

Kalman Filters Implemented in FVCOM

Changsheng Chen, Paola Malanotte-Rizzoli, Robert C. Beardsley, Zhigang Lai, Pengfei Xue, Jun Wei and Geoffrey W. Cowles

1. The Kalman Filters

Let \mathbf{x}^t be an array of the true values, \mathbf{x}^f be an array of the forecast values, \mathbf{x}^a an array of analysis values, and \mathbf{y} an array of observational values. We can define that

$$\text{Analysis error:} \quad \mathbf{e}_a = \mathbf{x}^a - \mathbf{x}^f \quad (1.1)$$

$$\text{Forecast error:} \quad \mathbf{e}_f = \mathbf{x}^t - \mathbf{x}^f \quad (1.2)$$

$$\text{Observational error:} \quad \mathbf{e}_o = \mathbf{y} - \mathbf{x}^f \quad (1.3)$$

The forecast error covariance \mathbf{P} and the observational error covariance \mathbf{R} thereafter can be defined as

$$\mathbf{P}^f = \overline{\mathbf{e}_f \mathbf{e}_f^T}, \quad \mathbf{R} = \overline{\mathbf{e}_o \mathbf{e}_o^T} \quad (1.4)$$

In a forecast model, the value of \mathbf{x}^f at time step i can be predicted by

$$\mathbf{x}^f(i) = \mathbf{M}_{i-1 \rightarrow i} [\mathbf{x}^a(i-1)] \quad (1.5)$$

where \mathbf{M} presents the linearized model operator. The forecast error covariance is equal to

$$\mathbf{P}^f = \mathbf{M}_{i-1 \rightarrow i} \mathbf{P}^a(i-1) \mathbf{M}_{i-1 \rightarrow i}^T + \mathbf{Q}(i-1) \quad (1.6)$$

where $\mathbf{Q}(i-1)$ is the system error covariance matrix. In the Kalman filter forecast model system, the analysis values \mathbf{x}^a is calculated by

$$\mathbf{x}^a(i) = \mathbf{x}^f(i) + \mathbf{K}(i) [\mathbf{y}(i) - \mathbf{H} \mathbf{x}^f(i)] \quad (1.7)$$

where \mathbf{K} is the Kalman gain matrix, which is equal to

$$\mathbf{K}(i) = \mathbf{P}^f(i) \mathbf{H}^T [\mathbf{H} \mathbf{P}^f(i) \mathbf{H}^T + \mathbf{R}(i)]^{-1} \quad (1.8)$$

and \mathbf{H} is an observation operator that functions as an objective map to interpolate the model data onto the observational points. The analysis error covariance is given as

$$\mathbf{P}^a(i) = [\mathbf{I} - \mathbf{K}(i)] \mathbf{P}^f(i). \quad (1.9)$$

In general, the size of the covariance matrix is huge. For example, $\mathbf{P}^f : [N \times N]$ and $\mathbf{M} : [N \times N]$, and N can be of $O(10^6 - 10^7)$, which makes it impractical to use this

method on most computers. For this reason, a family of Kalman Filters (Reduced Rank Kalman Filter, Ensemble Kalman Filter, Ensemble Square Root Kalman Filter and Ensemble Transform Kalman Filter) have been developed that require less computational power than the original filter. A brief description of these other Kalman Filters and how they are implemented in FVCOM is given below.

2. Reduced Rank Kalman Filter (RRKF)

Let \mathbf{x}^f be an array with a dimension of N (FVCOM output and RRKF input); \mathbf{x}^a an array with a dimension of N (that are output from RRKF to use to refresh the initial conditions for FVCOM input); \mathbf{y} an array with a dimension of N_o (that is an input for RRKF); \mathbf{E}_r the resolved empirical orthogonal functions (EOFs) with dimensions of $N \times N_e$ (the stationary input of RRKF); \mathbf{K}_r the stationary Kalman gain in the reduced space of $N_e \times N_o$; N_e the dimension of the EOFs subspace; \mathbf{i} and $\mathbf{i} + \Delta T$ two subsequent assimilation time steps of FVCOM; ΔT the assimilation interval; \mathbf{M}_i the forward (nonlinear) FVCOM model with initial conditions specified by the analysis solution; and \mathbf{D} is the spatially averaged standard deviation of each variable.

