

# Variational Ensemble Kalman Filtering on Parallel Computers

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## 1 Data Assimilation Methods

- 3D Variational Assimilation (3D-Var)
- 4D Variational Assimilation (4D-Var)
- The Extended Kalman Filter (EKF)
- The Variational Kalman Filter (VKF)

## 2 A Variational Ensemble Kalman Filter

- Ensemble Kalman Filters (EnKF)
- The Variational Ensemble Kalman Filter (VEnKF)

## 3 Computational Results

- The Lorenz '95 model
- Computational Results

## 4 Conclusions

# Overview

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# 3D Variational Assimilation (3D-Var)

## Algorithm

### Minimize

$$\begin{aligned} J(\mathbf{x}_0) &= J_b + J_o \\ &= \frac{1}{2}(\mathbf{x}_b - \mathbf{x}_0)^T \mathbf{S}_{apr}^{-1}(\mathbf{x}_b - \mathbf{x}_0) \\ &\quad + \frac{1}{2}(\mathbf{y}(0) - \mathcal{K}_t(\mathbf{x}_0))^T \mathbf{S}_e^{-1}(\mathbf{y}(0) - \mathcal{K}_t(\mathbf{x}_0)), \end{aligned}$$

# 3D Variational Assimilation (3D-Var)

## Where

- $\mathbf{x}_0$  is the analysis at time 0
- $\mathbf{x}_b$  is the background at time 0
- $\mathbf{y}$  is the vector of observations at time 0
- $\mathbf{S}_{apr}$  is the background error covariance matrix
- $\mathbf{S}e_t$  is the observation error covariance matrix
- $\mathcal{K}_t$  is the nonlinear observation operator

# 3D Variational Assimilation (3D-Var)

## Properties

- *3D-Var is computed at a snapshot in time where all observations are assumed contemporaneous*
- *3D-Var does not take into account atmospheric dynamics, by which*
- *It does not depend on the weather model*

# 4D Variational Assimilation (4D-Var)

## Algorithm

### Minimize

$$\begin{aligned} J(\mathbf{x}_0) &= J_b + J_o \\ &= \frac{1}{2}(\mathbf{x}_b - \mathbf{x}_0)^T \mathbf{S}_{apr}^{-1}(\mathbf{x}_b - \mathbf{x}_0) \\ &\quad + \frac{1}{2} \sum_{t=0}^T (\mathbf{y}(t) - \mathcal{K}_t(\mathcal{M}_t(\mathbf{x}_0)))^T \mathbf{S}_{e_t}^{-1}(\mathbf{y}(t) - \mathcal{K}_t(\mathcal{M}_t(\mathbf{x}_0))), \end{aligned}$$

# 4D Variational Assimilation (4D-Var)

## Where

- $\mathbf{x}_0$  is the analysis at the beginning of the assimilation window
- $\mathbf{x}_b$  is the background at the beginning of the assimilation window
- $\mathbf{S}_{apr}$  is the background error covariance matrix
- $\mathbf{S}e_t$  is the observation error covariance matrix
- $\mathcal{M}_t$  is the nonlinear weather model

# 4D Variational Assimilation (4D-Var)

## Properties

- *The model is assumed to be perfect*
- *Model integrations are carried out forward in time with the nonlinear model and the tangent linear model, and backward in time with the corresponding adjoint model*
- *Minimization is sequential*
- *The weather model can run in parallel*

# The Extended Kalman Filter (EKF)

## Algorithm

### Iterate in time

$$\mathbf{x}_a(t) = \mathcal{M}_t(\mathbf{x}_{est}(t-1))$$

$$\mathbf{S}_a(t) = \mathbf{M}_t \mathbf{S}_{est}(t-1) \mathbf{M}_t^T + \mathbf{S} \mathbf{E}_t$$

$$\mathbf{G}_t = \mathbf{S}_a(t) \mathbf{K}_t^T (\mathbf{K}_t \mathbf{S}_a(t) \mathbf{K}_t^T + \mathbf{S} \mathbf{e}_t)^{-1}$$

$$\mathbf{x}_{est}(t) = \mathbf{x}_a(t) + \mathbf{G}_t (\mathbf{y}(t) - \mathcal{K}_t(\mathbf{x}_a(t)))$$

$$\mathbf{S}_{est}(t) = \mathbf{S}_a(t) - \mathbf{G}_t \mathbf{K}_t \mathbf{S}_a(t),$$

