M}(\mathbf{E})\left(\mathbf{I} - \mathbf{1}\mathbf{1}^{\mathrm{T}}/m\right)/\varepsilon \tag{1.12c}$$

$$\mathbf{HMA} \quad \rightarrow \quad \mathcal{H} \circ \mathcal{M}(\mathbf{E})\left(\mathbf{I} - \mathbf{1}\mathbf{1}^{\mathrm{T}}/m\right)/\varepsilon. \tag{1.12d}$$

In this form the filter represents a derivative-less ensemble formulation of the EKF. In practice the difference between the EnKF formulation (1.11) and the EKF formulation (1.12) is that the latter is more sensitive to small-scale variability and therefore more prone to instability, similar to the difference in behaviour of the Newton and secant methods.

The forecast stage of the EnKF involves just propagating each ensemble member:

$$\mathbf{E}_i^f = \mathcal{M}_i(\mathbf{E}_{i-1}^a). \tag{1.13}$$

This is a remarkably simple equation compared to the KF forecast equations (1.7), even though the model error still needs to be accounted for in some way. Because propagation of each ensemble member is independent from the other members, the forecast stage in the EnKF is naturally parallelisable.

One way to handle model error in the EnKF is to include stochastic model error into the model operator in (1.13). (This would make it different to the model operator in the KF, which is deterministic.) Another option is to use the multiplicative inflation. The third option is to mimic the treatment of model error in the KF, although this would require the "rank reduction" (Verlaan and Heemink, 1997, eq. 28) to prevent increasing the ensemble size.

At the analysis stage one has to update the ensemble mean and ensemble anomalies to match (1.6). This involves handling ensemble as a whole, which is different to the forecast stage, when each ensemble member is propagated individually.

Note that factorisation (1.10b) is not unique: if $\mathbf{A}$ satisfies (1.10b), then $\tilde{\mathbf{A}} = \mathbf{A}\mathbf{U}$, where $\mathbf{U}$ is an arbitrary orthonormal matrix $\mathbf{U}\mathbf{U}^{\mathrm{T}} = \mathbf{I}$, also satisfies (1.10b). However, $\tilde{\mathbf{A}}$ should not only factorise $\mathbf{P}$, but also remain an ensemble anomalies matrix, $\tilde{\mathbf{A}}\mathbf{1} = \mathbf{0}$. This requires an additional constraint $\mathbf{U}\mathbf{1} = \mathbf{1}$. Summarising, if $\mathbf{E} = \mathbf{x}\mathbf{1}^{\mathrm{T}} + \mathbf{A}$ is an ensemble that satisfies (1.10), then ensemble

$$\tilde{\mathbf{E}} = \mathbf{x}\mathbf{1}^{\mathrm{T}} + \mathbf{A}\mathbf{U}^p, \quad \mathbf{U}^p : \ \mathbf{U}^p(\mathbf{U}^p)^{\mathrm{T}} = \mathbf{I}, \ \mathbf{U}^p\mathbf{1} = \mathbf{1} \tag{1.14}$$

also satisfies (1.10). If $\mathbf{E}$ is full rank (i.e. $\mathrm{rank}(\mathbf{E}) = \min(m, n)$, where n is the state dimension), then each unique $\mathbf{U}^p$ generates a unique ensemble, and (1.14) describes all possible ensembles matching a given SDAS of the KF. Such transformation of the ensemble is called ensemble *redrawing*. In the linear case (i.e. for affine model and observation operators) redrawing of the ensemble in the EnKF does not affect evolution of the underlying KF; and conversely, in the nonlinear case the redrawing does indeed affect evolution of the underlying KF.

1.3 EnKF analysis

In this section we will give a brief overview of solutions for the EnKF analysis, and then describe the particular schemes used in EnKF-C.

1.3.1 Overview

In the "baseline" EnKF (full-rank ensemble, no localisation) the analysed SDAS matches that of the KF, although the algebraic side is indeed different. The update of the ensemble mean is generally straightforward, in accordance with that in the KF (1.6a). The details may depend on the chosen algorithm to achieve better numerical efficiency (see sec. 1.3.3).

The update of ensemble anomalies can be done either via a right-multiplied or left-multiplied (or post/pre-multiplied) transform of the ensemble anomalies:

$$\mathbf{A}^a = \mathbf{T}_L \, \mathbf{A}^f, \tag{1.15}$$

or

$$\mathbf{A}^a = \mathbf{A}^f \, \mathbf{T}_R. \tag{1.16}$$

$\mathbf{T}_L$ and $\mathbf{T}_R$ are referred to hereafter as left-multiplied and right-multiplied ensemble transform matrices (ETMs), respectively. Note that to preserve the ensemble mean $\mathbf{T}_R$ has to satisfy $\mathbf{T}_R\mathbf{1} = \alpha\mathbf{1}$, where α is an arbitrary constant. It follows from (1.14) that if $\mathbf{T}_R$ is a particular solution for the right-multiplied ETM, then (for a full rank ensemble) any other solution can be written as

$$\tilde{\mathbf{T}}_R = \mathbf{T}_R(\mathbf{U}^p + \alpha\mathbf{1}\mathbf{1}^{\mathrm{T}}), \quad \mathbf{U}^p : \; \mathbf{U}^p(\mathbf{U}^p)^{\mathrm{T}} = \mathbf{I}, \; \mathbf{U}^p\mathbf{1} = \mathbf{1}. \tag{1.17}$$

Similarly, the analysis increment can be represented as a linear combination of the forecast ensemble anomalies:

$$\mathbf{x}^a = \mathbf{x}^f + \mathbf{A}^f\mathbf{w}. \tag{1.18}$$

Equations (1.16) and (1.18) can be combined into a single transform of the ensemble:

$$\mathbf{E}^a = \mathbf{E}^f\mathbf{X}_5, \tag{1.19}$$

$$\mathbf{X}_5 = \frac{1}{m}\mathbf{1}\mathbf{1}^{\mathrm{T}} + \left(\mathbf{I} - \frac{1}{m}\mathbf{1}\mathbf{1}^{\mathrm{T}}\right)\left(\mathbf{w}\mathbf{1}^{\mathrm{T}} + \mathbf{T}_R\right) = \frac{1}{m}\mathbf{1}\mathbf{1}^{\mathrm{T}} + \mathbf{w}\mathbf{1}^{\mathrm{T}} + \left(\mathbf{I} - \frac{1}{m}\mathbf{1}\mathbf{1}^{\mathrm{T}}\right)\mathbf{T}_R, \tag{1.20}$$

as $\mathbf{1}^{\mathrm{T}}\mathbf{w} = 0$. When $\mathbf{T}_R : \; \mathbf{T}_R^{\mathrm{T}} = \mathbf{T}_R, \; \mathbf{T}_R\mathbf{1} = \mathbf{1}$ (which is the case for e.g. the ETKF and DEnKF), $\mathbf{1}^{\mathrm{T}}\mathbf{T}_R = \mathbf{1}^{\mathrm{T}}$, and (1.20) simplifies to

$$\mathbf{X}_5 = \mathbf{w}\mathbf{1}^{\mathrm{T}} + \mathbf{T}_R. \tag{1.21}$$

The designation $\mathbf{X}_5$ is used for historic reasons, following Evensen (2003).

1.3.2 Some schemes

As follows from the previous section, there are multiple solutions for the ETM that match the KF covariance update equation (1.6b); however the particular solutions may have different properties in practice due to the DAS nonlinearity, their algorithmic convenience, or their robustness in suboptimal conditions. This section provides some background for the schemes used in EnKF-C:

- ETKF;
- DEnKF.

ETKF

It is easy to show using the definition of $\mathbf{K}$ (1.6c) and matrix shift lemma (1.23) that

$$(\mathbf{I}-\mathbf{KH})\,\mathbf{P}^f = (\mathbf{I}-\mathbf{KH})^{1/2}\,\mathbf{P}^f\,(\mathbf{I}-\mathbf{KH})^{\mathrm{T}/2},$$

which yields the following solution for the left-multiplied ETM:

$$\mathbf{T}_L = (\mathbf{I}-\mathbf{KH})^{1/2} \tag{1.22}$$

(Sakov and Oke, 2008b), that is

$$\mathbf{A}^a = (\mathbf{I}-\mathbf{KH})^{1/2}\mathbf{A}^f. \tag{1.22a}$$

Hereafter by $\mathbf{X}^{1/2}$ we denote the unique positive definite square root from a positive definite (generally, non-symmetric) matrix $\mathbf{X}$, defined as $\mathbf{X}^{1/2} = \mathbf{V}\mathbf{L}^{1/2}\mathbf{V}^{-1}$, where $\mathbf{X} = \mathbf{V}\mathbf{L}\mathbf{V}^{-1}$ is the eigenvalue decomposition of $\mathbf{X}$. By "matrix shift lemma" we refer to the following identity:

$$\mathcal{F}(\mathbf{AB})\,\mathbf{A} = \mathbf{A}\,\mathcal{F}(\mathbf{BA}), \tag{1.23}$$

where $\mathcal{F}$ is an arbitrary function expandable into Taylor series. Rewriting (1.22a) as

$$\mathbf{A}^a = \left[\mathbf{I} - \frac{1}{m-1}\mathbf{A}^f(\mathbf{H}\mathbf{A}^f)^{\mathrm{T}}(\mathbf{H}\mathbf{P}^f\mathbf{H}^{\mathrm{T}}+\mathbf{R})^{-1}\mathbf{H}\right]^{1/2}\mathbf{A}^f$$

and using the matrix shift lemma, we obtain:

$$\mathbf{A}^a = \mathbf{A}^f\left[\mathbf{I} - \frac{1}{m-1}(\mathbf{H}\mathbf{A}^f)^{\mathrm{T}}(\mathbf{H}\mathbf{P}^f\mathbf{H}^{\mathrm{T}}+\mathbf{R})^{-1}\mathbf{H}\mathbf{A}^f\right]^{1/2}$$

which yields the corresponding to (1.22) right-multiplied ETM:

$$\mathbf{T}_R = \left[\mathbf{I} - \frac{1}{m-1}(\mathbf{H}\mathbf{A}^f)^{\mathrm{T}}(\mathbf{H}\mathbf{P}^f\mathbf{H}^{\mathrm{T}}+\mathbf{R})^{-1}\mathbf{H}\mathbf{A}^f\right]^{1/2} \tag{1.24}$$

(Evensen, 2004). Applying the matrix inversion lemma

$$(\mathbf{A}+\mathbf{ULV})^{-1} = \mathbf{A}^{-1} - \mathbf{A}^{-1}\mathbf{U}(\mathbf{L}^{-1}+\mathbf{V}\mathbf{A}^{-1}\mathbf{U})^{-1}\mathbf{V}\mathbf{A}^{-1}, \tag{1.25}$$

(1.22) can be transformed to:

$$\mathbf{T}_L = (\mathbf{I}+\mathbf{P}^f\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H})^{-1/2} \tag{1.26}$$

(Sakov and Bertino, 2011); and applying the matrix shift lemma yields the corresponding right-multiplied ETM:

$$\mathbf{T}_R = \left[\mathbf{I} + \frac{1}{m-1}(\mathbf{H}\mathbf{A}^f)^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}\mathbf{A}^f\right]^{-1/2}, \tag{1.27}$$

also known as the ensemble transform Kalman filter, or ETKF (Bishop et al., 2001).

