Fundamentals of Data Assimilation

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2017 Joint DTC-EMC-JCSDA GSI Tutorial

Objective of This Lecture

- Introduction to
  - Basic concepts of Numerical Weather Prediction (NWP)
  - Practical approaches to Data Assimilation (DA)
- Introduction to
  - Maximum likelihood (ML) estimation, naturally for state
    →Variational forms of DA
  - Minimum variance (MV) estimation, naturally for state & covariance
    →(Ensemble) Kalman Filter-type DA
- Applications to DA

Focus: basic concepts and idealistic systems
(=setting hard problems of real systems aside)

Outline of This Lecture

- Background
  - NWP as DA: framework & elements
  - Basic ideas of probability for estimation

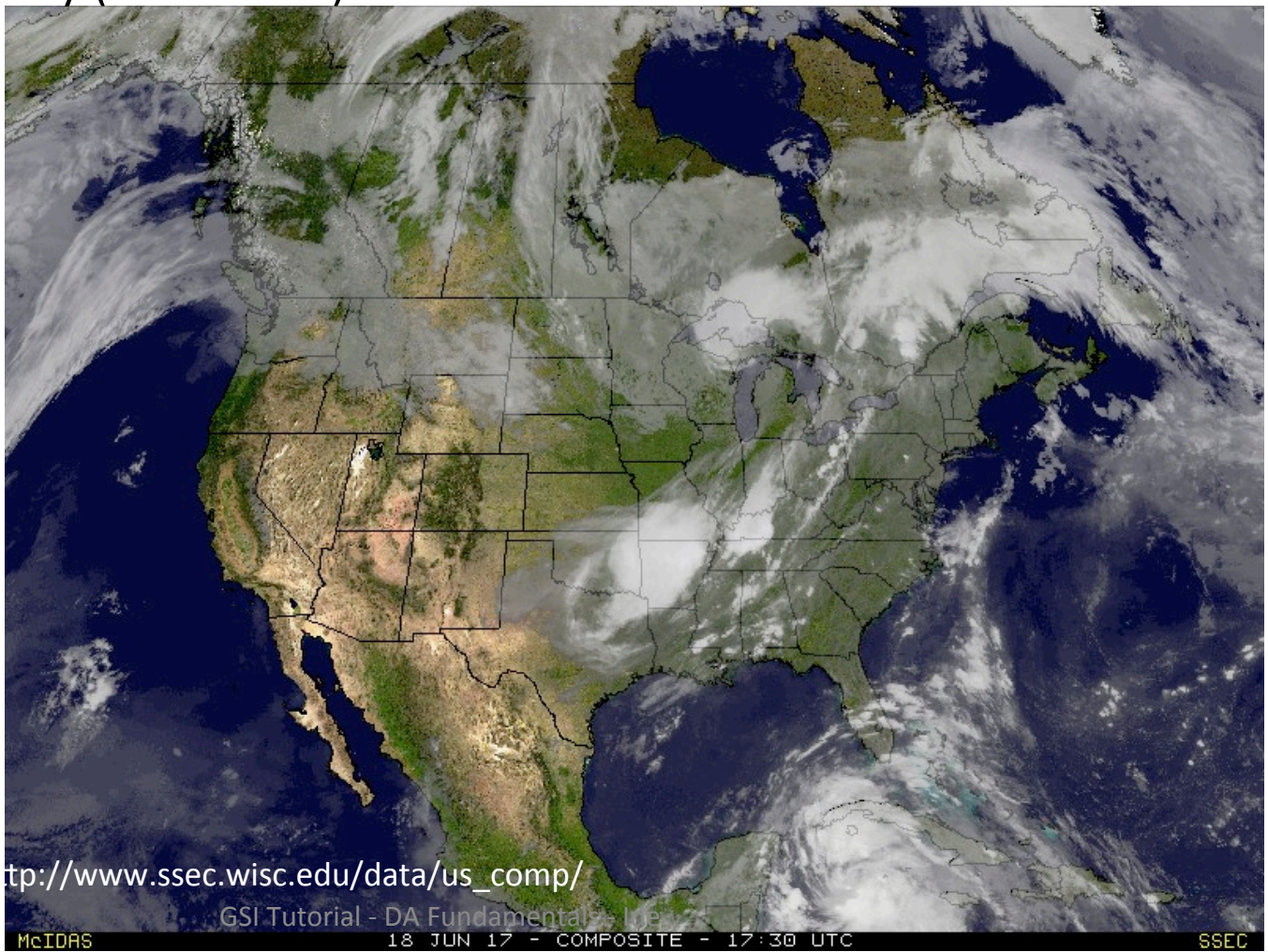
- Practical Methods of DA
  - 3D methods using static **B**
    - 3DVar = Variational (by likelihood)
    - OI = Optimal Interpolation (by risk reduction)
  - Towards 4D
    - FGAT = Asynchronized obs within one cycle
  - 4D methods using evolving **B**
    - 4DVar = Var along the model trajectory over a DA cycle
    - EKF/EnKF = Error evolution/explicit estimation of $\mathbf{B}_e$
    - 4DEnVar = Var analysis using $\mathbf{B}_e$
    - Hybrid 4DEnVar = Integration of 4DEnVar and 3DVar FGAT

duality

- Concluding Remarks

Basic Concepts of NWP

- Target: Forecasting evolution of atmosphere/weather system
  - As accurately as possible for the longest lead time possible
  - With uncertainty (confidence) estimate