# The Extended Kalman Filter (EKF)

## Where

- $\mathbf{x}_a$  is the prediction
- $\mathbf{x}_{est}$  is the analysis
- $\mathbf{S}_a$  is the prediction error covariance matrix
- $\mathbf{S}_{est}$  is the analysis error covariance matrix
- $\mathbf{SE}_t$  is the model error covariance matrix
- $\mathbf{G}_t$  is the Kalman gain matrix

# The Extended Kalman Filter (EKF)

## Properties

- *The model is not assumed to be perfect*
- *Model integrations are carried out forward in time with the nonlinear model for the state estimate and*
- *Forward and backward in time with the tangent linear model and the adjoint model, respectively, for updating the prediction error covariance matrix*
- *There is no minimization, just matrix products and inversions*
- *Computational cost of EKF is prohibitive, because  $\mathbf{S}_a$  is a huge full matrix*

# The Variational Kalman Filter (VKF)

## Algorithm

### Iterate in time

**Step 0:** *Select an initial guess  $\mathbf{x}_{est}(0)$  and a covariance  $\mathbf{S}_{est}(0)$ , and set  $t = 1$ .*

**Step 1:** *Compute the evolution model state estimate and the prior covariance estimate:*

(i) *Compute  $\mathbf{x}_a(t) = \mathcal{M}_t(\mathbf{x}_{est}(t-1))$ ;*

(ii) *Approximate  $(\mathbf{S}_a(t))^{-1} = (\mathbf{M}_t \mathbf{S}_{est}(t-1) \mathbf{M}_t^T + \mathbf{SE}_t)^{-1}$  by the LBFGS method;*

## Algorithm

**Step 2:** *Compute the Variational Kalman filter state estimate and the posterior covariance estimate:*

(i) *Minimize*

$$\ell(\mathbf{x}_{est}(t)|\mathbf{y}) = (\mathbf{x}_a(t) - \mathbf{x}_{est}(t))^T (\mathbf{S}_a(t))^{-1} (\mathbf{x}_a(t) - \mathbf{x}_{est}(t)) +$$

$$(\mathbf{y} - \mathcal{K}_t(\mathbf{x}_{est}(t)))^T (\mathbf{S}_{e_t})^{-1} (\mathbf{y} - \mathcal{K}_t(\mathbf{x}_{est}(t))) ;$$

*by the LBFGS method;*

(ii) *Store the result of the minimization as a VKF estimate  $\mathbf{x}_{est}(t)$ ;*

(iii) *Store the limited memory approximation to  $\mathbf{S}_{est}(t)$ ;*

**Step 3:** *Update  $t := t + 1$  and return to Step 1.*

# The Variational Kalman Filter (VKF)

## Where

- *Step 1(ii) is carried out with an auxiliary minimization that has a trivial solution but a random initial guess, and thereby generates a non-trivial minimization sequence*
- *$\mathbf{S}_a(t)$  and  $\mathbf{S}_{est}(t)$  are kept in vector format, as a sum of a diagonal or sparse background  $\mathbf{S}_{apr}$  and a low rank dynamical component  $\tilde{\mathbf{S}}_a(t)$  that*
- *Is obtained from the Hessian update formula of the Limited Memory BFGS iteration*
- *The Kalman gain matrix is not needed*

# The Variational Kalman Filter (VKF)

## Properties

- *The model is not assumed to be perfect*
- *Model integrations are carried out forward in time with the nonlinear model for the state estimate and*
- *Forward and backward in time for updating the prediction error covariance matrix*
- *There are no matrix inversions, just matrix products and minimizations*
- *Computational cost of VKF is similar to 4D-Var*
- *Minimizations are sequential*
- *Accuracy of analyses similar to EKF*

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# Ensemble Kalman Filters (EnKF)

## Properties

- *Ensemble Kalman Filters are generally simpler to program than variational assimilation methods or EKF, because*
- *EnKF codes are based on just the non-linear model and do not require tangent linear or adjoint codes, but they*
- *Tend to suffer from slow convergence and therefore inaccurate analyses*
- *Often underestimate analysis error covariance*

# Ensemble Kalman Filters (EnKF)

## Properties

- *Ensemble Kalman filters often base analysis error covariance on **bred vectors**, i.e. the difference between ensemble members and the background, or the ensemble mean*
- *One family of EnKF methods is based on perturbed observations, while*
- *Another family uses explicit linear transforms to build up the ensemble*