Historic reference. Another (and probably the first) solution for $\mathbf{T}_R$ equivalent to (1.24) and (1.27) was found by Andrews (1968):

$$\mathbf{T}_R = \mathbf{I} - \frac{1}{m-1}(\mathbf{H}\mathbf{A}^f)^{\mathrm{T}}\mathbf{M}^{-1/2}\left(\mathbf{M}^{1/2}+\mathbf{R}^{1/2}\right)^{-1}\mathbf{H}\mathbf{A}^f, \tag{1.28}$$

where $\mathbf{M} \equiv \mathbf{H}\mathbf{P}^f\mathbf{H}^{\mathrm{T}} + \mathbf{R}$.

Equations (1.24, 1.27, 1.28) yield algebraically different expressions for the (unique) symmetric right-multiplied solution. Apart from being the only symmetric solution, it also represents the minimum distance solution for the ensemble anomalies: its ensemble of analysed anomalies is closer to the ensemble of forecast anomalies with the inverse forecast (or analysis) covariance as the metric than any other ensemble of analysed anomalies given by (1.17) (Ott et al., 2003, rev. 2005). This means that in the above sense the symmetric right-multiplied solution preserves the identities of ensemble members during analysis in the best possible way.

Note that while the left-multiplied solutions (1.22, 1.26) correspond to the symmetric right-multiplied solution, they are not symmetric.

In a typical DAS with a large scale model one can expect $m = 100$, $p = 10^3 - 10^7$, $n = 10^6 - 10^9$; that is

$$m \ll p \ll n. \tag{1.29}$$

Therefore, considering the size of ETMs ($n \times n$ for left-multiplied ETMs and $m \times m$ for right-multiplied ETMs), only right-multiplied solutions are suitable for use with large scale models. The ETKF solution (1.27) represents the most popular option due to its simple form and numerical effectiveness: for a diagonal $\mathbf{R}$, it only requires to calculate inverse square root of a symmetric $m \times m$ matrix. Also, along with the left-multiplied solution (1.26), it generally has better numerical properties than solutions (1.22) and (1.24) due to the fact that the inverse square root in it is calculated from the sum of a positive definite and a positive semi-definite matrices.

DEnKF

Assuming that $\mathbf{KH}$ is small in some sense, one can approximate solution (1.22) by expanding it into Taylor series about $\mathbf{I}$ and keeping the first two terms of the expansion:

$$\mathbf{T}_L = \mathbf{I} - \frac{1}{2}\mathbf{KH}. \tag{1.30}$$

This approximation is known as the deterministic Kalman filter, or DEnKF (Sakov and Oke, 2008a). It has a simple interpretation of using half of the Kalman gain for updating the ensemble anomalies; but apart from that the DEnKF often represents a good practical choice due to its algorithmic convenience and good performance in suboptimal situations. The DEnKF is the default scheme in EnKF-C.

1.3.3 Some numerical considerations

Instead of using the forecast ensemble observation anomalies $\mathbf{H}\mathbf{A}^f$ and innovation $\mathbf{y} - \mathcal{H}(\mathbf{x}^f)$ it is convenient to use their standardised versions:

$$\mathbf{s} = \mathbf{R}^{-1/2}\left[\mathbf{y} - \mathcal{H}(\mathbf{x}^f)\right]/\sqrt{m-1}, \tag{1.31}$$

$$\mathbf{S} = \mathbf{R}^{-1/2}\mathbf{H}\mathbf{A}^f/\sqrt{m-1}. \tag{1.32}$$

Then

$$\mathbf{w} = \mathbf{G}\mathbf{s}; \tag{1.33}$$

for the ETKF

$$\mathbf{T}_R = (\mathbf{I} + \mathbf{S}^{\mathrm{T}}\mathbf{S})^{-1/2}, \tag{1.34}$$

and for the DEnKF

$$\mathbf{T}_R = \mathbf{I} - \frac{1}{2}\mathbf{G}\mathbf{S}, \tag{1.35}$$

where

$$\mathbf{G} \equiv (\mathbf{I} + \mathbf{S}^{\mathrm{T}}\mathbf{S})^{-1}\mathbf{S}^{\mathrm{T}}, \tag{1.36}$$

$$= \mathbf{S}^{\mathrm{T}}(\mathbf{I} + \mathbf{S}\mathbf{S}^{\mathrm{T}})^{-1}. \tag{1.37}$$

Here (1.36) involves inversion of an $m \times m$ matrix, while (1.37) involves inversion of a $p \times p$ matrix. Therefore, in the DEnKF it is possible to calculate $\mathbf{w}$ and $\mathbf{T}$ using a single inversion of either a $p \times p$ or $m \times m$ matrix, depending on the relation between the number of observations and the ensemble size. In contrast, the ETKF (1.34) requires calculation of the inverse square root of an $m \times m$ matrix. Then, one can use expression (1.36) for $\mathbf{G}$ and calculate both inversion in it and inverse square root in (1.34) from the same singular value decomposition (SVD). This makes the DEnKF somewhat more numerically effective because, firstly, one can exploit situations when $p < m$ to invert a matrix of lower dimension and, secondly, it requires only matrix inversion, which can be done via Cholesky decomposition instead of SVD.

1.4 Localisation

Localisation is a necessary attribute of the EnKF systems with large-scale models, aimed at overcoming the rank deficiency of the ensemble. It can also be seen as aimed at reducing spurious long range correlations occurring due to the finite size of the ensemble; or at limiting the impact of distant observations because of the unreliability of the corresponding covariances.

There are two common localisation methods for the EnKF – covariance localisation (CL, Hamill and Whitaker, 2001; Houtekamer and Mitchell, 2001), also known as covariance filtering, and local analysis (LA, Evensen, 2003; Ott et al., 2003, rev. 2005). Although CL may have advantages in certain situations (non-local observations, "strong" assimilation), in practice the two methods produce similar results (Sakov and Bertino, 2011). For algorithmic reasons EnKF-C uses LA.

Instead of calculating the global ensemble transform $\mathbf{X}_5$, LA involves calculating local ensemble transforms $\overset{i}{\mathbf{X}}_5$ for each element i of the state vector. This is done using local normalised ensemble observation anomalies $\overset{i}{\mathbf{S}}$ and local normalised innovation $\overset{i}{\mathbf{s}}$, obtained by tapering global $\mathbf{S}$ and $\mathbf{s}$:

$$\overset{i}{\mathbf{s}} \equiv \mathbf{s} \circ \overset{i}{\mathbf{f}}, \tag{1.38a}$$

$$\overset{i}{\mathbf{S}} \equiv \mathbf{S} \circ (\overset{i}{\mathbf{f}}\,\mathbf{1}^{\mathrm{T}}), \tag{1.38b}$$

where $\overset{i}{\mathbf{f}}$ is the vector of taper coefficients for element i, and $\mathbf{A} \circ \mathbf{B}$ denotes by-element, or Hadamard, or Schur product of matrices $\mathbf{A}$ and $\mathbf{B}$. We consider non-adaptive localisation only, when a taper coefficient is a function of locations of the state element i (denoted as $\overset{i}{\mathbf{r}}$) and observation o (denoted as $\overset{\{o\}}{\mathbf{r}}$): $\overset{i}{\mathbf{f}}_o = g(\overset{i}{\mathbf{r}}, \overset{\{o\}}{\mathbf{r}})$, where g is the taper function. In layered geophysical models g is often assumed to depend only on horizontal distance between these locations:

$$\overset{i}{\mathbf{f}}_o = g(|\overset{i}{\boldsymbol{\rho}} - \overset{\{o\}}{\boldsymbol{\rho}}|), \tag{1.39}$$

or on combination of horizontal and vertical distances, e.g.: $\overset{i}{f}_o = g_{xy}(|\overset{i}{\boldsymbol{\rho}} - \overset{\{o\}}{\boldsymbol{\rho}}|) g_z(|\overset{i}{z} - \overset{\{o\}}{z}|)$, where $\mathbf{r} = (\boldsymbol{\rho}, z)$, and $\boldsymbol{\rho} = (x, y)$. In the case (1.39) for a given set of observations the local ensemble transform $\overset{i}{\mathbf{X}}_5$ depends only on horizontal grid coordinates of the state element $\mathbf{x}_i$ and can be used for updating all state elements with the same horizontal grid coordinates. This is currently the only option in EnKF-C.

Smooth taper functions have advantage over non-smooth functions (such as the boxcar, or step function) because they maintain the spatial continuity of the analysis. EnKF-C uses the popular polynomial taper function by Gaspari and Cohn (1999), which has a number of nice properties.

1.5 Asynchronous DA

Observations assimilated at each cycle in the KF are assumed to be made simultaneously at the time of assimilation. In such cases observations and DA method are referred to as *synchronous*. In reality, observations assimilated at a given cycle are made over some period of time called "data assimilation window" (DAW). If the DA method accounts for the time of observations, observations and DA method are referred to as *asynchronous*.

The EnKF can be naturally extended for asynchronous DA. Let us consider the minimisation problem (1.1, 1.2) in the case of perfect model $\mathbf{Q} = 0$. It becomes

$$\mathbf{x}_1^a = \arg\min \; J(\mathbf{x}_1), \tag{1.40}$$

$$J(\mathbf{x}_1) = (\mathbf{x}_1 - \mathbf{x}_1^f)^{\mathrm{T}} (\mathbf{P}_1^f)^{-1} (\mathbf{x}_1 - \mathbf{x}_1^f) + \sum_{i=1}^{k} \left[\mathbf{y}_i - \mathcal{H}_i(\mathbf{x}_i)\right]^{\mathrm{T}} (\mathbf{R}_i)^{-1} \left[\mathbf{y}_i - \mathcal{H}_i(\mathbf{x}_i)\right], \tag{1.41}$$

$$\mathbf{x}_{i+1} = \mathcal{M}(\mathbf{x}_i), \quad i = 1, \ldots, k-1. \tag{1.42}$$

Compared to the original problem, the dimensionality of the solution is much reduced due to relations (1.42), which mean that the model state at any time can be found by propagating the initial state: $\mathbf{x}_2 = \mathcal{M}_2(\mathbf{x}_1)$, $\mathbf{x}_3 = \mathcal{M}_3 \circ \mathcal{M}_2(\mathbf{x}_1), \ldots$. The cost function (1.41) can then be written as

$$J(\mathbf{x}_1) = (\mathbf{x}_1 - \mathbf{x}_1^f)^{\mathrm{T}} (\mathbf{P}^f)^{-1} (\mathbf{x}_1 - \mathbf{x}_1^f) + \left[\mathbf{y} - \mathcal{H} \circ \mathcal{M}(\mathbf{x}_1)\right]^{\mathrm{T}} \mathbf{R}^{-1} \left[\mathbf{y} - \mathcal{H} \circ \mathcal{M}(\mathbf{x}_1)\right], \tag{1.43}$$

where observations $\mathbf{y}$ represent the augmented observation vector: $\mathbf{y} = [\mathbf{y}_1^{\mathrm{T}}, \ldots, \mathbf{y}_k^{\mathrm{T}}]^{\mathrm{T}}$, $\mathbf{R}$ is the corresponding observation error covariance, and forward operator $\mathcal{H} \circ \mathcal{M}(\mathbf{x}_1)$ relates the initial state $\mathbf{x}_1$ to observations.

