

# Data Assimilation as Parallel Minimization

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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)
- Ensemble 4DVar Data Assimilation (EDA)
- The Variational Ensemble Kalman Filter (VEnKF)
- The modified Local Ensemble Transform Kalman Filter (mLETK)

## 3 Computational Results

- The Lorenz '95 model
- Computational Results

## 4 Cost functions and parallelism

- Cost functions
- Parallelism

# Overview

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# 3D Variational Assimilation (3D-Var)

## Algorithm

### Minimize

$$\begin{aligned} J(\mathbf{x}(t_i)) &= J_b + J_o \\ &= \frac{1}{2}(\mathbf{x}(t_i) - \mathbf{x}^b(t_i))^T \mathbf{B}_0^{-1} (\mathbf{x}(t_i) - \mathbf{x}^b(t_i)) \\ &\quad + \frac{1}{2}(H(\mathbf{x}(t_i)) - \mathbf{y}_i^o)^T \mathbf{R}^{-1} (H(\mathbf{x}(t_i)) - \mathbf{y}_i^o), \end{aligned}$$

# 3D Variational Assimilation (3D-Var)

## Where

- $\mathbf{x}(t_i)$  is the analysis at time  $t_i$
- $\mathbf{x}^b(t_i)$  is the background at time  $t_i$
- $\mathbf{y}_i^o$  is the vector of observations at time  $t_i$
- $\mathbf{B}_0$  is the background error covariance matrix
- $\mathbf{R}$  is the observation error covariance matrix
- $H$  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

$$\begin{aligned} J(\mathbf{x}(t_0)) &= J_b + J_o \\ &= \frac{1}{2}(\mathbf{x}(t_0) - \mathbf{x}^b(t_0))^T \mathbf{B}_0^{-1}(\mathbf{x}(t_0) - \mathbf{x}^b(t_0)) \\ &+ \frac{1}{2} \sum_{i=0}^n (H(M(t_i, t_0)(\mathbf{x}(t_0))) - \mathbf{y}_i^o)^T \mathbf{R}^{-1} (H(M(t_i, t_0)(\mathbf{x}(t_0))) - \mathbf{y}_i^o) \end{aligned}$$

# 4D Variational Assimilation (4D-Var)

## Where

- $\mathbf{x}(t_0)$  is the analysis at the beginning of the assimilation window
- $\mathbf{x}^b(t_0)$  is the background at the beginning of the assimilation window
- $\mathbf{B}_0$  is the background error covariance matrix
- $\mathbf{R}$  is the observation error covariance matrix
- $H$  is the nonlinear observation operator
- $M$  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

$$\mathbf{x}^f(t_i) = M(t_i, t_{i-1})(\mathbf{x}^a(t_{i-1}))$$

$$\mathbf{P}_i^f = \mathbf{M}_i \mathbf{P}^a(t_{i-1}) \mathbf{M}_i^T + \mathbf{Q}$$

$$\mathbf{K}_i = \mathbf{P}^f(t_i) \mathbf{H}_i^T (\mathbf{H}_i \mathbf{P}^f(t_i) \mathbf{H}_i^T + \mathbf{R})^{-1}$$

$$\mathbf{x}^a(t_i) = \mathbf{x}^f(t_i) + \mathbf{K}_i (\mathbf{y}_i^o - H(\mathbf{x}^f(t_i)))$$

$$\mathbf{P}^a(t_i) = \mathbf{P}^f(t_i) - \mathbf{K}_i \mathbf{H}_i \mathbf{P}^f(t_i)$$

# The Extended Kalman Filter (EKF)

## Where

- $\mathbf{x}^f(t_i)$  is the prediction at time  $t_i$
- $\mathbf{x}^a(t_i)$  is the analysis at time  $t_i$
- $\mathbf{P}^f(t_i)$  is the prediction error covariance matrix at time  $t_i$
- $\mathbf{P}^a(t_i)$  is the analysis error covariance matrix at time  $t_i$
- $\mathbf{Q}$  is the model error covariance matrix
- $\mathbf{K}_i$  is the Kalman gain matrix at time  $t_i$
- $\mathbf{R}$  is the observation error covariance matrix
- $H$  is the nonlinear observation operator
- $\mathbf{H}_i$  is the linearized observation operator at time  $t_i$
- $\mathbf{M}_i$  is the linearized weather model at time  $t_i$