# The Variational Ensemble Kalman Filter (VEnKF)

## Properties

- *The goal of VEnKF is to produce an Ensemble Kalman filter that*
- *Will not require a tangent linear or adjoint code*
- *But will converge faster and thereby produce more accurate analyses than EnKF methods in general*
- *VEnKF is based on the **4D-LETKF** method by **Hunt, Kostelic and Szunyogh***
- *It incorporates certain features from VKF, in particular*
- *It uses an analysis produced by a 3D-Var minimization with LBFGS as the vector to base bred vectors on, and not the ensemble mean or background*

# The Variational Ensemble Kalman Filter (VEnKF)

## Properties

*The cost function to be minimized is a "dual 3D-Var" cost function that optimizes the weight of each ensemble member in the analysis, using the LBFGS method:*

$$J(\mathbf{w}) = \beta(n-1)\mathbf{w}^T\mathbf{w} + (1-\beta) \times \\ (y_{apr} - \mathcal{K}(\mathbf{x}_a^{(i)}(t)) - Y\mathbf{w})^T (\mathbf{S}e_t)^{-1} (y_{apr} - \mathcal{K}(\mathbf{x}_a^{(i)}(t)) - Y\mathbf{w})$$

# The Variational Ensemble Kalman Filter (VEnKF)

## Where

- $y_{apr}$  is the synthetic observation vector of the prior  
 $y_{apr} = \mathcal{K}(\mathbf{x}_{apr}(t))$
- $\mathbf{w}$  is the vector of the weights  $w^{(i)}$  of each ensemble member  
 $\mathbf{x}_a^{(i)}(t)$
- $Y$  is the matrix of synthetic observations of each ensemble member  
 $Y^{(i)} = \mathcal{K}(\mathbf{x}_a^{(i)}(t))$
- $n$  is the ensemble size
- $\beta$  is an empirical weight factor between 0 and 1

# The Variational Ensemble Kalman Filter (VEnKF)

## Algorithm

### Iterate in time

**Step 0:** Initialize the background state  $\mathbf{x}_{apr}(0)$  and the ensemble members  $\mathbf{x}_{est}^{(i)}(0)$  for  $i = 1, \dots, n$

**Step 1:** Compute  $\mathbf{x}_a^{(i)}(t) = \mathcal{M}_t(\mathbf{x}_{est}^{(i)}(t-1))$  and  $\mathbf{x}_{apr}(t) = \mathcal{M}_t(\mathbf{x}_{apr}(t-1))$ ;

**Step 2:** Perturb the members  $\mathbf{x}_a^{(i)}(t)$  and assemble them in matrix  $\Psi$ ;

**Step 3:** Compute the matrix  $X_a(t) : X_a^{(i)}(t) = \mathbf{x}_a^{(i)}(t) - \mathbf{x}_{apr}(t)$ ;

**Step 4:** Compute the matrix

$$Y_a(t) : Y_a^{(i)}(t) = \mathcal{K}(\mathbf{x}_a^{(i)}(t)) - \mathcal{K}(\mathbf{x}_{apr}(t));$$

# The Variational Ensemble Kalman Filter (VEnKF)

## Algorithm

**Step 5:** *Minimize the dual 3D-Var cost function  $J(\mathbf{w})$  using the LBFGS method.*

**Step 6:** *Compute the analysis  $\mathbf{x}_{apr}(t) = \mathbf{x}_{apr}(t) + X_a(t)\mathbf{w}$*

**Step 7:** *Compute the background ensemble*

$$X_{est}(t) : X_{est}^{(i)}(t) = X_a^{(i)}(t) + X_a(t)\mathbf{w}$$

**Step 8:** *Update  $t := t + 1$  and return to Step 1.*

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# The Lorenz '95 Model

## Properties

- *The Lorenz '95 model is computationally light and represents an analogue of mid-latitude atmospheric dynamics.*
- *The variables of the model can be thought of as representing some atmospheric quantity on a single latitude circle.*
- *The model consists of a system of coupled ordinary differential equations*

$$\frac{\partial c_i}{\partial t} = c_{i-1}c_{i+1} - c_{i-2}c_{i-1} - c_i + F,$$

- *Grid points range between  $i = 1, 2, \dots, k$  and  $F$  is a constant.*

# The Lorenz '95 Model

## Where

- *The domain is set to be cyclic, so that  $c_{-1} = c_{k-1}$ ,  $c_0 = c_k$  and  $c_{k+1} = c_1$ .*
- *The parameter values used in the simulation of the system were selected as follows:*
- *the number of grid points  $k = 40$ ,*
- *the climatological standard deviation of the model state,  $\sigma_{clim} \approx 3.64$ ,*
- *the observation noise matrix  $\mathbf{S}e_t = 0.15\sigma_{clim}\mathbf{I}$  and*
- *prediction error covariance  $\mathbf{S}E_t = 0.5\sigma_{clim}\mathbf{I}$ .*