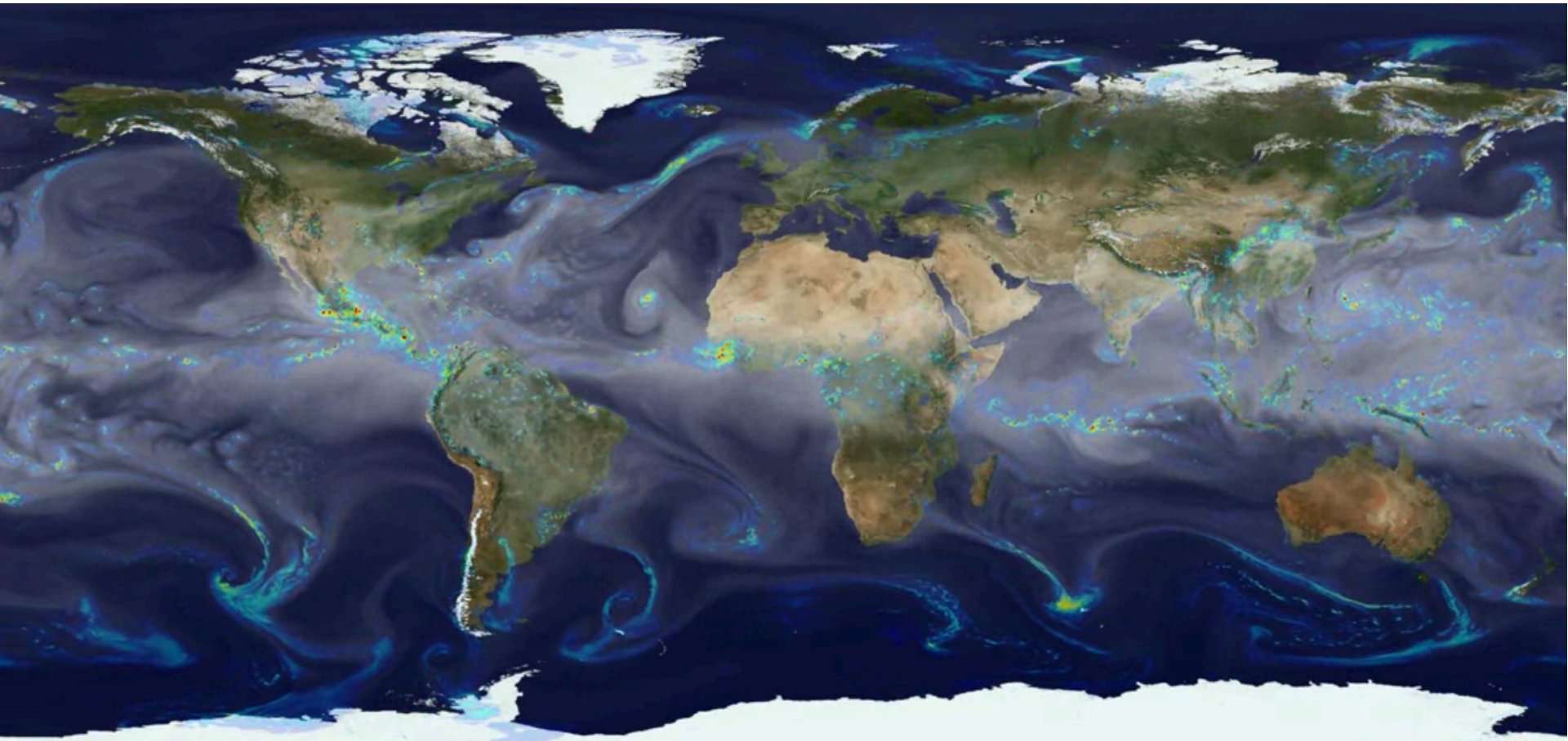


tp://www.ssec.wisc.edu/data/us_comp/

Basic Concepts of NWP

- Computational model for forecasting

  Ex) GEOS-5 Nature Run (NR) = 2yr-model simulation initialized on May 2005

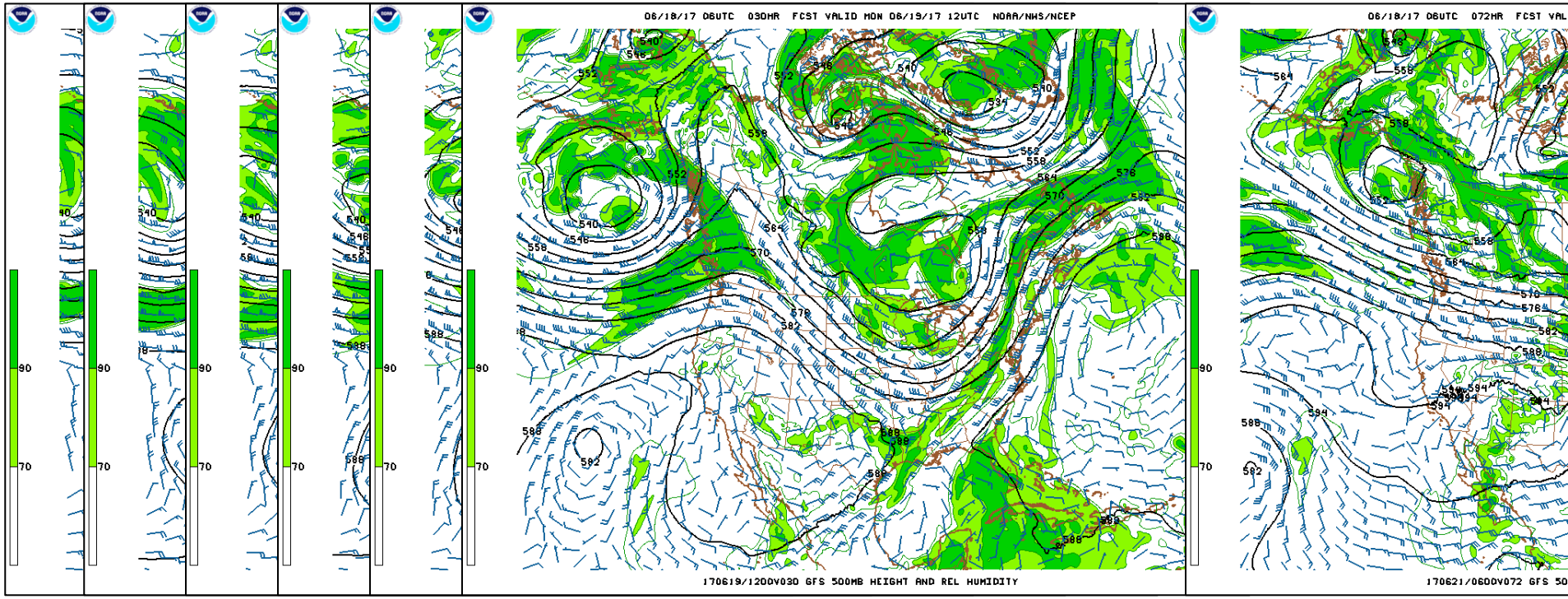


TPW (white) and rain fall (color: 0-15mm/hr) https://svs.gsfc.nasa.gov/30017

GEOS-5 7km NR (Gelaro et al, 2005)