Note that usually only $\mathcal{H}$ is a function that depends on assimilated observations; now by introducing $\mathcal{H} \circ \mathcal{M}(\mathbf{x}) = \mathcal{H}[\mathcal{M}(\mathbf{x})]$ we have to assume that $\mathcal{M}$ also depends on observations, propagating the

initial state to the time of each observation. It is also possible to interpret $\mathcal{M}(\mathbf{x})$ as the *trajectory* starting from $\mathbf{x}$, while $\mathcal{H}$ maps it to observations.

Apart from the operator $\mathcal{H} \circ \mathcal{M}$, the cost function (1.43) has the same form as that for a single DA cycle with synchronous observations. Consequently, in the linear case (1.3) one can use solutions for $\mathbf{w}$ and $\mathbf{T}$ from section 1.3.3, subject to extending definitions of $\mathbf{s}$ (1.31) and $\mathbf{S}$ (1.32) as follows:

$$\mathbf{s} = \mathbf{R}^{-1/2} \left[\mathbf{y} - \mathcal{H} \circ \mathcal{M}(\mathbf{x}_1^f) \right] / \sqrt{m-1}, \tag{1.44}$$

$$\mathbf{S} = \mathbf{R}^{-1/2} \, \mathbf{H} \circ \mathbf{M} \, \mathbf{A}_1^f / \sqrt{m-1}, \tag{1.45}$$

where $\mathbf{H} \circ \mathbf{M}$ is the tangent linear operator of $\mathcal{H} \circ \mathcal{M}$ about $\mathbf{x}_1^f$. This means that to account for the time of observations in the EnKF one simply needs calculate innovation and forecast ensemble observation anomalies using ensemble at the time of each observation. There are no specific restrictions on $\mathbf{R}$, so that in theory observation errors can be correlated in time.

The minimisation problem (1.40),(1.43) implies assimilation time $t = t_1$; however, in the linear case the standardised innovation and ensemble observation anomalies in form (1.44,1.45) represent objects invariant to assimilation time: the reference to $\mathbf{x}_1$ is only needed to define forward operator $\mathcal{H} \circ \mathcal{M}$. Consequently, the ensemble transform $\mathbf{X}_5$ calculated from $\mathbf{s}$ and $\mathbf{S}$ can be applied to ensemble at any particular time to yield (the same) analysed trajectories for the ensemble members: $\mathcal{M}(\mathbf{E}) \, \mathbf{X}_5 = \mathcal{M}(\mathbf{E} \, \mathbf{X}_5)$. This time invariance of ensemble transforms can be used to update ensemble back in time using observations from future cycles without the need in backward model (Evensen and van Leeuwen 2000, sec. 6, Evensen 2003, app. D).

Note. The background term $(\mathbf{x}_1 - \mathbf{x}_1^f)^{\mathrm{T}} (\mathbf{P}^f)^{-1} (\mathbf{x}_1 - \mathbf{x}_1^f)$ in (1.43) can be seen as accumulating the previous history of the system rather than characterising the initial uncertainty in the global problem. In this case it is natural to anchor it to the previous analysis:

$$J(\mathbf{x}) = (\mathbf{x} - \mathbf{x}^f)^{\mathrm{T}} (\mathbf{P}^f)^{-1} (\mathbf{x} - \mathbf{x}^f) + [\mathbf{y} - \mathcal{H} \circ \mathcal{M}(\mathbf{x})]^{\mathrm{T}} \, \mathbf{R}^{-1} \, [\mathbf{y} - \mathcal{H} \circ \mathcal{M}(\mathbf{x})] \, . \tag{1.46}$$

Here $\mathbf{x}^f$ is the analysed state at the end of the previous cycle (it yields the forecast trajectory for the current cycle), and $\mathbf{P}^f$ is the corresponding state error covariance. Minimising J yields the analysed initial model state $\mathbf{x}^a$, which in turn yields the analysed trajectory. The analysed state error covariance is defined so that the analysed background term absorbs the observation term:

$$\mathbf{x}^a = \arg\min \; J(\mathbf{x}),$$

$$\mathbf{P}^a : \; J(\mathbf{x}^a) = (\mathbf{x}^a - \mathbf{x}^f)^{\mathrm{T}} (\mathbf{P}^a)^{-1} (\mathbf{x}^a - \mathbf{x}^f) + \mathrm{Const.}$$

This framework is a natural extension of the problem (1.1) in the linear, perfect-model case to continuous time; and is convenient for iterative minimisation.

1.6 EnOI

The EnOI, or ensemble optimal interpolation (Evensen, 2003), can be defined as the EnKF with a static or, more generally, pre-defined, ensemble anomalies. It can be summarised as follows:

$$\mathbf{x}_i^b = \mathcal{M}_i(\mathbf{x}_{i-1}^a), \tag{1.47}$$

$$\mathbf{x}_i^a = \mathbf{x}_i^b + \mathbf{A}^b \, \mathbf{w}_i, \tag{1.48}$$

where $\mathbf{x}^b$ is the forecast model state estimate referred to as background, and $\mathbf{A}^b$ is an ensemble of static, or background, anomalies; the corresponding state error covariance $\mathbf{P}^b$ is also often referred to as the background covariance.

The main incentive for using the EnOI is its low computational cost due to the integration of only one instance of the model. Despite of the similarity with the EnKF, the EnOI is a rather different concept, as there is no global in time cost function associated with it. Conceptually the EnOI is closer to 3D-Var, as both methods use static (anisotropic, multivariate) covariance. It is an improvement on the optimal interpolation, which typically uses isotropic, homogeneous and univariate covariance.

In contrast to the EnKF, due to the use of a static ensemble the EnOI avoids potential problems related to the ensemble spread; but at the same time it does critically depend on the ensemble, while the EnKF with a stochastic model typically "forgets" the initial ensemble over time.

The EnOI can account for the time of observations by calculating innovation using forecast at observation time, as in (1.44). This approach is commonly known as "first guess at appropriate time", or FGAT.

Chapter 2

EnKF-C

2.1 Design considerations

EnKF-C is designed to use horizontal localisation only. While some may argue that using vertical localisation might help to decrease the ensemble size, we believe that, for example, in the ocean the vertical structure is too complicated and non-uniform to allow simple and robust solutions in this regard. Generally, dynamical processes include a variety of barotropic and baroclinic components, and introducing vertical localisation in one form or another can be detrimental for the model's balances. On the other hand, with an ensemble size of about 100, normally one can ignore the problem of spurious vertical correlations and leave the system to deal with the vertical covariances on its own.

With the system using horizontal localisation only the model state effectively becomes a collection of independent horizontal fields updated based on their correlations with local observations. The assimilation is conducted by calculating a common horizontal field of local ensemble transforms and applying them to each horizontal field of the model.

2.2 The workflow

EnKF-C conducts data assimilation in three stages: *prep*, *calc* and *update*.

prep preprocesses observations so that they are ready for DA. It has the following work flow:

- read original observations and fill each observation into a uniform structure `measurement`;
- write observations to file `observations-orig.nc`;
- combine observations into superobservations;
- write super observations to `observations.nc`.

calc calculates ensemble transforms for updating the forecast ensemble of model states (EnKF) or the background model state (EnOI) in the following stages:

- read observations from `observations.nc`;
- calculate ensemble of forecast observations $\mathbf{HE}^f$ (EnKF) or ensemble of background observation anomalies $\mathbf{HA}^f$ and background observations $\mathbf{Hx}^f$ (EnOI);
- for each horizontal grid cell calculate local ensemble transforms $\mathbf{X}_5$ (EnKF) or background update coefficients $\mathbf{w}$ (EnOI);
- save these transforms to `X5.nc` (EnKF) or `w.nc` (EnOI);
- calculate and report forecast and analysis innovation statistics;
- calculate observation impact metrics DFS and SRF (sec. 2.7.6) and save them to `enkf_diag.nc`;
- save ensemble, observations and transforms/weights for specified horizontal locations to pointlog files (sec. 2.10).

Apart from this main mode of operation, *calc* can also calculate forecast innovations only or operate in a single observation experiment mode.

update updates the ensemble (EnKF) or the background (EnOI) using transforms calculated by *calc*, and saves the analysis according to specifications. It also adds analysis information to the pointlog files, and can calculate and save the ensemble spread.

2.3 Starting up: example 1

It may be a good idea to start getting familiar with the system by running the example in `examples/1`. The example has been put up based on the runs of regional EnKF and EnOI reanalysis systems for Tasman Sea developed by Bureau of Meteorology. It allows one to conduct a single assimilation for 23 December 2007 (day 6565 since 1 January 1990) with either EnKF or EnOI. To reduce the size of the system, the model state has been stripped down to two vertical levels and 100×100 horizontal grid. Due to its size (almost 80 MB) the data for this example is available for download separately from the EnKF-C code – see `examples/1/README` for details.

2.4 Parameter files

EnKF-C requires 5 parameter files to run:

- main parameter file;
- model parameter file;
- grid parameter file;
- observation types parameter file;
- and observation parameter file.

Examples of these parameter files can be found in `examples/1`. Running EnKF-C binaries with `--describe-prm-format` in the command line provides information on the parameter file formats.

2.4.1 Main parameter file

The main parameter file specifies the main parameters of DA and 4 other parameter files. Its format is described by running `enkf_prep`, `enkf_calc` or `enkf_update` with option `--describe-prm-format`:

```
>./bin/enkf_prep --describe-prm-format

  Main parameter file format:

    MODE            = { ENKF | ENOI }
  [ SCHEME          = { DENKF* | ETKF } ]
  [ ALPHA           = <alpha> ]                              (1*)
    MODEL           = <model prm file>
    GRID            = <grid prm file>
    OBSTYPES        = <obs. types prm file>
    OBS             = <obs. data prm file>
    DATE            = <julian day of analysis>
  [ WINDOWMIN       = <start of obs window in days from analysis> ] (-inf*)
  [ WINDOWMAX       = <end of obs window in days from analysis> ]   (+inf*)
    ENSDIR          = <ensemble directory>
    BGDIR           = <background directory>                 (MODE = ENOI)
  [ KFACTOR         = <kfactor> ]                            (NaN*)
  [ RFACTOR         = <rfactor> ]                            (1*)
    ...
    LOCRAD          = <loc. radius in km>
  [ STRIDE          = <stride> ]                             (1*)
  [ SOBSTRIDE       = <stride> ]                             (1*)
  [ FIELDBUFFERSIZE = <fieldbuffersize> ]                    (1*)
  [ INFLATION       = <inflation> [ <VALUE>* | PLAIN ]       (0.5*)
    ...
  [ REGION          = <name> <lon1> <lon2> <lat1> <lat2> [[<z1> <z2>] ... ]
    ...
  [ POINTLOG        <i> <j> [grid name]]
    ...
  [ EXITACTION      = { BACKTRACE* | SEGFAULT } ]
  [ BADBATCHES      = <obstype> <max. bias> <max. mad> <min # obs.> ]
    ...

  Notes:
    1. { ... | ... | ... } denotes the list of possible choices
    2. [ ... ] denotes an optional input
    3. ( ... ) is a note
    4. * denotes the default value
    5. < ... > denotes a description of an entry
    6. ... denotes repeating the previous item an arbitrary number of times
```

Global analysis

It is possible to conduct global analysis by setting `LOCRAD` and `STRIDE` to large numbers. This is demonstrated by target "global" in example 1.

