# Variational Ensemble Kalman Filtering on Parallel Computers

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# Overview

# 3D Variational Assimilation (3D-Var)

## Algorithm

**Minimize**

$$\begin{aligned} J(\mathbf{x_0}) &= J_b + J_o \\ &= \frac{1}{2}(\mathbf{x_b} - \mathbf{x_0})^{\mathrm{T}} \mathbf{S}_{apr}^{-1} (\mathbf{x_b} - \mathbf{x_0}) \\ &+ \frac{1}{2}(\mathbf{y}(0) - \mathcal{K}_t(\mathbf{x_0}))^{\mathrm{T}} \mathbf{Se}_t^{-1} (\mathbf{y}(0) - \mathcal{K}_t(\mathbf{x_0})), \end{aligned}$$

# 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*
- $\mathbf{Se}_t$ *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**

$$\begin{aligned} J(\mathbf{x_0}) &= J_b + J_o \\ &= \frac{1}{2}(\mathbf{x_b} - \mathbf{x_0})^{\mathrm{T}} \mathbf{S}_{apr}^{-1} (\mathbf{x_b} - \mathbf{x_0}) \\ &+ \frac{1}{2} \sum_{t=0}^{T} (\mathbf{y}(t) - \mathcal{K}_t(\mathcal{M}_t(\mathbf{x_0})))^{\mathrm{T}} \mathbf{Se}_t^{-1} (\mathbf{y}(t) - \mathcal{K}_t(\mathcal{M}_t(\mathbf{x_0}))), \end{aligned}$$

# 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*
- $\mathbf{Se}_t$ *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**

$$\begin{aligned}
\mathbf{x}_a(t) &= \mathcal{M}_t(\mathbf{x}_{est}(t-1)) \\
\mathbf{S}_a(t) &= \mathbf{M}_t\mathbf{S}_{est}(t-1)\mathbf{M}_t^{\mathrm{T}} + \mathbf{SE}_t \\
\mathbf{G}_t &= \mathbf{S}_a(t)\mathbf{K}_t^{\mathrm{T}}(\mathbf{K}_t\mathbf{S}_a(t)\mathbf{K}_t^{\mathrm{T}} + \mathbf{Se}_t)^{-1} \\
\mathbf{x}_{est}(t) &= \mathbf{x}_a(t) + \mathbf{G}_t(\mathbf{y}(t) - \mathcal{K}_t(\mathbf{x}_a(t))) \\
\mathbf{S}_{est}(t) &= \mathbf{S}_a(t) - \mathbf{G}_t\mathbf{K}_t\mathbf{S}_a(t),
\end{aligned}$$

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

## Algorithm

**Step 2:** *Compute the Variational Kalman filter state estimate and the posterior covariance estimate:*
*(i) Minimize*

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

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

*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* $\breve{\mathbf{S}}_a(t)$ *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 sequantial*
- *Accuracy of analyses similar to EKF*

# Overview

# 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:*

$$J(\mathbf{w}) = \beta(n-1)\mathbf{w}^{\mathrm{T}}\mathbf{w} + (1-\beta)\times$$

$$(y_{apr} - \mathcal{K}(\mathbf{x}_a^{(i)}(t)) - Y\mathbf{w})^{\mathrm{T}}(\mathbf{Se}_t)^{-1}(y_{apr} - \mathcal{K}(\mathbf{x}_a^{(i)}(t)) - Y\mathbf{w})$$

# 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* $i = 1, \ldots, n$

**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* $X_a(t) : X_a^{(i)}(t) = \mathbf{x}_{apr}(t) - \Psi^{(i)}$;

**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.*

# Overview

# 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* $i = 1, 2, ..., k$ *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* $\mathbf{Se}_t = 0.15\sigma_{clim}\mathbf{I}$ *and*
- *prediction error covariance* $\mathbf{SE}_t = 0.5\sigma_{clim}\mathbf{I}$.

# 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* $j \in \mathcal{I} := \{8i \mid i = 1, 2, \ldots, 100\}$ *and define*

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

# The Lorenz '95 Model

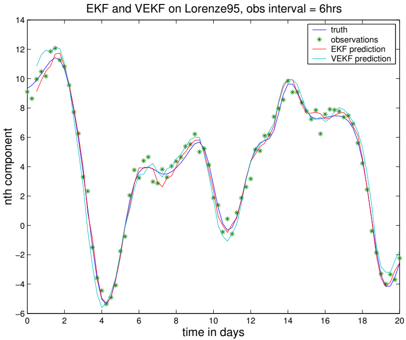
## Where

- *$\mathcal{M}_n$ 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*

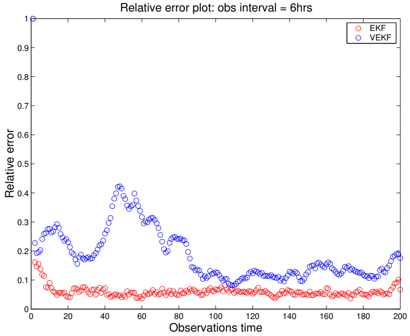
$$[\textbf{forecast\_skill}]_i = \frac{1}{\sigma_{\text{clim}}} \sqrt{\frac{1}{100} \sum_{j \in \mathcal{I}} [\textbf{forecast\_error}_j]_i},$$

*i=1,. . . ,20,*

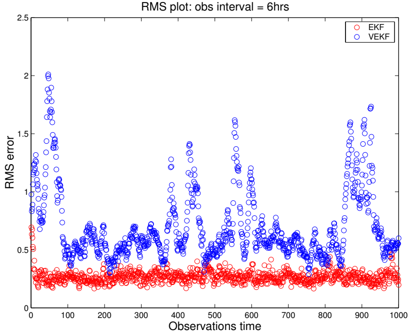
# Computational Results



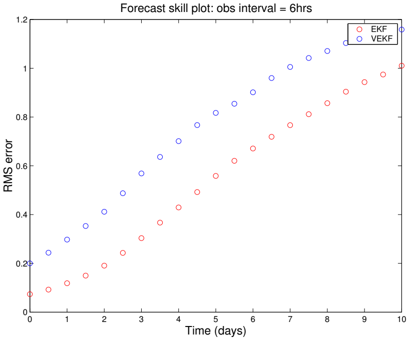
# Computational Results



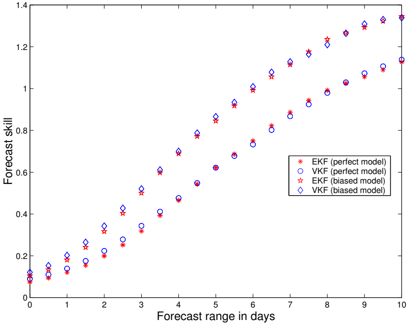
# Computational Results



# Computational Results



# Computational Results



# Overview

# 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!**