# 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  $\mathbf{P}^f(t_i)$  and  $\mathbf{P}^a(t_i)$  are huge full matrices*

# The Variational Kalman Filter (VKF)

## Algorithm

### Iterate in time

**Step 0:** *Select an initial guess  $\mathbf{x}^a(t_0)$  and a covariance  $\mathbf{P}^a(t_0)$ , and set  $i = 1$ .*

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

(i) *Compute  $\mathbf{x}^f(t_i) = M(t_i, t_{i-1})(\mathbf{x}^a(t_{i-1}))$ ;*

(ii) **Minimize**

$$(\mathbf{P}^f(t_i))^{-1} = (\mathbf{M}_i \mathbf{P}^a(t_{i-1}) \mathbf{M}_i^T + \mathbf{Q})^{-1}$$

*by the LBFGS method - or CG, as in incremental 4DVar;*

# The Variational Kalman Filter (VKF)

## Algorithm

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

(i) **Minimize**

$$\begin{aligned} & \lambda(\mathbf{x}^a(t_j) | \mathbf{y}_j^o) \\ & = (\mathbf{y}_j^o - \mathbf{H}_j \mathbf{x}^a(t_j))^T \mathbf{R}^{-1} (\mathbf{y}_j^o - \mathbf{H}_j \mathbf{x}^a(t_j)) \\ & \quad + (\mathbf{x}^f(t_j) - \mathbf{x}^a(t_j))^T (\mathbf{P}^f(t_j))^{-1} (\mathbf{x}^f(t_j) - \mathbf{x}^a(t_j)) \end{aligned}$$

by the LBFGS method - or CG, as in incremental 3DVar;

(ii) Store the result of the minimization as a VKF estimate  $\mathbf{x}^a(t_j)$ ;

(iii) Store the limited memory approximation to  $\mathbf{P}^a(t_j)$ ;

**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*
- *$\mathbf{P}^f(t_i)$  and  $\mathbf{P}^a(t_i)$  are kept in vector format, as a weighted sum of a diagonal or sparse background  $\mathbf{B}_0$ , a diagonal model error variance matrix  $\mathbf{Q}$  and a low rank dynamical component  $\mathbf{P}^f(t_i)$  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*

# EnKF Cost functions

## Algorithm

### Minimize

$$(\mathbf{P}^f(t_i))^{-1} = (\beta \mathbf{B}_0 + (1 - \beta) \frac{1}{N} \mathbf{X}^f(t_i) \mathbf{X}^f(t_i)^T)^{-1}$$

## Algorithm

### Minimize

$$\begin{aligned} \ell(\mathbf{x}^a(t_i) | \mathbf{y}_i^o) &= (\mathbf{y}_i^o - H(\mathbf{x}^a(t_i)))^T \mathbf{R}^{-1} (\mathbf{y}_i^o - H(\mathbf{x}^a(t_i))) \\ &+ \frac{1}{N} \sum_{j=1}^N (\mathbf{x}_j^f(t_i) - \mathbf{x}^a(t_i))^T (\mathbf{P}^f(t_i))^{-1} (\mathbf{x}_j^f(t_i) - \mathbf{x}^a(t_i)) \end{aligned}$$

# Ensemble 4DVar Data Assimilation (EDA)

## Algorithm

**Step 0:** *Select an initial guess  $\mathbf{x}^a(t_0)$  and a covariance  $\mathbf{B}_0$  and set  $i = 1$*

**Step 1:** *Compute perturbed observations and physics:*

*(i) Create an ensemble of observations by  $\delta_k \mathbf{y}_i^o \sim N(\mathbf{y}_i^o, \mathbf{R}_i)$ ;*