2.4.2 Model parameter file

The model parameter file mainly describes the composition of the state vector by listing the model variables and specifying the associated grids.

```
>./bin/enkf_prep --describe-prm-format model

  Model parameter file format:

    NAME      = <name>

    VAR       = <name>
  [ GRID      = <name> ]                    (# grids > 1)
  [ INFLATION = <value> [<value> | PLAIN] ]
  [ RANDOMISE <deflation> <sigma> ]

  [ <more of the above blocks> ]
```

Each model variable is described in a block started by the entry for the variable name. The inflation parameters for a variable, if specified, override the common values set in the main parameter file (sec. 2.8.1). Entry RANDOMISE makes it possible to specify a "forgetting" model for a variable (sec. 2.12).

EnKF-C permits using multiple model grids. In this case each model variable must be associated with one of the grids defined in the grid parameter file. See `examples/4` for an example.

2.4.3 Grid parameter file

Grid parameter file describes grids used for model variables. Each grid is described in a section started by the grid name entry and contains the grid name, grid data file, and names of the dimensions and coordinates in the grid data file. It also contains variable names for the depth and for number of layers in a vertical column (z grids) or land mask (sigma grids):

```
>./bin/enkf_prep --describe-prm-format grid

  Grid parameter file format:

    NAME             = <name> [ PREP | CALC ]
    VTYPE            = { z | sigma | hybrid }
  [ VDIR             = { fromsurf* | tosurf } ]
  [ MAPTYPE          = { binary* | kdtree } (curvilinear grids) ]
    DATA             = <data file name>
    XVARNAME         = <X variable name>
    YVARNAME         = <Y variable name>
    ZVARNAME         = <Z variable name> (z | sigma)
  [ ZCVARNAME        = <ZC variable name> (z | sigma) ]
  [ HCVARNAME        = <hc variable name> (0.0*) (sigma) ]
  [ DEPTHVARNAME     = <depth variable name> (z | sigma) ]
  [ NUMLEVELSVARNAME = <# of levels variable name> (z) ]
  [ MASKVARNAME      = <land mask variable name> (sigma | hybrid) ]
```

```
  AVARNAME          = <A variable name> (hybrid)
  BVARNAME          = <B variable name> (hybrid)
[ ACVARNAME         = <AC variable name> (hybrid) ]
[ BCVARNAME         = <BC variable name> (hybrid) ]
  P1VARNAME         = <P1 variable name> (hybrid)
  P2VARNAME         = <P2 variable name> (hybrid)
[ STRIDE            = <stride> (common*) ]
[ SOBSTRIDE         = <sobstride> (common*) ]
[ SFACTOR           = <spread factor> (1.0*) ]
[ ZSTATINTS         = [<z1> <z2>] ... ]

[ <more of the above blocks> ]
```

The code is supposed to automatically identify the type of horizontal grid used, while the type of the vertical grid has to be specified explicitly.

Horizontal grids

At the moment, EnKF-C supports 3 main types of horizontal grids:

- equidistant rectangular grids aligned with physical coordinates;
- non-equidistant rectangular grids aligned with physical coordinates;
- quadrilateral simply connected grids (via libgu).

For rectangular grids the code tries to determine and handle periodicity in X or Y directions.

With some effort EnKF-C can also handle non-simply connected grids (like tri-polar ORCA grids). This is achieved by creating an auxiliary grid that is simply connected in grid index space by masking some nodes (replacing their coordinates with NaNs) in the original grid. Because only *prep* requires mapping from physical to grid space, this auxiliary grid is then used in *prep* only, while the original grid is used in *calc* and *update*. To specify that a grid entry is to be used in *prep* only one needs to add qualifier "PREP" after its name; and to specify that it is to be used in *calc* and *update* one needs to add qualifier "CALC". See `examples/3` for an example.

From version 1.37.0 such grids can also be handled by using grid mapping via kd-tree instead of the default mapping via spatial binary tree, which is now available from package gridutils-c. This is done by setting parameter `MAPTYPE` to "k".

Vertical grids

The vertical coordinates are used for mapping the depth/height (pressure) of non-surface observations to fractional layer index. The observation depth or height are assumed to be positive.

EnKF-C supports 3 types of vertical grids: Z; σ; and hybrid σ-p (σ - pressure).

For Z grids one needs to define vertical coordinates of layer centres (entry `ZVARNAME`) and (optionally) the coordinates of layer corners (`ZCVARNAME`). If coordinates of layer corners are not specified they are built by the code assuming that the surface layer starts at $z = 0$.

For σ grids the code implements the "new" vertical coordinate formulation from ROMS as described in `https://www.myroms.org/wiki/Vertical_S-coordinate`, Eq. 2 and elaborated by Shchepetkin in `https://www.myroms.org/forum/viewtopic.php?f=20&t=2189`. This formulation reduces to the "standard" σ grid if the entry `HCVARNAME` is not specified or if the corresponding variable in the grid file is set to zero. Similarly to Z grid, one needs to define the vertical coordinates of layer centres (entry `CSRVARNAME`) and (optionally) the coordinates of layer corners (entry `CSWVARNAME`).

The hybrid σ-p grids are implemented as described in `https://journals.ametsoc.org/doi/pdf/10.1175/2008MWR2537.1`. One needs to specify the A (`AVARNAME`) and B (`BVARNAME`) arrays for layer centres as well as the top and surface pressure (`P1VARNAME` and `P2VARNAME`). One can also specify optional A and B arrays for layer corners (`ACVARNAME`, `BCVARNAME`). The entry `DEPTHVARNAME` needs only to be specified for variables with non-surface observations.

By default, the code assumes that the surface starts at layer 0. If this is not the case, one needs to specify this explicitly by `VDIR = TOSURF`.

2.4.4 Observation types parameter file

Observation types are the interface that connects model and observations. They are specified in a separate parameter file. Each observation type is described in a separate section identified by the entry `NAME`. Apart from the type name, the section must contain the tag for the observation kind; associated model variable; the tag for the associated observation operator; and the allowed range. The optional parameters include the R-factor for the type (sec. 2.9) and spatial limits on corresponding observations. For example:

```
>./bin/enkf_prep --describe-prm-format obstypes

  Observation types parameter file format:

    NAME        = <name>
    ISSURFACE   = {0 | 1}
    VAR         = <model variable name> [...]
  [ OFFSET      = <file name> <variable name> ]    (none*)
  [ MLD_VARNAME = <model varname> ]                (none*)
  [ MLD_THRESH  = <threshold> ]                    (NaN*)
    HFUNCTION   = <H function tag>
  [ ASYNC       = <time interval> [c*|e]]          (synchronous*)
  [ LOCRAD      = <locrad> ... ]                   (global*)
  [ WEIGHT      = <weight> ... ]                   (1*)
  [ RFACTOR     = <rfactor> ]                      (1*)
  [ MINVALUE    = <minimal allowed value> ]        (-inf*)
  [ MAXVALUE    = <maximal allowed value> ]        (+inf*)
  [ XMIN        = <minimal allowed X coordinate> ] (-inf*)
  [ XMAX        = <maximal allowed X coordinate> ] (+inf*)
  [ YMIN        = <minimal allowed Y coordinate> ] (-inf*)
  [ YMAX        = <maximal allowed Y coordinate> ] (+inf*)
  [ ZMIN        = <minimal allowed Z coordinate> ] (-inf*)
  [ ZMAX        = <maximal allowed Z coordinate> ] (+inf*)
  [ WINDOWMIN   = <start of obs window in days from analysis> ] (-inf*)
  [ WINDOWMAX   = <end of obs window in days from analysis> ]   (+inf*)
```

```
  [ <more of the above blocks> ]
```

The tags for available observation operators are listed in array `allhentries` in file `calc/allhs.c`.

The `OFFSET` entry may be used for adding the known model bias to observations, for example, to specify the mean dynamic topography (MDT) when assimilating sea level anomaly (SLA) observations.

The localisation radius for an observation type, if specified, overrides the common value from the main parameter file. The R-factors for each observation type are obtained by multiplying the common value by the observation type value. (More on localisation radius and R-factor in sec. 2.9.)

The entry `OFFSET` allows one to add a new observation type without re-compiling the code. This can be useful e.g. for evaluating a new instrument (by getting an independent statistics for the new instrument and seeing the change in statistics for the old instruments).

The entries `MLD_VARNAME` and `MLD_THRESH` are used to calculate the model mixed layer depth for projecting the surface bias.

`WINDOWMIN` and `WINDOWMAX` override the corresponding common settings in the main parameter file for this observation type.

2.4.5 Observation data parameter file

Observation data parameter file specifies observations to be assimilated. EnKF-C has a simple policy in this regard: if a data file is listed in the observation data parameter file, then observations from this file are assimilated. This allows one using custom observation windows for particular observation types, instruments etc., specifying details on the script level during the parameter file generation.

In practice some of observations specified in the observation data parameter file can be outside the observation time window for the cycle. In this case the exact boundaries of the observation window can be specified by entries `WINDOWMIN` and `WINDOWMAX` in the main parameter file; observations with time outside interval `[DATE-WINDOWMIN, DATE+WINDOWMAX)` will be discarded.

The observation parameter file contains an arbitrary number of sections identified by entries `PRODUCT`. Each section specifies the observation type, input files, reader and, possibly, observation error:

```
./bin/enkf_prep --describe-prm-format obsdata

  Observation data parameter file format:

    PRODUCT   = <product>
    READER    = <reader>
  [ PARAMETER <name> = <value> ]
    ...
    TYPE      = <observation type>
```

```
  FILE      = <data file wildcard>
  ...
[ ERROR_STD = { <value> | <data file> } [ EQ* | PL | MU | MI | MA ] ]
  ...

[ <more of the above blocks> ]
```

Observation files can be defined using wildcards "*" and "?". Missing a file is reported in the log and is not considered to be a fatal error.

The line in the above example starting with `ERROR_STD` specifies the observation error. It can contain either a number or a file name. In the case of entering the file name there also should be another entry in the same line specifying the name of the variable to be read. The variable should have the same dimension (2D or 3D) as the associated observation kind as described by the field `issurface` in the array `allkinds` in file `common/obstypes.c` (sec. 2.4.4).

The line with observation error can also have another token specifying the type of operation to be conducted: `EQUAL` ($\sigma_{tot} \leftarrow \sigma_{now}$, default), `PLUS` ($\sigma_{tot} \leftarrow \sqrt{\sigma_{tot}^2 + \sigma_{now}^2}$), `MULT` ($\sigma_{tot} \leftarrow \sigma_{tot}\sigma_{now}$), `MIN` ($\sigma_{tot} = \max(\sigma_{tot}, \sigma_{now})$), or `MAX` ($\sigma_{tot} = \min(\sigma_{tot}, \sigma_{now})$). There can be several error entries in a section in the observation parameter file.