Basic Concepts of NWP

- Forecast: future model trajectory, given IC (current condition)



NOAA Global Forecast System (GFS) forecast hr

http://mag.ncep.noaa.gov/

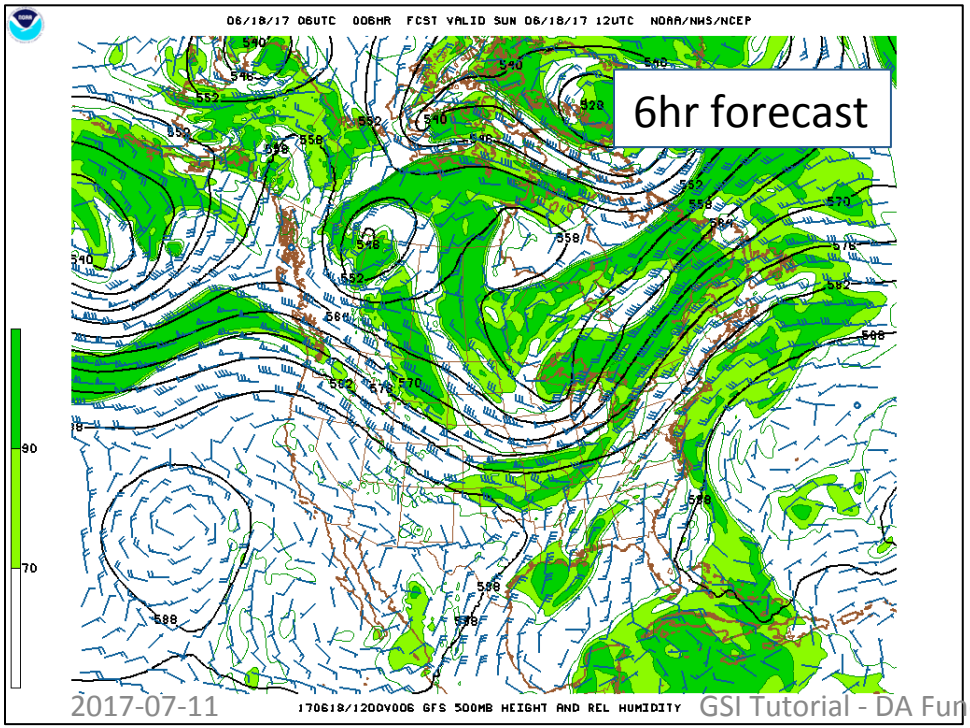
00….06 ……12 ….18 ….24 ….30 ……72……

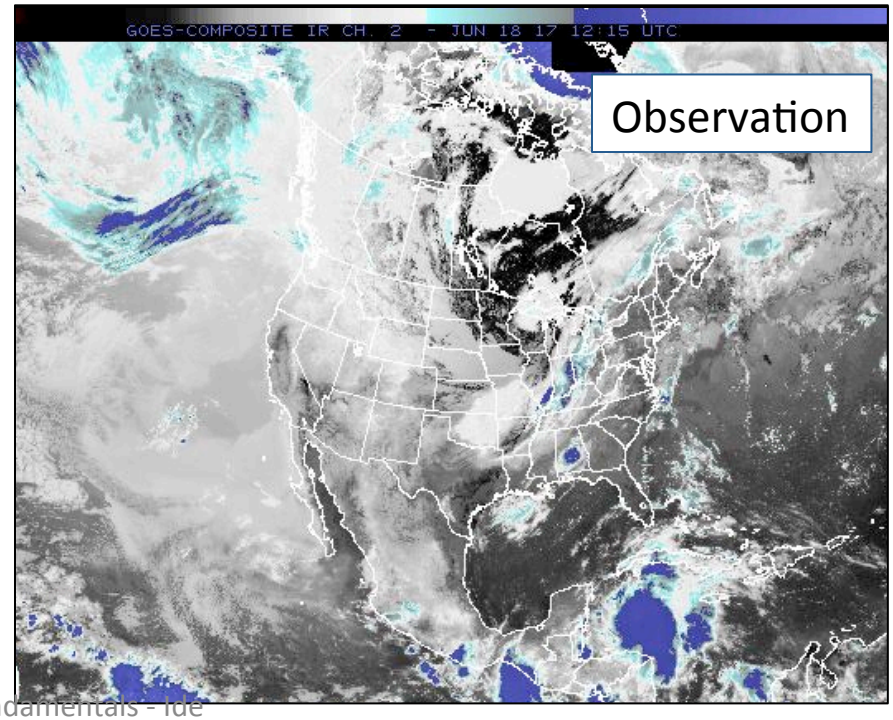
(=IC)

Challenges and Limitations of NWP

- Initialization (determination of IC)