**Step 2:** *(i) Minimize, for each  $k$*

$$\begin{aligned} J(\mathbf{x}(t_{i-1})) &= J_b + J_o \\ &= \frac{1}{2}(\mathbf{x}(t_0) - \mathbf{x}^b(t_0))^T \mathbf{B}_0^{-1} (\mathbf{x}(t_0) - \mathbf{x}^b(t_0)) \\ &+ \frac{1}{2} \sum_{j=0}^n (H(M(t_j, t_0)(\mathbf{x}(t_0))) - (\mathbf{y}_j^o + \delta_k \mathbf{y}_j^o))^T \mathbf{R}^{-1} \\ &\times (H(M(t_j, t_0)(\mathbf{x}(t_0))) - (\mathbf{y}_j^o + \delta_k \mathbf{y}_j^o)), \end{aligned}$$

*to obtain an ensemble of analyses from  $\mathbf{X}^f(t_{i-1})$  to  $\mathbf{X}^f(t_i)$  by the LBFGS method;*

# Ensemble 4DVar Data Assimilation (EDA)

## Algorithm

(ii) Compute the updated error covariance for each time step in the assimilation window

$(\mathbf{P}^a(t_j))^{-1} = (\mathbf{B}_0 + \mathbf{X}^f(t_j)\mathbf{X}^f(t_j)^\top)^{-1}$ ,  $j = t_{i-1} \dots t_i$   
by the LBFGS method;

**Step 3: (i) Minimize:**

$$\begin{aligned} J(\mathbf{x}(t_{i-1}), \dots, \mathbf{x}(t_i)) &= J_b + J_o + J_M \\ &= \frac{1}{2} \sum_{j=t_{i-1}}^{t_i} (\mathbf{x}(t_j) - \mathbf{x}^b(t_j))^\top (\mathbf{P}^a(t_j))^{-1} (\mathbf{x}(t_j) - \mathbf{x}^b(t_j)) \\ &\quad + \frac{1}{2} \sum_{i=0}^n (H(\mathbf{x}(t_j)) - \mathbf{y}_j^o)^\top \mathbf{R}^{-1} (H(\mathbf{x}(t_j)) - \mathbf{y}_j^o) \\ &\quad + \frac{1}{2} \sum_{j=t_{i-1}}^{t_i} (\mathbf{x}(t_j) - M(t_j, t_{j-1})(\mathbf{x}(t_{j-1})))^\top \mathbf{Q}^{-1} \\ &\quad \times (\mathbf{x}(t_j) - M(t_j, t_{j-1})(\mathbf{x}(t_{j-1}))), \end{aligned}$$

Store the result as the EDA estimate  $\mathbf{x}^a(t_{i-1}), \dots, \mathbf{x}^a(t_i)$ ;

(ii) Update  $i := i + 1$  and return to Step 1.

# The Variational Ensemble Kalman Filter (VEnKF)

## Algorithm

### Iterate in time

**Step 0:** *Select a state  $\mathbf{x}^a(t_0)$  and a covariance  $\mathbf{P}^a(t_0)$  and set  $i = 1$*

**Step 1:** *Evolve the state and the prior covariance estimate:*

(i) *Compute  $\mathbf{x}^f(t_i) = M(t_i, t_{i-1})(\mathbf{x}^a(t_{i-1}))$ ;*

(ii) *Compute the ensemble forecast*

$\mathbf{X}^f(t_i) = M(t_i, t_{i-1})(\mathbf{X}^a(t_{i-1}))$ ;

(iii) **Minimize** *from a random initial guess*

$(\mathbf{P}^f(t_i))^{-1} = (\beta \mathbf{B}_0 + (1 - \beta) \frac{1}{N} \mathbf{X}^f(t_i) \mathbf{X}^f(t_i)^T + \mathbf{Q}_i)^{-1}$

*by the LBFGS method;*

# The Variational Ensemble Kalman Filter (VEnKF)

## Algorithm

**Step 2:** Compute the Variational Ensemble Kalman Filter posterior state and covariance estimates:

(i) Minimize

$$\begin{aligned} & \ell(\mathbf{x}^a(t_i) | \mathbf{y}_i^o) \\ &= (\mathbf{y}_i^o - H(\mathbf{x}^a(t_i)))^T \mathbf{R}^{-1} (\mathbf{y}_i^o - H(\mathbf{x}^a(t_i))) \\ &+ (\mathbf{x}^f(t_i) - \mathbf{x}^a(t_i))^T (\mathbf{P}^f(t_i))^{-1} (\mathbf{x}^f(t_i) - \mathbf{x}^a(t_i)) \end{aligned}$$

by the LBFGS method;