The observation time only matters if the observation type is specified to be "asynchronous" (see sec. 2.6.2). In this case the model estimation for the observation is made by using model state at the appropriate time. Otherwise, observations are assumed to be made at the time of assimilation, regardless of the actual observation time.

Note that there can be multiple blocks with the same product. This enables custom treatment of some specific data. For example, the following entries override observation error for Geosat (files with prefix `g1_`) on 23 May 2006:

```
# set observation error for Geosat to 7cm
product == RADS
type = SLA
reader = standard2
file=/short/p93/pxs599/obs/RADS-IB/y2006/m05/g?_d23.nc
error_std = 0.07

# use default errors for other altimeters
product == RADS
type = SLA
reader = standard2
file=/short/p93/pxs599/obs/RADS-IB/y2006/m05/[!g]?_d23.nc
```

2.5 File name conventions

EnKF-C assumes that the ensemble and background file names have some predefined formats. The file name for member `mid` and model variable `varname` is assumed to be `sprintf("mem%03d_%s.nc", mid, varname)`. The background file (EnOI only) for variable `varname` is assumed to be `sprintf("bg_%s.nc", varname)`. The above names are used for reading forecast states for synchronous DA and for

writing analyses, in the case if the analyses are appended to forecasts (true by default). For asynchronous DA the member and background file names for the time slot `t` are assumed to be `sprintf("mem%03d_%s_%d.nc", mid, varname, t)` and `sprintf("bg_%s_%d.nc", varname, t)`, correspondingly.

2.6 *prep*

prep is the first stage of data assimilation in EnKF-C. Its preprocesses observations by bringing them to a common form and merging close observations into so called superobservations.

By design, *prep* is supposed to be light-weight, so that it does not read either the ensemble or background, and the only model information it needs is the model grid. (Note that this may require some additional processing at later stages for models with dynamic grid, such as HYCOM.)

The name of the binary (executable) for *prep* is `enkf_prep`. It has the following usage and options:

```
>./bin/enkf_prep
  Usage: enkf_prep <prm file> [<options>]
  Options:
  --consider-subgrid-variability
      increase error of superobservations according to subgrid variability
  --describe-prm-format [main|model|grid|obstypes|obsdata]
      describe format of the parameter file and exit
  --describe-superob <sob #>
      print composition of this superobservation and exit
  --log-all-obs
      put all obs into observations.nc (default: obs within model domain only)
  --no-superobing
  --no-superobing-across-instruments
  --no-writing-orig-obs
  --version
      print version and exit
```

`enkf_prep` writes the preprocessed observations to file `observatons.nc`. It also writes original (not superobed) observations to `observatons-orig.nc` (provided that superobing has not been switched off by flag `--no-superobing`). By default, only observations within the model grid are written to it, but the the option `--log-all-obs` changes this behaviour to writing all observations from the input files.

2.6.1 Observation types, products, instruments, batches, readers

Types

Each observation has a number of attributes defined by the fields of the structure `observation`. One of them is observation type, which characterises the observation in a general way and relates it to the model state. For example, typical oceanographic observations may have tags SLA (for sea level anomalies), SST (sea surface temperature), TEM (subsurface temperature) and SAL (subsurface

salinity). Different types can be related to the same model variable, as do SST and TEM in the above example. Observation types are described in the corresponding parameter file (sec. 2.4.4).

Products

An observation is also characterised by "product". It can be a tag for an organisation that provides data from certain observational platforms, e.g.:

```
PRODUCT == RADS
TYPE = SLA
READER = standard2
FILE = obs/RADS-IB/y2007/m12/??_d19.nc
FILE = obs/RADS-IB/y2007/m12/??_d20.nc
FILE = obs/RADS-IB/y2007/m12/??_d21.nc
FILE = obs/RADS-IB/y2007/m12/??_d22.nc
FILE = obs/RADS-IB/y2007/m12/??_d23.nc

PRODUCT == NAVO
TYPE = SST
READER = standard
FILE = obs/NAVO/navo_20071219.nc
FILE = obs/NAVO/navo_20071220.nc
FILE = obs/NAVO/navo_20071221.nc
FILE = obs/NAVO/navo_20071222.nc
FILE = obs/NAVO/navo_20071223.nc
```

Instruments

The observational data from a product can be collected by a number of instruments. The corresponding field in the `measurement` structure is supposed to be filled by the observation reader.

Batches

An observation can be attributed to one of the groups called "batches", such as altimeter passes, Argo profiles etc., to enable detection and discarding of bad batches. Programmatically, to switch on capabilities associated with observation batches for a particular kind of observations, the observation batch ID needs to be set by the corresponding observation reader.

A batch of observations is considered bad if either the magnitude of its innovation bias or the mean magnitude of innovation exceed specified thresholds. Specifications for bad batches can be set in the parameter file as follows:

```
BADBATCHES = SLA 0.06 0.10 500
BBADBATCHES = TEM 4 5 0
BADBATCHES = SST 0.5 2 10000
BADBATCHES = SAL 1.5 2 0
```

The above entry means that any batch of observations of type SLA (typically, an orbit) containing more than 500 observations and having either mean innovation greater than 0.06 (meter) in magnitude or mean absolute innovation greater than 0.10 is considered to be bad. Similarly, a TEM batch (typically, a profile) is considered bad if the mean innovation exceeds 4 (degrees) or the mean absolute innovation exceeds 5 (degrees). The parameter file can have arbitrary number of such entries. Information about bad batches is written by `enkf_calc` to the file `badbatches.out`. When `enkf_prep` detects the presence of such file, it marks the corresponding observations as bad.

Therefore, the workflow for detecting and eliminating bad batches of observations is as follows:

1. specify bad batches in the parameter file;
2. make a pilot run of `enkf_prep`;
3. run `enkf_calc` with the flag `--forecast-stats-only`;
4. remove `observations.nc` and `observations-orig.nc`;
5. calculate analysis in a "normal" way by running `enkf_prep`, `enkf_calc` and `enkf_update`.

Note that bad batches are identified at stage 2 based on superobservations formed by observations from the same batch only. Consequently, detection of bad batches may become unreliable if there are not enough such "clean" superobservations. It is possible to alleviate this problem by (1) switching off superobing by setting `SOBSTRIDE = 0` or specifying `--no-superobing` for `enkf_prep` and/or (2) by processing observations by parts, one type (or instrument) at a time, and repeating stages 1 and 2 as many times as necessary.

Readers

The function of data readers is to read observations in specified files and parse them sequentially into `struct observation` defined in `common/observations.h`.

At the moment there are few agreed standards for observational data. Even data of similar nature may have specific features that require creating a new or modify an existing observation data reader. It is therefore likely that developing a completely new system will require add new data readers.

The new readers can be created based on existing ones, or developed from scratch. The available readers are listed by the variable `allreaders` defined in `prep/allreaders.c`. Each reader can be specified in the observation data parameter file with an arbitrary number of parameters. For example, the following section changes the default minimal depth for using altimetry observations to 150 m:

```
(...)
product == RADS
type = SLA
reader = standard2
parameter MINDEPTH = 150
(...)
```

There are also several generic readers:

```
reader_xy_scattered
reader_xy_gridded
reader_xyz_scattered
reader_xyz_gridded
```

These readers allow one to specify a number of parameters by means of the entry `PARAMETER` of the observation data parameter file. At the moment the only obligatory parameter for these readers is `VARNAME`; a number of other obligatory parameters (e.g. `LONNAME`, `LATNAME`) can be specified either via the entry `PARAMETER` or by using default variable names in data files.

2.6.2 Asynchronous DA / FGAT

An observation type can be specified as "asynchronous" by specifying entry `ASYNC` in the observation types parameter file (sec. 2.4.4), e.g.:

```
NAME = SST
(...)
ASYNC = 1
(...)
```

The above means that SST observations are considered to be asynchronous with time bins of 1 day. If, for example, the assimilation time is specified as "6085.5 days since 1990-01-01", then the interval 0 is centred (by default) at the time of assimilation, i.e. will be from day 6080.0 to day 6081.0; interval -1 – from day 6079.0 to day 6080.0, interval 1 – from day 6081.0 to day 6082.0, and so on. It is possible to shift the asynchronous intervals so that not the centre but the start of interval 0 is located at the time of assimilation. In this case one needs to add qualifier "e" after the length of the interval, i.e.

```
NAME = SST
(...)
ASYNC = 1 e
(...)
```

The interval 0 will then be from day 6085.5 to day 6086.5.

The model states for each asynchronous interval are read from files with names `mem<xxx>_<variable name>_<time shift>.nc` in the ensemble directory (for the EnKF) or `bg_<variable name>_<time shift>.nc` in the background directory (for the EnOI). Here "time shift" is the interval ID (with the interval 0 being centred/starting at the observation time). If the corresponding members (or the background files, in the case of EnOI) are found, the observations are assimilated asynchronously; if they are not found, then the observations are assimilated synchronously. This can be tracked from the *calc* log file, e.g.:

```
calculating ensemble observations:
2014-03-22 06:28:28
  ensemble size = 96
  distributing iterations:
    all processes get 6 iterations
    process 0: 0 - 5
  SST |aaaaaa|aaaaaa|aaaaaa|aaaaaa|aaaaaa
  SLA |aaaaaa|aaaaaa|aaaaaa|aaaaaa|aaaaaa
  TEM ......
  SAL ......
```

The entries "a" mean that the observations are assimilated asynchronously and the files and the corresponding (by name) files have been found. These entris would be replaced by "s" if the observations were assimilated synchronously because of lacking the corresponding files. The vertical lines indicate the time slots for asynchronous DA; in the above example the DAW has 5 time slots. The entries "." indicate calculating ensemble observations for synchronous observations. Note that only the master process is writing to the log here, which explains why there is only output from 6 members in the log above. For EnOI there also will be "+" at the end of the line for each observation type indicating reading of the corresponding background field.

2.6.3 Superobing

"Superobing" is the process of reduction of the number of observations by merging spatially close observations before their assimilation. EnKF-C merges observations if:

- they belong to the same model grid cell;
- are of the same type;
- for asynchronous observations – belong to the same time slot.

The horizontal size of superobing cells can be increased from the default of 1 model grid cell to $N \times N$ cells by setting `SOBSTRIDE = <N>` in the parameter file; the vertical size is always equal to 1 layer. Setting `SOBSTRIDE = 0` switches superobing off.

The observations are merged by averaging their values, coordinates and times with weights inversely proportional to the observation error variance. The observation error variance of a superobservation is set to the inverse of the sum of inverse observation error variances of the merged observations. The product and instrument fields of the superobservation are set either to those of the merged observations or to -1, depending on whether the merged observations have the same values for these fields or not.

Command line parameter `--consider-subgrid-variability` switches on considering the subgrid variability by calculating standard deviation of the merged observations σ_{sub} and using $\sigma_{obs} = \max(\sigma_{obs}, \sigma_{sub})$. The calculation of σ_{sub} is currently done in a rather crude way, assuming equal weights for all merged observations.