A detailed description of RRKF was given in *Buehner and Malanotte-Rizzoli* [2003]. S. Lyu, who worked with P. Rizzoli as a postdoctoral investigator at MIT, helped us implement RRKF into FVCOM. He worked together with P. Xue, Q. Xu and Z. Lai in testing the RRKF code in idealized cases.

The RRKF is developed based on linear theory. In a linear system, if the observational network, observational and model error covariances are stationary and all neutrally stable and unstable modes are measurable, the forecast error covariance reaches an asymptotically stationary result and then a stationary Kalman gain (\mathbf{K}_r) can be derived efficiently by the doubling algorithm [*Anderson and Moore*, 1979]. This stationary \mathbf{K}_r is calculated from the control model run and it is applied in the data assimilation process of the RRKF.

The RRKF in FVCOM is operated following the procedure given below:

Step 1: Determination the number of resolved EOFs (E_r) from the control model run:

$$\mathbf{D}^{-1} \hat{\mathbf{X}}_f \hat{\mathbf{X}}_f^T \mathbf{D}^{-1} = \mathbf{E} \mathbf{\Lambda} \mathbf{E}^T \quad (2.1)$$

where $\hat{X}_f = x^f - \bar{x}^f$, \bar{x}^f the mean of x^f , E the EOF matrix; and Λ is the diagonal covariance eigenvalue matrix.

Step 2: Linearization of the model in the resolved EOF subspace (build M_r from E_r):

$$M_{ri} = \frac{1}{\alpha} E_r^T D^{-1} [M(x_0 + \alpha D e_i) - M(x_0)] \quad (2.2)$$

where M presents the nonlinear model; subscripts “ r ” and “ i ” of M denote the linearized model in the resolved subspace and the i th column of M_r ; α is the perturbation size; e_i the i th retained EOF; and x_0 is the specified time mean of a long model run without assimilation.

Step 3: Projection of the error covariance into the resolved EOFs subspace and estimation of the model and observation errors:

$$P_r^f = E_r^T P^f E_r; P_r^a = E_r^T P^a E_r; M_r = E_r^T M E_r; Q_r = \gamma \Lambda \quad (2.3)$$

$$R = R_m + H_u P_u^f H_u^T \quad (2.4)$$

where P_r^a is the analysis error covariance matrix in the resolved subspace; Q_r the ‘pesudo’ model error covariances; R the observational error covariance; R_m the actual measurement error; and P_r^f the forecast error covariance matrix in the resolved subspace.

Step 4: Calculation of the stationary Kalman gain K_r in the reduced subspace by the doubling algorithm, estimation of the difference between the observations and forecast and projection to the full space by multiplying E_r

$$K_r(t) = P_r^f(t) (H_r P_r^f(t) H_r^T + R)^{-1} \quad (2.5)$$

$$P_r^a(t) = (I - K_r(t) H_r) P_r^f(t) \quad (2.6)$$

$$P_r^f(t+1) = M_r P_r^a(t) M_r^T + Q_r \quad (2.7)$$

where $H_r = H D E_r$ and P_r^f is asymptotically stationary as $t \rightarrow \infty$ if H , R and Q is stationary with linear dynamics.

Step 5: Data assimilation by using a stationary Kalman gain K_r

$$x^a(t) = x^f(t) + D E_r K_r [y(t) - H x^f(t)] \quad (2.8)$$

RRKF works efficiently in a linear system but not for a nonlinear system. We tested it for various idealized cases such as tidal waves in the circular lakes, the flooding/drying

process in the rectangular shape estuary. It produces a fast convergence solution for the linear tidal wave case, but never converges in the estuarine case characterized with nonlinear dynamics.

3. Ensemble Kalman Filter (EnKF)

Evensen (1994) suggested that the error covariance relative to the mean of ensemble model results could provide a better estimation of the error covariance defined in the classical Kalman Filter. The EnKF is constructed by running a forecast model driven by a set of initial conditions and then estimate the error covariance relative to the ensemble mean to determine the ensemble analysis values for the next time step forecast.