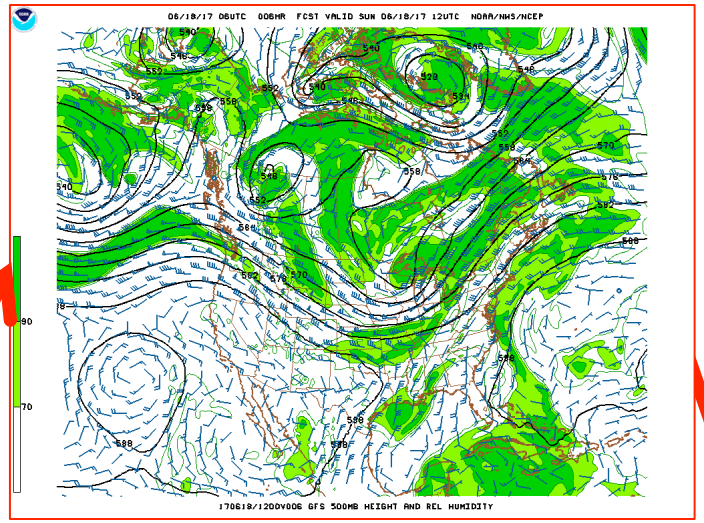
- Departure of forecast (given an IC) from the "true" evolution
  - Due to: >> Intrinsic predictability limits (nonlinearity)
    >> Practical predictability limits (IC, modeling, ….)
  - Quantification of departure: Observations (noisy sampling of the "truth")



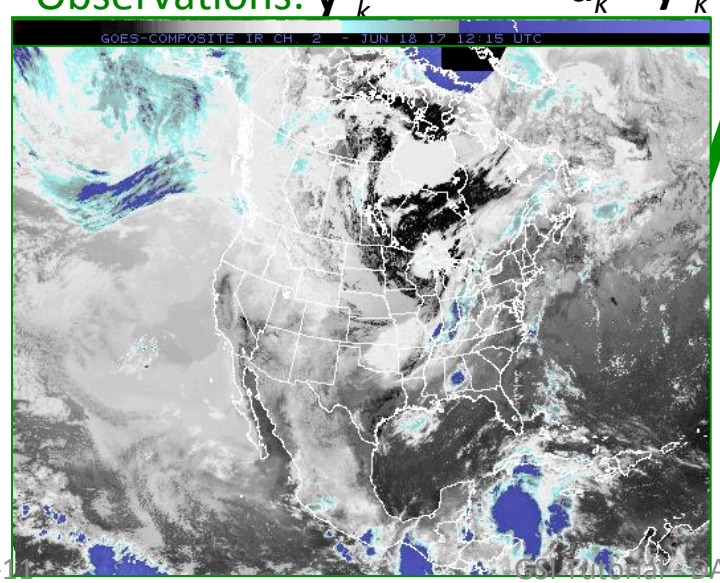


DA Schematic

- Model forecast: $\mathbf{x}^b_k$

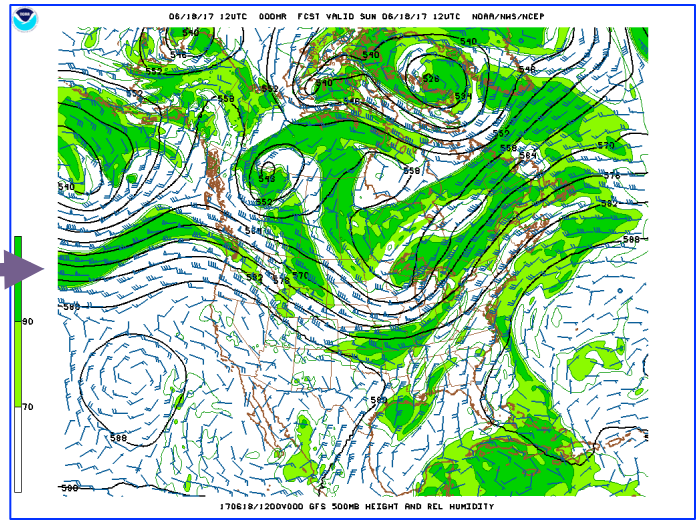


- Observations: $\mathbf{y}^o_k$



$$\mathbf{d}_k = \mathbf{y}^o_k - \mathbf{h}(\mathbf{x}^b_k)$$

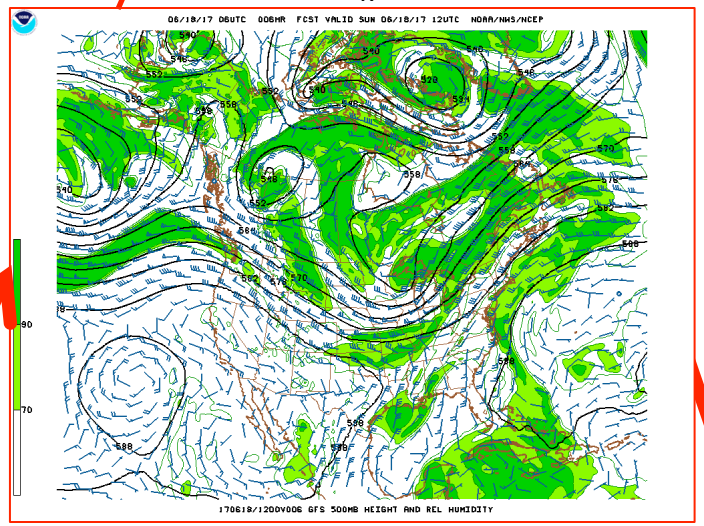
- Analysis model state: $\mathbf{x}^a_k = \mathbf{x}^b_k + \Delta\mathbf{x}^a_k$



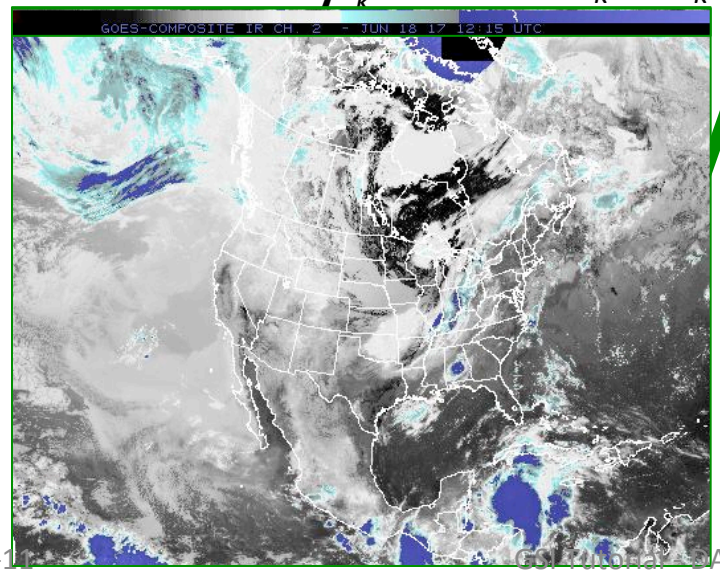
$\Delta\mathbf{x}^a_k$: increments by $\mathbf{d}_k$