(ii) Store the result of the minimization as  $\mathbf{x}^a(t_i)$ ;

(iii) Store the limited memory approximation to  $\mathbf{P}^a(t_i)$ ;

(iv) Generate a new ensemble  $\mathbf{X}^a(t_i) \sim N(\mathbf{x}^a(t_i), \mathbf{P}^a(t_i))$ ;

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



# The Variational Ensemble Kalman Filter (VEnKF)

## Properties

- *Follows the algorithmic structure of VKF*
- *Bred vectors are centered on the **mode**, not the mean, of the ensemble, as in Bayesian estimation*
- *Like in VKF, a new ensemble and a new error covariance matrix is generated at every observation time*
- *No covariance leakage*
- *No tangent linear or adjoint code*
- *Asymptotically equivalent to VKF and therefore EKF when ensemble size increases*

# The modified Local Ensemble Transform Kalman Filter (mLETKF)

## Properties

- *The goal of mLETKF 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*
- *mLETKF 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*

# The modified Local Ensemble Transform Kalman Filter (mLETKF)

## 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:*

$$J(\mathbf{w}) = \beta(n-1)\mathbf{w}^T\mathbf{w} + (1-\beta) \times (\mathbf{y}^f - H(\mathbf{x}_k^a(t_i)) - \mathbf{w}^T Y)^T \mathbf{R}^{-1} (\mathbf{y}^f - H(\mathbf{x}_k^a(t_i)) - \mathbf{w}^T Y)$$

# The modified Local Ensemble Transform Kalman Filter (mLETKF)

## Where

- $\mathbf{y}^f$  is the synthetic observation vector of the prior  
 $\mathbf{y}^f = H(\mathbf{x}^f(t_i))$
- $\mathbf{w}$  is the vector of the weights  $w^k$  of each ensemble member  $\mathbf{x}_k^a(t_i)$
- $Y$  is the matrix of synthetic observations of each ensemble member  $\mathbf{y}_k^f = H(\mathbf{x}_k^a(t_i))$
- $N$  is the ensemble size
- $\beta$  is an empirical weight factor between 0 and 1

# The modified Local Ensemble Transform Kalman Filter (mLETKF)

## Algorithm

### Iterate in time

**Step 0:** Initialize the background state  $\mathbf{x}^a(t_0)$  and the ensemble members  $\mathbf{x}_k^a(t_0)$  for  $k = 1, \dots, N$

**Step 1:** Compute  $\mathbf{x}_k^f(t_i) = M(\mathbf{x}_k^a(t_{i-1}))$  and  $\mathbf{x}^f(t_i) = M(\mathbf{x}^a(t_{i-1}))$ ;

**Step 2:** Perturb the members  $\mathbf{x}_k^f(t_i)$  and assemble them in matrix  $\Psi$ ;

**Step 3:** Compute the matrix  $X^f(t_i) : \mathbf{x}_k^f(t_i) = \mathbf{x}^f(t_i) - \Psi^k$ ;

**Step 4:** Compute the matrix

$$Y^f(t_i) : \mathbf{y}_k^f(t_i) = H(\mathbf{x}_k^f(t_i)) - H(\mathbf{x}^f(t_i));$$

# The modified Local Ensemble Transform Kalman Filter (mLETKF)

## Algorithm

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

**Step 6:** *Compute the analysis  $\mathbf{x}^a(t_i) = \mathbf{x}^f(t_i) + \mathbf{w}^T X^f(t_i)$*

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

$$X^a(t_i) : \mathbf{x}_k^a(t_i) = \mathbf{x}_k^f(t_i) + \mathbf{w}^T X^f(t_i)$$

**Step 8:** *Update  $i := i + 1$  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*

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

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



# 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  $\mathbf{R} = 0.15\sigma_{clim}\mathbf{I}$  and*
- *prediction error covariance  $\mathbf{B}_0 = 0.5\sigma_{clim}\mathbf{I}$ .*