Let k denote the k th ensemble member and N_E the total number of the ensemble members selected in the forecast model run. The forecast value at time step i for the k th ensemble model run can be estimated by

$$\mathbf{x}_k^f(i) = \mathbf{M}_{i-\Delta t \rightarrow i}[\mathbf{x}_k^a(i-1)], \quad k = 1, 2, \dots, N_e \quad (3.1)$$

and the analysis values at time step i for the k th ensemble model run are calculated by

$$\mathbf{x}_k^a(i) = \mathbf{x}_k^f(i) + \mathbf{K}(i)[\mathbf{y}_k(i) - \mathbf{H}\mathbf{x}_k^f(i)], \quad k = 1, 2, \dots, N_e \quad (3.2)$$

Define that

$$\mathbf{X}_f = \left\{ [\mathbf{x}_k^f - \bar{\mathbf{x}}^f] / \sqrt{N_e - 1} \right\} \quad k = 1, 2, \dots, N_e \quad (3.3)$$

then the forecast error covariance can be estimated by

$$\mathbf{P}^f(i) \approx \mathbf{X}_f(i) \mathbf{X}_f^T(i): \quad [N \times N_e][N_e \times N] \quad (3.4)$$

The Kalman gain is equal to

$$\mathbf{K}(i) = \mathbf{X}_f \mathbf{X}_f^T \mathbf{H}^T (\mathbf{H} \mathbf{X}_f \mathbf{X}_f^T \mathbf{H}^T + \mathbf{R})^{-1} \quad (3.5)$$

To conduct the EnKF, we need to create an ensemble of the observational data constructed with the perturbation relative to the real value, *i. e.*,

$$\mathbf{y}_k = \mathbf{y} + \delta_k, \quad \delta_k = N(0, \sqrt{R}) \quad (3.6)$$

where

$$\mathbf{R} = \overline{\delta\delta^T} \quad (3.7)$$

In the situation with a sufficiently large number of ensembles, the ensemble analysis error covariance matrix can be updated with a relationship as

$$\mathbf{P}_e^a(t) = (\mathbf{I} - \mathbf{K}_r(t)\mathbf{H})\mathbf{P}_e^f(t) \quad (3.8)$$

With assumption of Gaussian distribution, this will give us optimal analysis values in the maximum likelihood sense and in the minimum variance sense. In the situation with a small number of ensembles, the perturbed observations required by EnKF may cause a rank deficiency problem for the estimation of \mathbf{P}^f and an underestimate of \mathbf{P}^a , which leads to filter divergence [Whitaker and Hamill, 2002]. The filter divergence problem can be controlled by using the covariance localization [Houterkamer and Mitchell, 2001] and covariance inflation [Wang and Bishop, 200]. EnKF is suitable for both linear and nonlinear systems. For a linear system, RRKF works well and also fast, but it sometimes fails to resolve linear waves in the idealized, linear coastal ocean system. In such a case, EnKF works well.

4. Ensemble Square-Root Kalman Filter (EnSKF)

The EnKF is a filter that requires perturbed sets of observational values. In this system, the perturbed observational values are usually constructed by a control observation in addition to random noise sampled from the assumed observational error distribution. There are derivatives of EnKF that are conducted with deterministic observational ensembles. These filters are known as the EnSKF [Whitaker and Hamill, 2002], Ensemble Transform Kalman Filter (EnTKF) [Bishop et al., 2001] and the Ensemble Adjustment Kalman Filter (EnAKF) [Anderson, 2001]. Actually, these filters are a family of the deterministic square root filters [Tippett et al., 2003]. A brief description of one type of EnSKF is given below.

Assuming that the forecast and observational error covariance is Gaussian distributed, the ensemble Kalman Filter provides optimal analysis values which satisfy the classical Kalman Filter covariance form as

$$\mathbf{P}_e^a = (\mathbf{I} - \mathbf{K}_e \mathbf{H}) \mathbf{P}_e^f \quad (4.1)$$

and the Kalman gain is

$$\mathbf{K}_e = \mathbf{P}_e^f \mathbf{H}^T [\mathbf{H} \mathbf{P}_e^f \mathbf{H}^T + \mathbf{R}_e]^{-1} \quad (4.2)$$

Eq. (4.1) can be rewritten into

$$\mathbf{P}_e^a = \mathbf{X}_a \mathbf{X}_a^T \quad (4.3)$$

where

$$\mathbf{X}_a = \mathbf{X}_f \hat{\mathbf{T}} \quad (4.4)$$

and $\hat{\mathbf{T}}$ is the square root matrix defined as

$$\hat{\mathbf{T}} = \{ \mathbf{I} - \mathbf{X}_f \mathbf{H}^T [\mathbf{H} \mathbf{X}_f \mathbf{X}_f^T \mathbf{H}^T + \mathbf{R}]^{-1} \mathbf{H} \mathbf{X}_f \} \quad (4.5)$$

where \mathbf{I} is $N_e \times N_e$ unit matrix. In this case, an ensemble of the analysis deviation \mathbf{X}_a can be estimated deterministically from an ensemble of the forecast deviation, and also the analysis ensemble has a desired error covariance.