DA Schematic

- Model forecast: $\mathbf{x}^b_k$

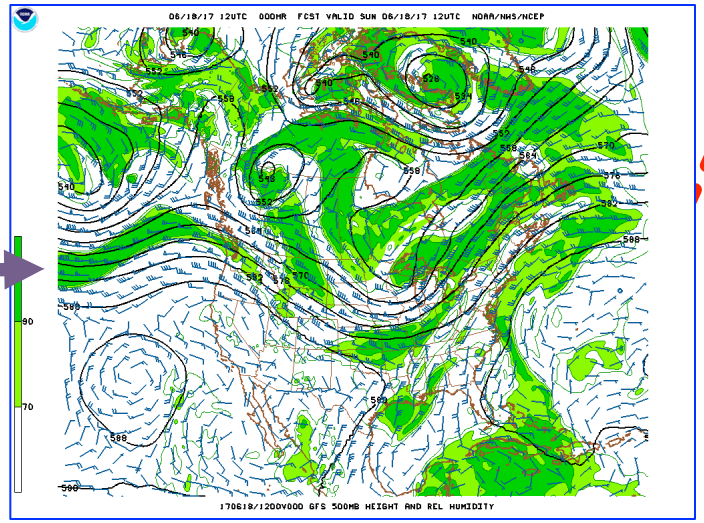


- Observations: $\mathbf{y}^o_k$



$$\mathbf{d}_k = \mathbf{y}^o_k - \mathbf{h}(\mathbf{x}^b_k)$$

- Analysis model state: $\mathbf{x}^a_k$

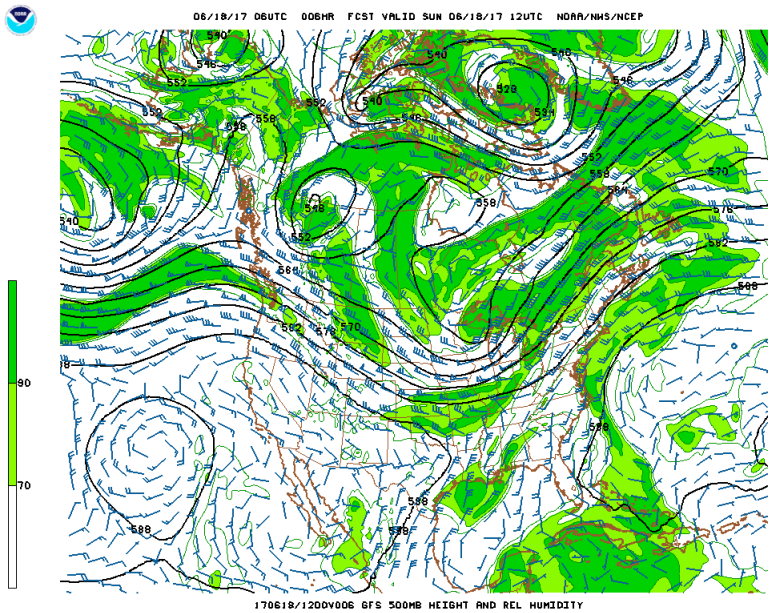


DA provides a framework for NWP using
- $\mathbf{x}^b_k$
- $\mathbf{y}^o_k$ [or $\mathbf{d}_k$]

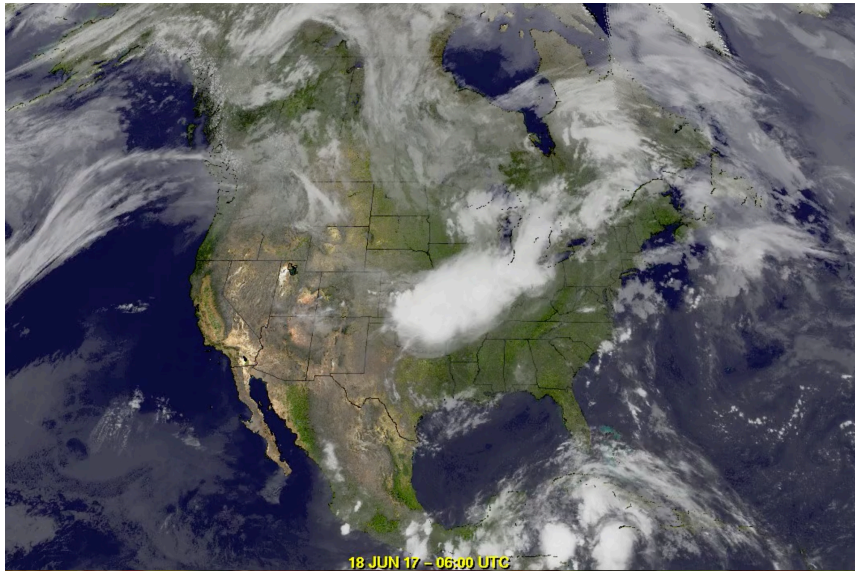
6hr for Operational System

DA Elements: State **x** and Forecast Model **m**

- Forecast model



- Nature



Computational model (from time t_{k-1} to t_k)

$\mathbf{x}_k = \mathbf{m}_{k,k-1}(\mathbf{x}_{k-1})$

m: model

x: *N*-dim spatially discretized vector of atmospheric variables ($N \sim 10^9$)