# 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*

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

# The Lorenz '95 Model

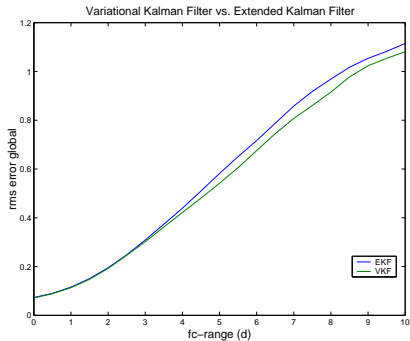
## Where

- $M_n$  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

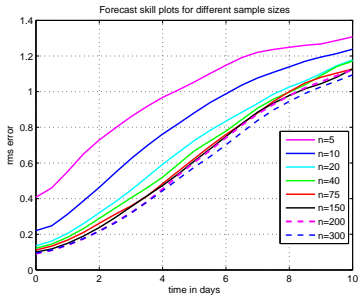
$$[\text{forecast\_skill}]_i = \frac{1}{\sigma_{\text{clim}}} \sqrt{\frac{1}{100} \sum_{j \in \mathcal{I}} [\text{forecast\_error}_j]_i^2}$$

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

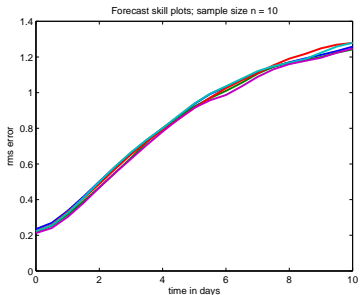
# VKF vs. EKF



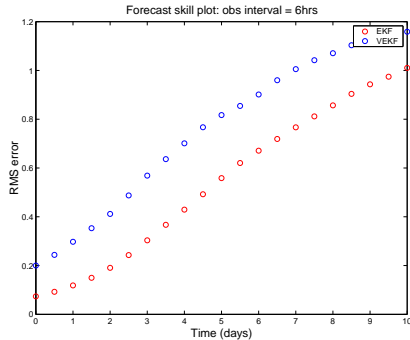
# VEEnKF, $N = 5, \dots, 300$



# Skills of several VEnKF analyses, N=10



# mLETKF (N=150) vs. EKF



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### • Cost functions



## 3D-Var Cost function

### Algorithm

#### Minimize

$$\begin{aligned} J(\mathbf{x}(t_i)) &= J_b + J_o \\ &= \frac{1}{2}(\mathbf{x}(t_i) - \mathbf{x}^b(t_i))^T \mathbf{B}_0^{-1} (\mathbf{x}(t_i) - \mathbf{x}^b(t_i)) \\ &\quad + \frac{1}{2}(H(\mathbf{x}(t_i)) - \mathbf{y}_i^o)^T \mathbf{R}^{-1} (H(\mathbf{x}(t_i)) - \mathbf{y}_i^o) \end{aligned}$$

## 4D-Var Cost function

### Algorithm

#### Minimize

$$\begin{aligned} J(\mathbf{x}(t_0)) &= J_b + J_o \\ &= \frac{1}{2}(\mathbf{x}(t_0) - \mathbf{x}^b(t_0))^T \mathbf{B}_0^{-1}(\mathbf{x}(t_0) - \mathbf{x}^b(t_0)) \\ &\quad + \frac{1}{2} \sum_{i=0}^n (H(M(t_i, t_0)(\mathbf{x}(t_0))) - \mathbf{y}_i^o)^T \mathbf{R}^{-1} (H(M(t_i, t_0)(\mathbf{x}(t_0))) - \mathbf{y}_i^o) \end{aligned}$$

# EnKF Cost functions

## Algorithm

### Minimize

$$(\mathbf{P}^f(t_i))^{-1} = (\beta \mathbf{B}_0 + (1 - \beta) \frac{1}{N} \mathbf{X}^f(t_i) \mathbf{X}^f(t_i)^T)^{-1}$$