2.7 *calc*

calc is the second stage of data assimilation in EnKF-C. It calculates 2D arrays of local ensemble transforms $\mathbf{X}_5$ (for EnKF) or coefficients $\mathbf{w}$ (for EnOI).

The name of the binary for *calc* is `enkf_calc`. It has the following usage and options:

```
>./bin/enkf_calc
  Usage: enkf_calc <prm file> [<options>]
  Options:
  --describe-prm-format [main|model|grid|obstypes]
      describe format of a parameter file and exit
  --forecast-stats-only
      calculate and print forecast observation stats only
  --ignore-no-obs
      proceed even if there are no observations
  --no-mean-update
      update ensemble anomalies only
  --point-logs-only
      skip calculating transforms for the whole grid and observation stats
  --print-batch-stats
       calculate and print global biases for each batch of observations
  --single-observation-xyz <lon> <lat> <depth> <type> <inn> <std>
      assimilate single observation with these parameters
  --single-observation-ijk <fi> <fj> <fk> <type> <inn> <std>
      assimilate single observation with these parameters
  --use-rmsd-for-obsstats
      use RMSD instead of MAD when printing observation stats
  --use-these-obs <obs file>
      assimilate observations from this file; the file format must be compatible
      with that of observations.nc produced by 'enkf_prep'
  --version
      print version and exit
```

The option `--forecast-stats-only` can be used for quick calculation of the innovation statistics for a given background (or ensemble). This can be used, for example, for obtaining the persistence statistics, that is, the innovation statistics for the previous analysis.

The options `--single-observation-xyz` and `--single-observation-ijk` provide an easy way to conduct the so called single observation experiments, with the observation coordinates provided either in spatial or grid coordinates, correspondingly. Parameter `<value>` defines innovation rather than the observation value. Normally, this experiments would be conducted in the EnOI mode, calculating increment (option `--output-increment` of `enkf_update`) rather than analysis. When run in the EnKF mode, the increment (or analysis, depending on specifications) for each member is calculated.

Note that the calculated transforms *do not* incorporate inflation. Inflation is applied during *update* according to specifications (sec. 2.8.1).

2.7.1 Observation functions

Model estimations for observations of each type are calculated using observation functions specified for this type by entry `HFUNCTIONS` in the observation types parameter file, e.g.:

```
NAME = SLA
...
HFUNCTION = standard
...
```

The available functions for each observation type are specified by the variable `allhentries` in `calc/allhs.c`. The "standard" functions do normally perform 2D or 3D linear interpolation from the corner model grid nodes for the cell containing the observation.

2.7.2 Interpolation of ensemble transforms

Local ensemble transforms $\mathbf{X}_5$ (EnKF) or local ensemble weights $\mathbf{w}$ (EnOI) represent smooth fields with the characteristic spatial variability scale of the localisation radius. This smoothness allows one to reduce the computational load in *calc* by calculating local transforms or weights on a subgrid with a specified stride only, and using linearly interpolated transforms or weights in the intermediate grid cells. The value of the stride is defined by the `STRIDE` entry in the parameter file and can be overwritten for a particular grid in the grid parameter file.

2.7.3 Adaptive moderation of observations

One of standard quality control (QC) procedures in DA is the so called background check, when an observation is compared with the forecast and discarded if the innovation magnitude exceeds some specified threshold. The downside of this approach is that it can not distinguish between situations of an outlier, big model error (e.g. because of an error in forcing), or model divergence. While one probably would like to discard an outlier, it is usually desirable to make use of valid observations, although, perhaps, with a reduced impact, to avoid "over-stressing" the model. In EnKF-C this is achieved by adaptive moderation of the observation impact by restricting the magnitude of the increment from a given observation in observation space by K times magnitude of the spread of the forecast ensemble (Sakov and Sandery, 2017).

Specifically, the adaptive moderation of the observation impact is conducted by smoothly increasing the observation error depending on the magnitude of innovation as follows:

$$\sigma_{obs}^2 \leftarrow \left[(\sigma_f^2 + \sigma_{obs}^2)^2 + \sigma_f^2\, d^2/K^2\right]^{1/2} - \sigma_f^2,$$

where σ_{obs} is the observation error standard deviation, σ_f – forecast ensemble spread, d – innovation, and K – the so called K-factor defined in the main parameter file (sec. 2.4.1). Tests with small models show that setting the K-factor to say 2-3 or above makes a marginal impact (if any) on performance of weakly suboptimal systems, while still can be quite beneficial in stressful situations.

2.7.4 Moderation of spread reduction

The moderating parameter $\alpha \in (0, 1]$ specified in the main parameter file via the entry `ALPHA` allows one to reduce the contraction of ensemble during assimilation, while leaving the increment unchanged. It modifies the DEnKF expression (1.35) for $\mathbf{T}_R$ as

$$\mathbf{T}_R = \mathbf{I} - \frac{\alpha}{2}\,\mathbf{GS},$$

and the ETKF expression (1.34) as

$$\mathbf{T}_R = (\mathbf{I} + \alpha\,\mathbf{S}^{\mathrm{T}}\mathbf{S})^{-1/2}.$$

2.7.5 Innovation statistics

In its course *calc* calculates some basic innovation statistics: number of observations, mean absolute forecast innovation, mean absolute analysis innovation, mean forecast innovation, mean analysis innovation, mean forecast ensemble spread, and mean analysis ensemble spread. This statistics is provided for each region defined in the main parameter file (sec. 2.4.1), as well as for each time slot defined for asynchronous DA, and for each instrument. By default, EnKF-C defines one statistical region "Global" with domain $[x_1, x_2] = [-999, 999], [y_1, y_2] = [-999, 999]$.

In addition, for 3D observations *calc* also calculates observation statistics in specified depth intervals. These intervals can be set via the entry `ZSTATINTS` in the grid parameter file; by default, three intervals are defined: `[0 DEPTH_SHALLOW]`, `[DEPTH_SHALLOW DEPTH_DEEP]`, and `[DEPTH_DEEP DEPTH_MAX]`, where `DEPTH_SHALLOW`, `DEPTH_DEEP` and `DEPTH_MAX` are the macros defined in `common/definitions.h`.

Following is an example of innovation statistics written to the log (standard output) of `enkf_calc`:

```
printing observation statistics:
  region obs.type   # obs.  |for.inn.| |an.inn.|   for.inn.   an.inn.  for.spread  an.spread
  ---------------------------------------------------------------------------------------
  Tasman
         SLA          3003    0.067      0.038      0.033      0.012      0.035      0.025
          -4           712    0.058      0.038      0.035      0.013      0.028      0.021
          -3           785    0.093      0.040      0.060      0.019      0.052      0.034
          -2           700    0.062      0.043      0.030      0.016      0.027      0.021
          -1           668    0.049      0.031      0.017      0.004      0.028      0.021
           0           138    0.078      0.033     -0.043     -0.016      0.045      0.029
           j1         1323    0.070      0.033      0.041      0.016      0.037      0.024
           n1          876    0.073      0.042      0.052      0.025      0.036      0.026
           g1          785    0.054      0.042     -0.004     -0.009      0.029      0.024
           N/A          19    0.101      0.037      0.097      0.031      0.059      0.036
         SST          9316    0.346      0.174     -0.215     -0.094      0.358      0.254
          -4          2946    0.327      0.166     -0.236     -0.092      0.342      0.245
          -3          2733    0.368      0.183     -0.270     -0.133      0.362      0.256
          -2          2560    0.352      0.169     -0.167     -0.057      0.370      0.262
          -1           580    0.342      0.191     -0.148     -0.093      0.414      0.291
           0           497    0.305      0.182     -0.126     -0.075      0.307      0.225
           AVHRR      9316    0.346      0.174     -0.215     -0.094      0.358      0.254
         TEM           768    0.581      0.365     -0.245     -0.151      0.320      0.251
           ARGO        768    0.581      0.365     -0.245     -0.151      0.320      0.251
```

```
    0-50m       125   0.418    0.230     0.049     0.027    0.365    0.281
    50-500m     451   0.678    0.403    -0.266    -0.141    0.360    0.278
    >500m       192   0.458    0.365    -0.387    -0.291    0.196    0.170
  SAL           768   0.079    0.060     0.014     0.019    0.033    0.028
    ARGO        768   0.079    0.060     0.014     0.019    0.033    0.028
    0-50m       125   0.079    0.063     0.031     0.035    0.034    0.030
    50-500m     451   0.092    0.067     0.026     0.032    0.039    0.032
    >500m       192   0.048    0.041    -0.027    -0.021    0.018    0.016
```

This excerpt shows innovation statistics for the region "Tasman". It contains sections for SST, SLA and TEM observations. The summary statistics for each observation type is shown at the top of each section; then statistics for days -4, -3, -2, -1 and 0 of a 5-day DAW are shown for the two asynchronous types, SST and SLA. After that, statistics for particular instruments is shown; "N/A" corresponds to superobservations resulted from merging observations from two or more instruments. (One can avoid superobing across different instruments by using option `--no-superobing-across-instruments` in `enkf_prep`.) For subsurface temperature also statistics for shallow (0–50 m), deep (>500 m), and intermediate (50–500 m) observations is given.

The analysis innovation statistics is calculated from the updated (analysis) ensemble observations by *calc*, thus avoiding the need to access analysis files produced later by *update*. The update of ensemble observations is performed in the same way as that of any other element of the state vector: for the EnKF – by applying the appropriate local ensemble transforms to the forecast ensemble observations,

$$\mathcal{H}(\mathbf{E}^a) \leftarrow \mathcal{H}(\mathbf{E}^f)\,\mathbf{X}_5;$$

and for the EnOI – by applying the appropriate local linear combination of the ensemble observation anomalies:

$$\mathcal{H}(\mathbf{E}^a) \leftarrow \left[\mathcal{H}(\mathbf{x}^f) + (\mathbf{H}\mathbf{A}^f)\mathbf{w}\right]\mathbf{1}^{\mathrm{T}} + \mathbf{H}\mathbf{A}^f.$$

2.7.6 Impact of observations

In the course of its work *calc* routinely calculates two metrics for assessing the impact of observations, degrees of freedom of signal (DFS) and spread reduction factor (SRF):

$$\mathrm{DFS} = \mathrm{tr}(\mathbf{K}\mathbf{H}) = \mathrm{tr}(\mathbf{G}\mathbf{S}),$$
$$\mathrm{SRF} = \sqrt{\frac{\mathrm{tr}(\mathbf{H}\mathbf{P}^f\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1})}{\mathrm{tr}(\mathbf{H}\mathbf{P}^a\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1})}} - 1 = \sqrt{\frac{\mathrm{tr}(\mathbf{S}^{\mathrm{T}}\mathbf{S})}{\mathrm{tr}(\mathbf{G}\mathbf{S})}} - 1,$$

where $\mathrm{tr}(\cdot)$ is the trace function. The values of these metrics for each local analysis, calculated both for all observations and for observations of each type only, are written to file `enkf_diagn.nc`. Note that the in EnKF-C DFS and SRF are calculated from the above expressions and represent theoretical values for the EnKF analysis; they coincide with the actual DFS and SRF values only for the ETKF, but not for the DEnKF, which is an approximation of the KF (and indeed not for the EnOI, which is not even an approximation).