# The Lorenz '95 Model

## Properties

- *The system was assimilated using each of EKF, VKF and VEnKF.*
- *In order to compare the quality of analyses produced by all three methods, we compute the following forecast statistics at every 8th observation.*
- *Take  $j \in \mathcal{I} := \{8i \mid i = 1, 2, \dots, 100\}$  and define*

$$[\text{forecast\_error}_j]_i = \frac{1}{40} \|\mathcal{M}_{4i}(\mathbf{x}_j^{\text{est}}) - \mathbf{x}_{j+4i}^{\text{true}}\|^2, \quad i = 1, \dots, 20,$$

# The Lorenz '95 Model

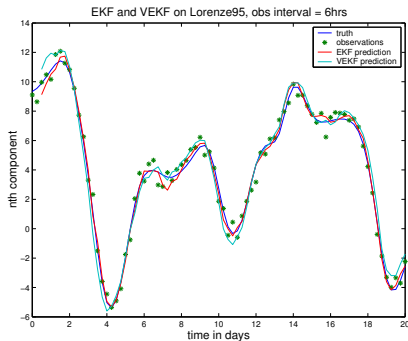
## Where

- $\mathcal{M}_n$  denotes a forward integration of the model by  $n$  time steps with the RK4 method.
- This vector gives a measure of forecast accuracy given by the respective filter estimate up to 80 time steps, or 10 days out.
- This allows us to define the forecast skill vector

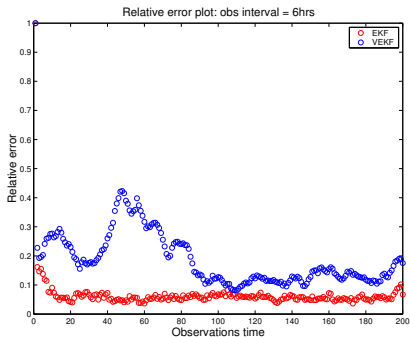
$$[\text{forecast\_skill}]_i = \frac{1}{\sigma_{\text{clim}}} \sqrt{\frac{1}{100} \sum_{j \in \mathcal{I}} [\text{forecast\_error}_j]_i^2}$$

$$i=1, \dots, 20,$$

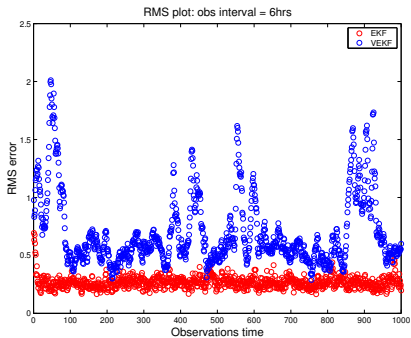
# Computational Results



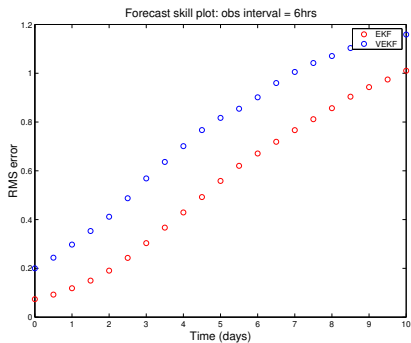
# Computational Results



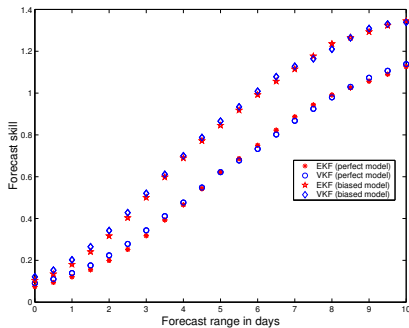
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# Conclusions

- VKF performs as well as EKF, with a computational cost comparable to 4D-Var, on Lorentz '95
- VEnKF is less good than EKF or VKF in forecast skill, but can be run without an adjoint code
- VEnKF is embarrassingly parallel
- Another version of VKF also parallelizes well, but has a higher serial complexity
- VKF and VEnKF are attractive candidates to replace 4D-Var and Optimum Interpolation, respectively, in operational weather data assimilation

Thank You

**Thank You!**