### Minimize

$$\begin{aligned} & \ell(\mathbf{x}^a(t_i) | \mathbf{y}_i^o) \\ &= (\mathbf{y}_i^o - H(\mathbf{x}^a(t_i)))^T \mathbf{R}^{-1} (\mathbf{y}_i^o - H(\mathbf{x}^a(t_i))) \\ &+ \frac{1}{N} \sum_{j=1}^N (\mathbf{x}_j^f(t_i) - \mathbf{x}^a(t_i))^T (\mathbf{P}^f(t_i))^{-1} (\mathbf{x}_j^f(t_i) - \mathbf{x}^a(t_i)) \end{aligned}$$

# EDA Cost functions - 1

## Algorithm

Minimize, for each perturbation  $\delta_k \mathbf{y}_j^o$

$$\begin{aligned} J(\mathbf{x}(t_{i-1})) &= J_b + J_o \\ &= \frac{1}{2}(\mathbf{x}(t_0) - \mathbf{x}^b(t_0))^T \mathbf{B}_0^{-1} (\mathbf{x}(t_0) - \mathbf{x}^b(t_0)) \\ &+ \frac{1}{2} \sum_{i=0}^n (H(M(t_i, t_0)(\mathbf{x}(t_0))) - (\mathbf{y}_j^o + \delta_k \mathbf{y}_j^o))^T \mathbf{R}^{-1} \\ &\times (H(M(t_i, t_0)(\mathbf{x}(t_0))) - (\mathbf{y}_j^o + \delta_k \mathbf{y}_j^o)) \end{aligned}$$

## EDA Cost functions - 2

### Algorithm

#### Minimize

$$(\mathbf{P}^a(t_j))^{-1} = (\beta \mathbf{B}_0 + (1 - \beta) \frac{1}{N} \mathbf{X}^f(t_j) \mathbf{X}^f(t_j)^T)^{-1}, \quad j = t_{i-1} \dots t_i$$

## EDA Cost functions - 3

### Algorithm

#### Minimize

$$\begin{aligned} J(\mathbf{x}(t_{i-1})) &= J_b + J_o + J_M \\ &= \frac{1}{2} \sum_{j=t_{i-1}}^{t_i} (\mathbf{x}(t_j) - \mathbf{x}^b(t_j))^T (\mathbf{P}^a(t_j))^{-1} (\mathbf{x}(t_j) - \mathbf{x}^b(t_j)) \\ &\quad + \frac{1}{2} \sum_{i=0}^n (H(\mathbf{x}(t_j)) - \mathbf{y}_j^o)^T \mathbf{R}^{-1} (H(\mathbf{x}(t_j)) - \mathbf{y}_j^o) \\ &\quad + \frac{1}{2} \sum_{j=t_{i-1}}^{t_i} (\mathbf{x}(t_j) - M(t_j, t_{j-1})(\mathbf{x}(t_{j-1})))^T \mathbf{Q}^{-1} (\mathbf{x}(t_j) - M(t_j, t_{j-1})(\mathbf{x}(t_{j-1}))), \end{aligned}$$

# VEnKF Cost functions

## Algorithm

### Minimize

$$(\mathbf{P}^f(t_i))^{-1} = (\beta \mathbf{B}_0 + (1 - \beta) \frac{1}{N} \mathbf{X}^f(t_i) \mathbf{X}^f(t_i)^T + \mathbf{Q})^{-1}$$

### Minimize

$$\begin{aligned} \ell(\mathbf{x}^a(t_i) | \mathbf{y}_i^o) &= (\mathbf{y}_i^o - H(\mathbf{x}^a(t_i)))^T \mathbf{R}^{-1} (\mathbf{y}_i^o - H(\mathbf{x}^a(t_i))) \\ &+ (\mathbf{x}^f(t_i) - \mathbf{x}^a(t_i))^T (\mathbf{P}^f(t_i))^{-1} (\mathbf{x}^f(t_i) - \mathbf{x}^a(t_i)) \end{aligned}$$