In the EnKF context DFS is a useful indicator of potential rank problems. Normally, it should not exceed a fraction (a half, or better, a quarter) of the ensemble size. SRF shows the "strength"

of DA. "Strong" DA implies a close to optimal system, which indeed never happens in practice. Therefore, ideally, SRF should be small (below 1, on average).

2.7.7 Multiple model grids

EnKF-C permits using multiple model grids, in which case the ensemble transforms are calculated sequentially for each of the grids. These transforms are then used for updating of the model variables defined on the corresponding grids.

2.7.8 "Multi-scale" localisation

It is possible to specify the localisation taper function as a linear combination of the Gaspari and Cohn's taper functions with different support radii:

$$f(r) = \sum_{i=1}^{N} w_i f_0(\frac{r}{R_i}),$$

where w_i is the weight, r is the distance, R_i is the support radius, and

$$f_0(\frac{x}{2}) = \begin{cases} 1 - \frac{5}{3}x^2 + \frac{5}{8}x^3 + \frac{1}{2}x^4 - \frac{1}{4}x^5, & 0 \le x \le 1, \\ -\frac{2}{3}x^{-1} + 4 - 5x + \frac{5}{3}x^2 + \frac{5}{8}x^3 - \frac{1}{2}x^4 + \frac{1}{12}x^5, & 1 < x \le 2, \\ 0, & 2 < x. \end{cases}$$

This can be set by entries `LOCRAD` and `WEIGHT` either in the main parameter file or in the observation types parameter file, e.g.:

```
LOCRAD 150 500
WEIGHT 0.9 0.1
```

(recall that entries in the observation types parameter file for particular observation types override the common settings in the main parameter file). Note that the weights are normalised so that their sum is equal to 1.

2.8 *update*

update is the third and final stage of data assimilation in EnKF-C. It updates the ensemble (EnKF) or the background (EnOI) by applying the transforms calculated by *calc*.

The name of the binary for *update* is `enkf_update`. It has the following usage and options:

```
>./bin/enkf_update
  Usage: enkf_update <prm file> [<options>]
  Options:
  --calculate-spread
```

```
    calculate ensemble spread and write to spread.nc
--describe-prm-format [main|model|grid]
    describe format of a parameter file and exit
--direct-write
    write fields directly to the output file (default: write to tiles first)
--joint-output
    append analyses to forecast files (default: write to separate files)
--leave-tiles
    do not delete tiles
--no-fields-write
    do not write analysis fields
--output-increment
    output analysis increment (default: output analysis)
--write-inflation
    write adaptive inflation magnitudes to inflation.nc
--version
    print version and exit
```

The option `--joint-output` tells *update* to append analyses to the corresponding forecast files, using new variable names constructed by concatenating the forecast variable names and suffix `_an`. By default the analyses are written to separate files, using the same variable names as the forecast files, but with an extra suffix `.analysis` or `.increment` added to the file name, depending on whether the analysis or increment is written.

By default, *update* first writes each updated horizontal field of the model to a separate file (referred to here as a tile), and then concatenates these fields into analysis files. The tiles are removed after writing the analysis files; one may save time for allocating them on disk in the next cycle by leaving them on disk by using option `--leave-tiles`. This approach is somewhat less effective than direct writing to analysis files (without intermediate tiles), but, unfortunately, the direct writing is generally not reliable due to parallel I/O issues with NetCDF. Note that in some cases it proved to be possible to obtain robust performance with direct write using "classic" or "64-bit-offset" NetCDF formats.

2.8.1 Capping of inflation

Applying spatially uniform ensemble inflation involves areas with no local observations, where no assimilation is conducted. It can gradually inject energy into the model and deteriorate performance of the DAS over time. Similar problems may arise due to lack of correlation between some state elements updated with the same transforms, so that even in presence of local observations the ensemble spread for some elements may hardly reduce after assimilation, yet the ensemble anomalies are inflated.

To avoid this behaviour EnKF-C currently restricts inflation by specified fraction (half by default) of the the spread reduction factor calculated directly for each element of the state vector during the update. For example, if inflation is specified as

```
INFLATION = 1.06 0.5
```

then the ensemble anomalies for any model state element will be inflated by 6 %, but no more than

$1 + 0.5(\sigma_f/\sigma_a - 1)$, where σ_f and σ_a represent the forecast and analysis ensemble spreads for this element. Specification

```
INFLATION = 1.06
```

is equivalent to

```
INFLATION = 1.06 1
```

Capping inflation by the magnitude of reduction of the ensemble spread is a default mode of application of inflation in EnKF-C; to revert to the uniform inflation add qualifier `PLAIN` to the entry `INFLATION` in the main parameter file, e.g.:

```
INFLATION = 1.06 PLAIN
```

The common inflation settings in the main parmater file can be overwritten by settings for particular model variables specified in the model parameter file (sec. 2.4.2).

2.9 DA tuning

Following are the main parameters for DAS tuning in EnKF-C:

- R-factors;
- inflation magnitudes;
- localisation radii.

The R-factors can be defined for each observation type. They represent scaling coefficients for the corresponding observation error variances and affect the impact of these observations: increasing R-factor decreases the impact of observations and vice versa. Specifying R-factor equal k produces the same increment as reducing the ensemble spread by $k^{1/2}$ times.

The main parameter file defines the base R-factor common for all observation types. It is possible to specify additional R-factors for observations of each type (sec. 2.4.4); the resulting R-factor for an observation is then given by multiplication of the common R-factor and the additional R-factor specified for observations of this type.

Multiplicative inflation can be seen as an additional forgetting factor in the KF. In EnKF-C one can specify the inflation multiple for analysed ensemble anomalies, e.g.:

```
> grep INFLATION main.prm
INFLATION = 1.05 PLAIN
> grep temp -A 1 model.prm
VAR = temp
INFLATION = 1.07 PLAIN
```

In this case all model variables except "temp" will have inflation of 5 %, while "temp" will have inflation of 7 %. The ability to define different inflation rates for different variables can be useful for non-dynamical variables, such as estimated biases, helping to avoid the ensemble collapse for them. In general, to retain dynamical balances one should rather avoid using different inflation magnitudes across model variables. Note that even small inflation can substantially affect the ensemble spread established in the course of evolution of the system. By default EnKF-C applies adaptive capping of inflation (sec. 2.8.1).

Localisation radius is defined by the entry `LOCRAD` in the parameter file. Specifically, this entry defines the support localisation radius (in km). This is different to the "effective" localisation radius, which is defined sometimes as $e^{1/2} \approx 1.65$ - folding distance. For the Gaspary and Cohn's taper function used in EnKF-C the effective radius is approximately 3.5 times smaller than the support radius.

Increasing the localisation radius increases the number of local observations and hence the overall impact of observations. To compensate this in a system with horizontal localisation one has to change the R-factor as the square of the localisation radius.

2.10 Point logs

It is often desirable to investigate sensitivity of model variables to observations or, more generally, analyse certain features of the DAS and their behaviour over time. In practice such analysis can be logistically complicated due to limitations on storage and/or access to it. Yet, it is usually feasible to save this information in a number of specified locations.

EnKF-C provides capability of saving complete DA related information for specified horizontal locations in so called "point logs". The locations are specified in the main parameter file, e.g.:

```
POINTLOG 94 134
POINTLOG 78 111
POINTLOG 57 51
POINTLOG 86 191
```

Here the information will be saved for points with horizontal grid coordinates (94, 134), (78, 111), (67, 51), and (86, 191) in files `pointlog_94,134.nc`, `pointlog_78,111.nc`, and so on. By default the coordinates are defined on the first grid in the grid parameter file (sec. 2.4.3); otherwhile the grid can be specified by entering the grid name as an additional parameter, .e.g:

```
POINTLOG 86 191 t-grid
```

Following is an example of the header of the saved point log file in NetCDF format:

```
netcdf pointlog_57\,51 {
dimensions:
        m = 96 ;
        p = 515 ;
```

```
        nk-0 = 25 ;
        nk-1 = 25 ;
        nk-2 = 25 ;
variables:
        int obs_ids(p) ;
        float lcoeffs(p) ;
        float lon(p) ;
        float lat(p) ;
        float depth(p) ;
        float obs_val(p) ;
        float obs_std(p) ;
        float obs_fi(p) ;
        float obs_fj(p) ;
        float obs_fk(p) ;
        int obs_type(p) ;
                obs_type:SLA = 0 ;
                obs_type:RFACTOR_SLA = 2. ;
                obs_type:LOCRAD_SLA = 200. ;
                obs_type:SST = 1 ;
                obs_type:RFACTOR_SST = 4. ;
                obs_type:LOCRAD_SST = 200. ;
                obs_type:TEM = 2 ;
                obs_type:RFACTOR_TEM = 8. ;
                obs_type:LOCRAD_TEM = 800. ;
                obs_type:SAL = 3 ;
                obs_type:RFACTOR_SAL = 8. ;
                obs_type:LOCRAD_TEM = 800. ;
        float obs_date(p) ;
                obs_date:units = "days from 5875.5 days since 1990-01-01" ;
        float s(p) ;
        float S(m, p) ;
        double X5(m, m) ;
                X5:long_name = "ensemble transform calculated for this (i,j) location in grid-0
                   (rho-grid)" ;
        float X5_actual(m, m) ;
                X5_actual:long_name = "the actual (interpolated) ensemble transform used at this
                          (i,j) location in grid-0 (rho-grid)" ;
        float zeta(m) ;
        float zeta_an(m) ;
                zeta_an:INFLATION = 1.1f, 0.5f ;
        float temp(nk-0, m) ;
        float temp_an(nk-0, m) ;
                temp_an:INFLATION = 1.1f, 0.5f ;
        float salt(nk-0, m) ;
        float salt_an(nk-0, m) ;
                salt_an:INFLATION = 1.1f, 0.5f ;
        float u(nk-1, m) ;
        float u_an(nk-1, m) ;
                u_an:INFLATION = 1.1f, 0.5f ;
        float v(nk-2, m) ;
        float v_an(nk-2, m) ;
                v_an:INFLATION = 1.1f, 0.5f ;
        float ubar(m) ;
        float ubar_an(m) ;
                ubar_an:INFLATION = 1.1f, 0.5f ;
        float vbar(m) ;
        float vbar_an(m) ;
                vbar_an:INFLATION = 1.1f, 0.5f ;
```

```
// global attributes:
                :date = "5875.5 days since 1990-01-01" ;
                :i = 57 ;
                :j = 51 ;
                :lon = 151.75 ;
                :lat = -39.849998 ;
                :depth = 4632.623046875 ;
```

This data makes it possible to check DA algorithms by reproducing the ensemble transforms (for EnKF) or weights (for EnOI) calculated by EnKF-C from $\mathbf{S}$ and $\mathbf{s}$ according to section 1.3.3; restore observations from $\mathbf{s}$ by using the corresponding R-factors and localisation coefficients; to monitor the ensemble spread for each model variable; calculate inflation applied to the analysed anomalies; calculate impacts of particular observations; and so on.