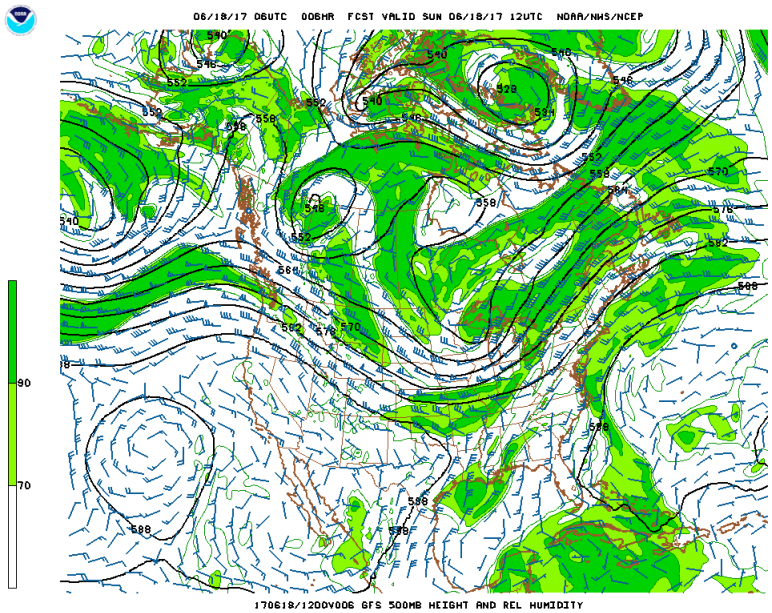
"true state" $\mathbf{x}^t_k$

= projection of real state onto **x**

- representation of $\mathbf{x}^t$ has uncertainty
- Probability $p(\mathbf{x})$ ~Likelihood [0,1] of the value being **x**

DA Elements: State **x** and Forecast Model **m**

- Forecast model



- Modeling of error ($\mathbf{e}_0$) in IC & error growth ($\mathbf{e}_k$) in forecast
  - Practical limits
    - Quality of model $\mathbf{m}_{k,0}$
    - Quality of IC $\mathbf{x}_0$
  - Intrinsic limits
    - Nonlinear dynamics
    - Stochastic processes

→ DA should estimate and reduce **e**

Computational model (from time t_{k-1} to t_k)

$\mathbf{x}_k = \mathbf{m}_{k,k-1}(\mathbf{x}_{k-1})$

m: model

x: N-dim spatially discretized vector of atmospheric variables ($N \sim 10^7$)

"true state" $\mathbf{x}^t_k$

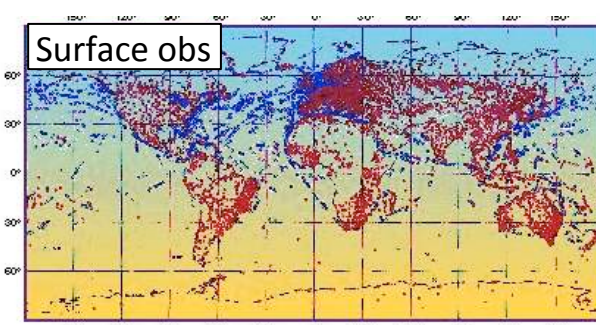
= projection of real state onto **x**

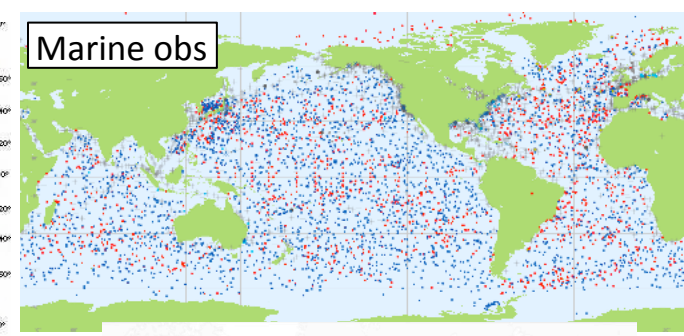
- representation of $\mathbf{x}^t$ has uncertainty
- Probability $p(\mathbf{x})$ ~Likelihood [0,1] of the value being **x**

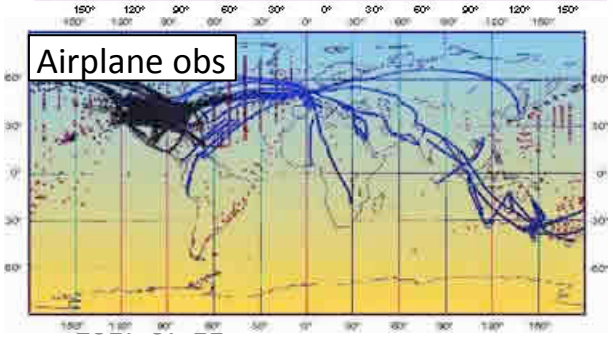
DA Elements: Observation **y** and Forward Model **h**(**x**)

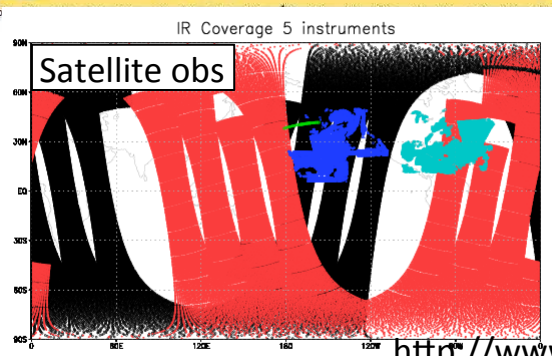
- Characteristics of $\mathbf{y}^o$
  - Noisy sampling of $\mathbf{x}^t$
  - Heterogeneous, spatially inhomogeneous, and temporally asynchronous
- Forward model $\mathbf{h}(\mathbf{x})=\mathbf{y}$
  - Needed for DA to sample **y** from the model state **x**
  - Uncertainty in the representation $\mathbf{y}=\mathbf{h}(\mathbf{x})$ [$\mathbf{y}^t=\mathbf{h}(\mathbf{x}^t)$?]