Assuming that the observation errors are uncorrelated, the observations can be assimilated serially. In this case, $\mathbf{H} \mathbf{X}_f \mathbf{X}_f^T \mathbf{H}^T + \mathbf{R}$ in (4.5) is simplified to be a scalar in the case of a single observation. Then the square root matrix can be easily calculated as

$$\hat{\mathbf{T}} = [1 - \beta \mathbf{X}_f^T \mathbf{H}^T \mathbf{H} \mathbf{X}_f] [1 - \beta \mathbf{X}_f^T \mathbf{H}^T \mathbf{H} \mathbf{X}_f]^T \quad (4.6)$$

where $\beta = [a + \sqrt{Ra}]^{-1}$.

EnSKF does not require a perturbed observation set, so that the ensemble mean of analysis values $\bar{\mathbf{x}}^a$ can be updated directly by the mean of forecast ensemble produced from a traditional Kalman Filter equation as

$$\bar{\mathbf{x}}^a(i) = \bar{\mathbf{x}}^f(i) + \mathbf{X}_f \mathbf{X}_f^T \mathbf{H}^T [\mathbf{H} \mathbf{X}_f \mathbf{X}_f^T \mathbf{H}^T + \mathbf{R}]^{-1} (\mathbf{y} - \mathbf{H} \bar{\mathbf{x}}^f) \quad (4.7)$$

and each analysis member \mathbf{x}_k^a can be calculated by

$$\bar{\mathbf{x}}_k^a(i) = \bar{\mathbf{x}}^a(i) + \mathbf{X}_k^a \sqrt{N_e - 1} \quad k = 1, 2, \dots, N_e \quad (4.8)$$

5. Ensemble Transform Kalman Filter (EnTKF)

The EnTKF is very similar to EnSKF with a linear transformation of the forecast perturbation into the analysis perturbation by $\hat{\mathbf{T}}$

$$\mathbf{X}_a = \mathbf{X}_f \hat{\mathbf{T}} \quad (5.1)$$

Bishop et al. [2001] proposed the form of the transformation matrix \mathbf{T} as:

$$\hat{\mathbf{T}} = \mathbf{C}(\tilde{\mathbf{A}} + \mathbf{I})^{-1/2} \quad (5.2)$$

where columns of the matrix \mathbf{C} contain the eigenvectors of $\mathbf{X}_f^T \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H} \mathbf{X}_f$ and $\tilde{\mathbf{A}}$ is the nonzero diagonal matrix that satisfies a relationship with \mathbf{C} as

$$\mathbf{X}_f^T \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H} \mathbf{X}_f = \mathbf{C} \tilde{\mathbf{A}} \mathbf{C}^T \quad (5.3)$$

In this case,

$$\mathbf{x}^a(i) = \bar{\mathbf{x}}^f(i) + \mathbf{X}_f \mathbf{C} \tilde{\mathbf{A}}^{1/2} (\tilde{\mathbf{A}} + \mathbf{I})^{-1} \mathbf{E}^T \{ \mathbf{R}^{-1/2} \mathbf{y} - \mathbf{H} \bar{\mathbf{x}}^f \} \quad (5.4)$$

where

$$\mathbf{E} = \mathbf{H} \mathbf{X}_f \mathbf{C} \tilde{\mathbf{A}}^{-1/2} \quad (5.5)$$

In FVCOM, EnTKF is used for adaptive observation optimization in which \mathbf{X}_a is used to evaluate the analysis ensemble error covariance under different observational strategies. This approach allows us to use the model to determine the optimal observational network for a selected region.