2.11 Use of innovation statistics for model validation

EnKF-C can calculate innovation statistics for validating a model against observations only, without data assimilation. The pre-requisites are (i) observations and (ii) model dump readable by the code, and possibly (iii) auxiliary files for projecting the model state to observation space (e.g. grid specs and mean SSH). To get the innovation statistics one needs to:

- set up the parameter files in a normal way (`MODE = EnOI`), omitting the ensemble directory and assimilation related parameters;
- run `enkf_prep`;
- run `enkf_calc` with additional parameter `--forecast-stats-only`.

The results will be written to the log of `enkf_calc`. An example of using this functionality is available by running `make stats` in `examples/1` (see sec. 2.3).

2.12 Bias correction

It is possible to estimate and correct bias for a model variable with the EnKF by generating and using an ensemble of bias fields. These bias fields need to be subtracted from the corresponding observation forecasts. This is accomplished by specifying a secondary variable in the observation type entry `VAR` and by passing the name of this variable to the corresponding observation functions, which need to take care for subtracting the bias from the model forecasts.

Because bias fields are usually assumed to persist (not change) during propagation, one may need to make specific settings for their inflation to avoid their collapse (loss of spread) over time. Another possibility is to introduce a "forgetting" stochastic model for bias fields, for example:

$$\mathbf{x}_{i+1} = \lambda\,\mathbf{x}_i + (1-\lambda^2)^{1/2}\boldsymbol{\sigma},$$

where λ is the forgetting factor, $0 < \lambda < 1,\ 1-\lambda \ll 1$, and $\boldsymbol{\sigma} \sim \sigma_0 N(0,1)$, where σ_0 is the error standard deviation of $\mathbf{x}$. This can be specified for a model variable via entry `RANDOMISE` in the corresponding section of the model parameter file (sec. 2.4.2).

2.13 Grids

Currently EnKF-C makes three main general assumptions about grids:

- the vertical grid coordinates correspond to layer centres, either for Z or sigma layers;
- the horizontal coordinates are geographic (longitude, latitude);
- the order of vertical coordinate (top to bottom or bottom to top) corresponds to that of 3D model fields.

If the available model grids do not meet the above assumptions, one needs to generate the corresponding auxiliary grids and use them instead.

Further, the horizontal grid must be either rectangular in longitude-latitude, with constant or irregular step; or represent a structured simply connected quadrilateral grid, referred to elsewhere as "curvilinear". In the first case mapping from physical to grid space is done independently by X and Y coordinates; in the second case the grid is rendered into spatial binary tree to achieve logarithmic search time. Note that some curvilinear grids used in practice (e.g. tri-polar ORCA grids) are not simply connected in grid space. Such grids can be used in EnKF-C as described in section 2.4.3.

2.14 System issues

2.14.1 Memory footprint

To reduce the memory usage, most of the potentially big arrays in EnKF-C use `float` data type.

The memory footprint of *prep* is defined by the size of the `measurement` structure and the number of observations. It is rarely a problem.

For *calc* it is mainly defined by the size of ensemble observation anomalies, which require $p \times m \times 4$ bytes for storage. For example, with $3 \cdot 10^6$ superobservations and 10^2 ensemble members the size of this array would be about 1.2 GB per CPU, which should be manageable on most contemporary systems. If the footprint becomes too big, one may consider reducing the number of observations by a coarser superobing (setting the parameter `SOBSTRIDE` to 2 or more) or reducing the number of cores per node used.

From version 1.74, it is possible to substantially reduce the memory footprint in *calc* by using shared memory for the ensemble observations. For that, *calc* needs to be compiled with flag `-DHE_VIASHMEM`. It is likely to become a default option in future.

The footprint of *update* is mainly defined by the size of the array of simultaneously updated horizontal fields. For example, for a 1500×3600 horizontal field, 100 ensemble members and simultaneous update of 2 fields the size of this array would be about 4.3 GB per CPU. It can be reduced to 2.15 GB by setting the parameter `FIELDBUFFERSIZE` to 1. Note that reducing the number of simultaneously updated fields specified by parameter `FIELDBUFFERSIZE` increases I/O (the $\mathbf{X}_5$ array is read from disk N_f/N_b times, where N_f is the total number of horizontal fields, and N_b is the

number of simultaneously updated fields) and reduces computational effectiveness (the $\mathbf{X}_5$ array needs to be interpolated horizontally N_f/N_b times).

2.14.2 Exit action

When exiting on an error, EnKF-C by default prints the stack trace, which allows to trace the exit location in the code. Another option – to generate a segmentation fault – can be activated by setting `EXITACTION = SEGFAULT` in the parameter file. Note that when run on multiple processors, this can result in segmentation faults on more than one processor (but not necessarily on every engaged processor, as some processes can also be forced to exit by `MPI_abort()`). If the system is set to generate core dumps, they can indeed be used for investigating the final state of the program.

2.14.3 Dependencies and compilation issues

Compiling EnKF-C requires the following external libraries:

- netcdf;
- lapack (or mkl_rt);
- openmpi;
- gridutils.

EnKF-C also relies on `qsort_r()`, which may be lacking in older systems. In such cases use compile flag `-DINTERNAL_QSORT_R` to activate the internal version of this procedure.

Notes:

1. Using Intel's version of Lapack library – Intel Math Kernel Library – can improve performance over Lapack compiled with gfortran.
2. Grid utilities (libgu) is necessary for handling curvilinear grids only. Add compile flag `-DNO_GRIDUTILS` to compile without it.

2.15 Possible problems

2.15.1 *calc* becomes too slow after increasing localisation radius

This is due to the increased number of local observations.

The local observations are sought by using so called k-d tree. Normally it works well, but can become a bottleneck when the number of local observations becomes very large. If this happens, one may use a coarser superobing to reduce the number of assimilated observations, by increasing parameter `SOBSTRIDE` from the default value of 1 to 2 or more.

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EnKF-C has been developed during author's work with Bureau of Meteorology on Bluelink project. The author has used his knowledge of TOPAZ (Sakov et al., 2012) and BODAS (Oke et al., 2008) systems and borrowed from them a number of design solutions and features. Paul Sandery was the first user of this code (apart from the author), and his enthusiastic support is cheerfully acknowledged.

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Abbreviations

CL	-	covariance localisation
DEnKF	-	deterministic EnKF
DA	-	data assimilation
DAS	-	data assimilation system
DAW	-	data assimilation window
DFS	-	degrees of freedom of signal
EKF	-	extended Kalman filter
EnKF	-	ensemble Kalman filter
EnOI	-	ensemble optimal interpolation
ETKF	-	ensemble transform Kalman filter
ETM	-	ensemble transform matrix
FGAT	-	first guess at appropriate time
KF	-	Kalman filter
KS	-	Kalman smoother
LA	-	local analysis
SDAS	-	state of data assimilation system
SRF	-	spread reduction factor
SVD	-	singular value decomposition

Symbols

General symbols

$\mathbf{x}$ (small, bold)	-	a vector
$\mathbf{1}$	-	a vector with all elements equal to 1
$\mathbf{0}$	-	a vector with all elements equal to 0
$\mathbf{A}$ (capital, bold)	-	a matrix
$\mathbf{I}$	-	an identity matrix
$\mathbf{U}$	-	a unitary matrix, $\mathbf{U}\mathbf{U}^{\mathrm{T}} = \mathbf{I}$
$\mathbf{A}^{\mathrm{T}}$	-	transposed matrix $\mathbf{A}$
$\mathbf{A}^{1/2}$	-	the unique positive definite square root of a positive definite matrix $\mathbf{A}$
$\mathrm{tr}(\mathbf{A})$	-	trace of $\mathbf{A}$
$\mathcal{H} \circ \mathcal{M}(\mathbf{x})$	-	$\mathcal{H}\left[\mathcal{M}(\mathbf{x})\right]$
$\mathbf{A} \circ \mathbf{B}$	-	by-element, or Hadamard, or Schur product of matrices

DA related symbols

m	-	ensemble size
n	-	state size
p	-	number of observations
$\mathbf{A}$	-	ensemble anomalies, $\mathbf{A} = \mathbf{E} - \mathbf{x}\mathbf{1}^{\mathrm{T}}$
$\mathbf{E}$	-	ensemble
$\mathbf{G}$	-	an intermediate matrix in the EnKF analysis, $\mathbf{G} \equiv (\mathbf{I} + \mathbf{S}^{\mathrm{T}}\mathbf{S})^{-1}\mathbf{S}^{\mathrm{T}} = \mathbf{S}^{\mathrm{T}}(\mathbf{I} + \mathbf{S}\mathbf{S}^{\mathrm{T}})^{-1}$
$\mathcal{H}$	-	nonlinear observation operator; in linear case – affine observation operator
$\mathbf{H}$	-	linearised observation operator, $\mathbf{H} = \nabla\mathcal{H}(\mathbf{x})$
J	-	cost function
$\mathcal{M}$	-	nonlinear model operator; in linear case – affine model operator
$\mathbf{M}$	-	linearised model operator, $\mathbf{M} = \nabla\mathcal{M}(\mathbf{x})$
$\mathbf{P}$	-	state error covariance estimate; also used as abbreviation for $\mathbf{A}\mathbf{A}^{\mathrm{T}}/(m-1)$
$\mathbf{Q}$	-	model error covariance
$\mathbf{R}$	-	observation error covariance
$\mathbf{S}$	-	normalised ensemble observation anomalies, $\mathbf{S} = \mathbf{R}^{-1/2}\mathbf{H}\mathbf{A}/\sqrt{m-1}$
$\mathbf{T}_L$	-	left-multiplied ensemble transform matrix, $\mathbf{A}^a = \mathbf{T}_L\mathbf{A}^f$
$\mathbf{T}_R$	-	right-multiplied ensemble transform matrix, $\mathbf{A}^a = \mathbf{A}^f\mathbf{T}_R$
$\mathbf{U}^p$	-	a unitary mean-preserving matrix, $\mathbf{U}^p(\mathbf{U}^p)^{\mathrm{T}} = \mathbf{I}$, $\mathbf{U}^p\mathbf{1} = \mathbf{1}$
$\mathbf{X}_5$	-	historic symbol for the full ensemble transform matrix, $\mathbf{E}^a = \mathbf{E}^f\mathbf{X}_5$
$\mathbf{s}$	-	normalised innovation, $\mathbf{s} = \mathbf{R}^{-1/2}\left[\mathbf{y} - \mathcal{H}(\mathbf{x}^f)\right]/\sqrt{m-1}$
$\mathbf{x}$	-	state estimate
$\mathbf{y}$	-	observation vector
$\mathbf{w}$	-	vector of linear coefficients for updating the mean, $\mathbf{x}^a = \mathbf{x}^f + \mathbf{A}^f\mathbf{w}$
$(\cdot)^f$	-	forecast expression
$(\cdot)^a$	-	analysis expression
$(\cdot)_i$	-	either expression at cycle i or ith element of a vector
$\overset{i}{(\cdot)}$	-	local expression for state element i
$\overset{\{o\}}{(\cdot)}$	-	local expression for observation o