➔ Modeling of observation likelihood: $p(\mathbf{y}|\mathbf{x})$





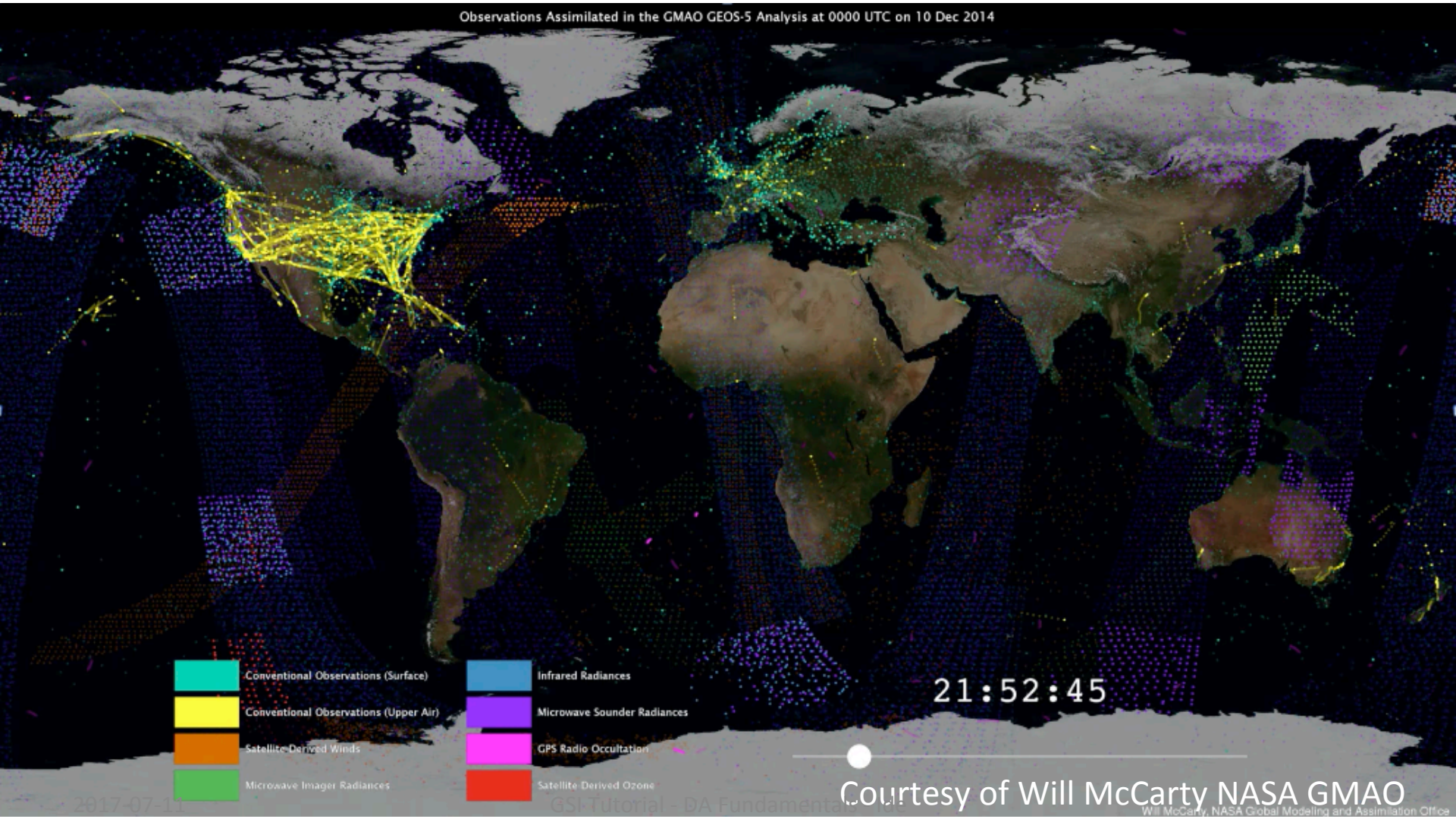




http://www.wmo.int/pages/prog/www/OSY/GOS.html

DA Elements: Observation **y** and **h**(**x**)

- Observations for numerical weather prediction over 6hrs



Courtesy of Will McCarty NASA GMAO

DA Challenges: Model

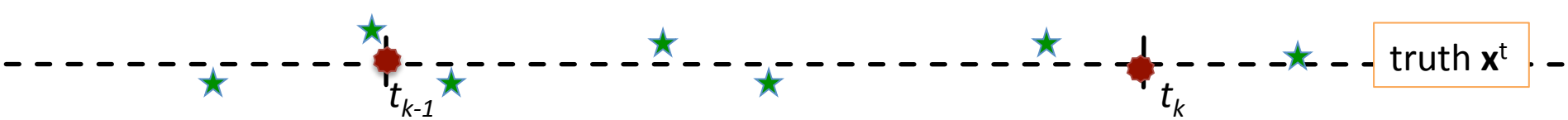
$\mathbf{m}_{k,k-1}$ is
- nonlinear
- imperfect

Step 1. Model Forecast
Forecast→Background: $\mathbf{x}^b_k$
$\mathbf{x}_k=\mathbf{m}_{k,k-1}(\mathbf{x}_{k-1})$