References

- Anderson, B. and J. B. Moore (1979), *Optimal Filtering*, Prentice-Hall, 357pp.
- Anderson, J. L. (2001), An ensemble adjustment Kalman filter for data assimilation. *Mon Weather Rev* 129: 2884–2903.
- Bishop, C. H., B. J. Etherton and S. J. Majumdar (2001), Adaptive sampling with the Ensemble Transform Kalman Filter. Part I: theoretical aspects, *Mon. Wea. Rev.*, 129, 420-436.
- Buehner, M. and P. Malanotte-Rizzoli (2003), Reduced-rank Kalman filters applied to an idealized model of the wind-driven ocean circulation, *J. Geophys. Res.*, 108, 3192, doi:10.1029/2001JC000873
- Evensen, G. (1994), Sequential data assimilation with a nonlinear quasi-geostrophic model using Monte Carlo methods to forecast error statistics. *J. Geophys. Res.*, 99, 10,143-10,162.
- Houtekamer, P. and H. L. Mitchell (1998), Data assimilation using an ensemble Kalman filter technique. *Mon. Wea. Rev.*, 126, 796-811.
- Tippett, M. K., J. L. Anderson, C. H. Bishop, T. M. Hamill and J. S. Whitaker (2003).

- Ensemble square root filters. *Mon. Wea. Rev.*, 131, 1485-1490.
- Wang, X., and C. H. Bishop (2003), A comparison of breeding and ensemble transform Kalman filter ensemble forecast schemes. *J. Atmos. Sci.*, 60, 1140-1158.
- Whitaker, J. S. and T. M. Hamill (2002), Data assimilation without perturbed observations. *Mon. Wea. Rev.*, 130, 1913-1924.

Figure Caption

Figure S1: Schematic of the implementation of RRKF into FVCOM.

Figure S2: Schematic of the implementation of EnKF (EnSKF/EnTKF) into FVCOM.