# VKF Cost functions

## Algorithm

### Minimize

$$(\mathbf{P}^f(t_i))^{-1} = (\mathbf{M}_i \mathbf{P}^a(t_{i-1}) \mathbf{M}_i^T + \mathbf{Q})^{-1}$$

### Minimize

$$\begin{aligned} & \lambda(\mathbf{x}^a(t_i) | \mathbf{y}_i^o) \\ &= (\mathbf{y}_i^o - \mathbf{H}_i \mathbf{x}^a(t_i))^T \mathbf{R}^{-1} (\mathbf{y}_i^o - \mathbf{H}_i \mathbf{x}^a(t_i)) \\ &+ (\mathbf{x}^f(t_i) - \mathbf{x}^a(t_i))^T (\mathbf{P}^f(t_i))^{-1} (\mathbf{x}^f(t_i) - \mathbf{x}^a(t_i)) \end{aligned}$$



# mLETKF Cost function

## Algorithm

### Minimize

$$J(\mathbf{w}) = \beta(n-1)\mathbf{w}^T\mathbf{w} + (1-\beta) \times \\ (\mathbf{y}^f - H(\mathbf{x}_k^a(t_i)) - \mathbf{w}^T \mathbf{Y})^T \mathbf{R}^{-1} (\mathbf{y}^f - H(\mathbf{x}_k^a(t_i)) - \mathbf{w}^T \mathbf{Y})$$

# Parallelism - 1

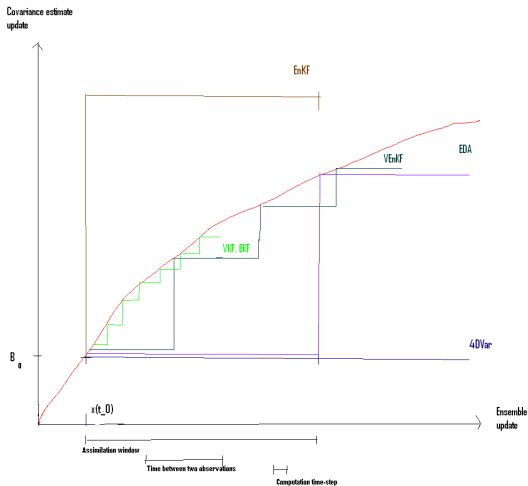
- Ensemble methods generally use their ensemble as a sample to approximate error covariance
- But the most accurate methods, such as 3DVar, 4DVar and VKF, are based on Krylov space approximation of the covariance
- Krylov space approximation is inherently serial, since a Krylov space is defined by iterative application of an operator on a vector:

$$\mathbf{K}_k(A, \mathbf{b}) = \text{Span}(\mathbf{b}, A\mathbf{b}, A^2\mathbf{b}, \dots, A^k\mathbf{b})$$

## Parallelism - 2

- EnKF variants can be embarrassingly parallel and evolve its ensemble in parallel
- But the most accurate of them, such as VEnKF and EDA, still use a Krylov space method to approximate covariance: LBFGS, CG or Lanczos
- These methods are therefore inherently sequential, too
- The best accuracy of analysis in L95 tests follows from frequent and smooth updating of both the ensemble and the error covariance estimate

# Updates to Ensemble and Error Covariance



# Overview

## 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)
- Ensemble 4DVar Data Assimilation (EDA)
- The Variational Ensemble Kalman Filter (VEnKF)
- The modified Local Ensemble Transform Kalman Filter (mLETK)

## 3 Computational Results

- The Lorenz '95 model
- Computational Results

## 4 Cost functions and parallelism

- Cost functions

## Conclusions - 1

- VKF performs as well as EKF, with a computational cost comparable to 4D-Var, on Lorentz '95
- VEnKF is asymptotically as good as EKF or VKF in forecast skill, but can be run without an adjoint code
- VEnKF attains equal quality to EKF only on large ensemble sizes, but
- VEnKF performs better than EnKF especially with small ensemble size

## Conclusions - 2

- The more frequent the inter-linked updates of the ensemble and the error covariance estimate, the more accurate the analysis
- There appears to be a trade-off between the accuracy of an assimilation method and its parallelism that needs to be decided by experiments

Thank You

**Thank You!**