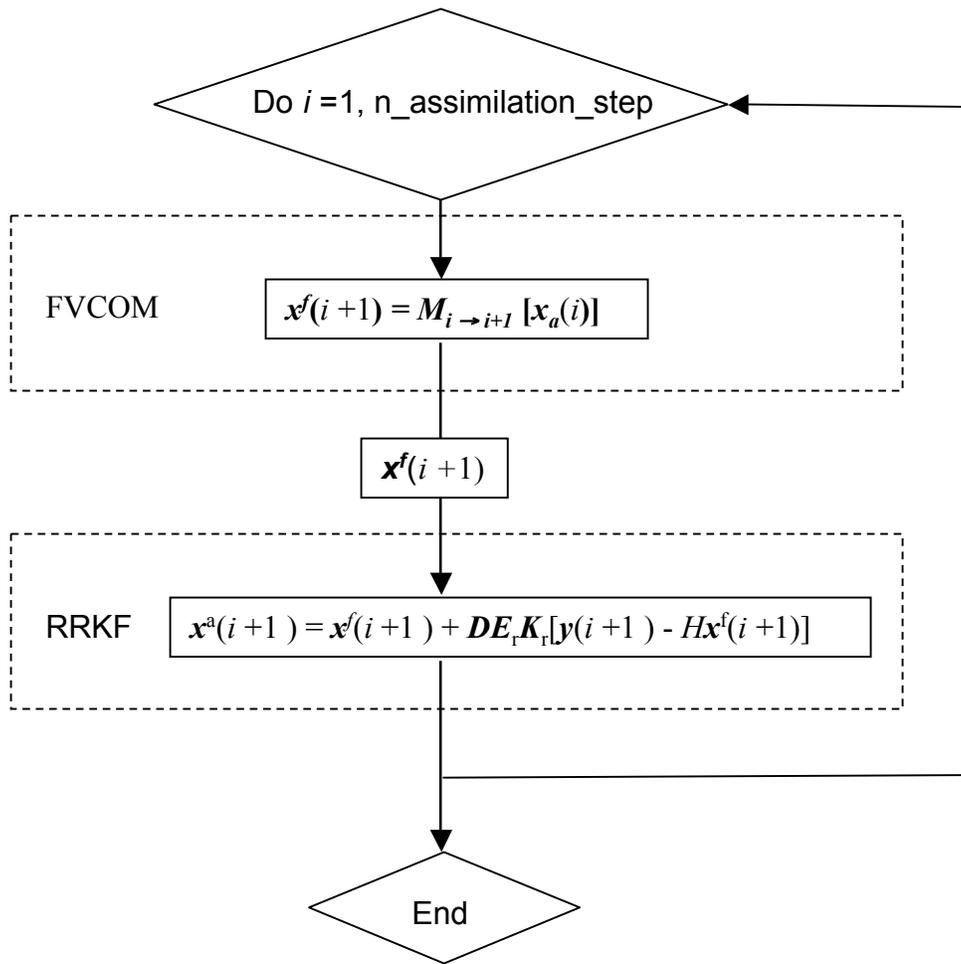


Fig. S1

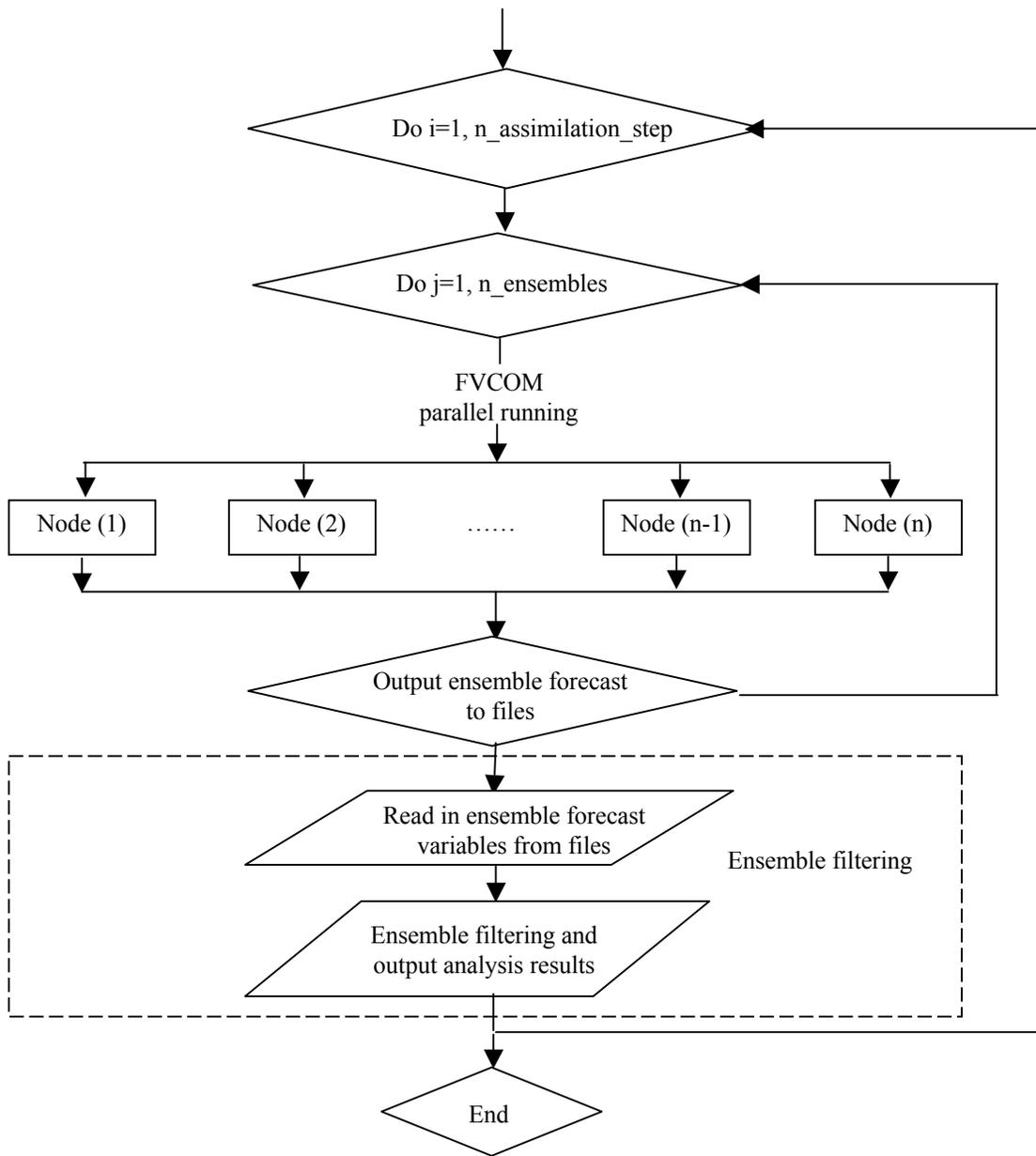


Fig. S2