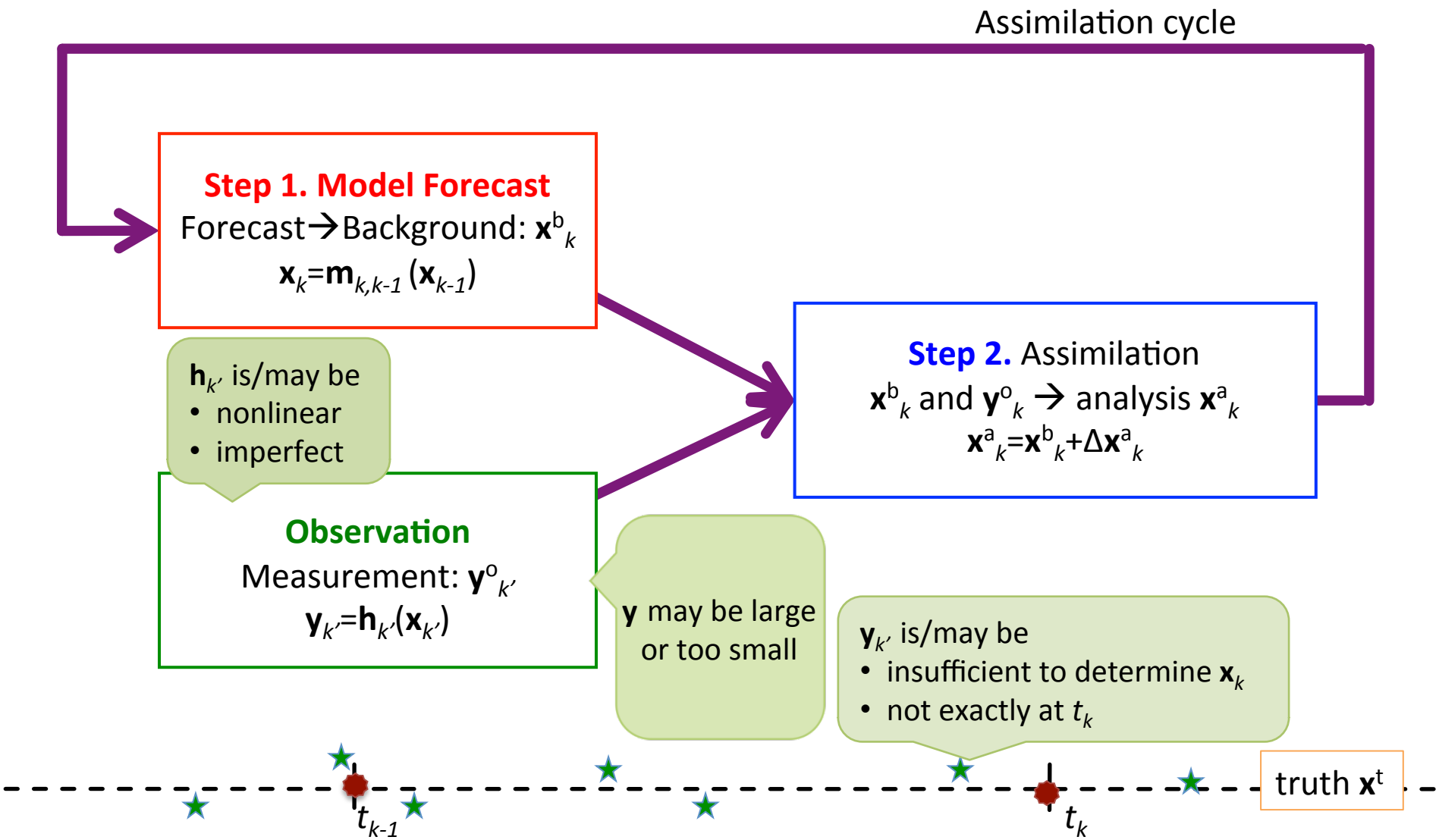
$\mathbf{x}$ can be large

Step 2. Assimilation
$\mathbf{x}^b_k$ and $\mathbf{y}^o_k$ → Analysis $\mathbf{x}^a_k$
$\mathbf{x}^a_k=\mathbf{x}^b_k+\Delta\mathbf{x}^a_k$

Observation
Measurement: $\mathbf{y}^o_{k'}$
$\mathbf{y}_{k'}=\mathbf{h}_{k'}(\mathbf{x}_{k'})$



DA Challenges: Observations



DA Challenges: Uncertainty

Uncertainty
$\mathbf{x}^b_k = \mathbf{x}^t_k + \mathbf{e}^b_k$

Step 1. Model Forecast
Forecast→Background: $\mathbf{x}^b_k$
$\mathbf{x}_k = \mathbf{m}_{k,k-1}(\mathbf{x}_{k-1})$

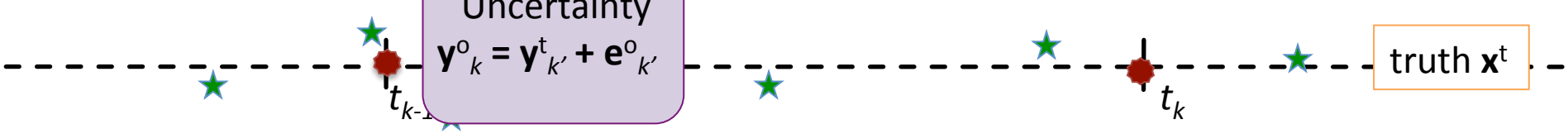
Uncertainty
$\mathbf{x}^a_k = \mathbf{x}^t_k + \mathbf{e}^a_k$

Step 2. Assimilation
$\mathbf{x}^b_k$ and $\mathbf{y}^o_k$ → analysis $\mathbf{x}^a_k$
$\mathbf{x}^a_k = \mathbf{x}^b_k + \Delta\mathbf{x}^a_k$

Observation
Measurement: $\mathbf{y}^o_{k'}$
$\mathbf{y}_{k'} = \mathbf{h}_{k'}(\mathbf{x}_{k'})$

DA: a framework for NWP
so that $\mathbf{x}^a$ is better than $\mathbf{x}^b$
- $\mathbf{e}^a$ is smaller than $\mathbf{e}^b$
- $\mathbf{h}(\mathbf{x}^a)$ is closer $\mathbf{y}^o$ than $\mathbf{h}(\mathbf{x}^b)$

Uncertainty
$\mathbf{y}^o_k = \mathbf{y}^t_{k'} + \mathbf{e}^o_{k'}$



Probability in Practical DA

- Idealistic assumptions/representation of uncertainty $p(\mathbf{x})$ [= likelihood of $\mathbf{x}$]
  - Unbiased

$$E[\mathbf{x}] = \mathbf{x}^*$$

$$E[\mathbf{e}] = \mathbf{0}$$

  - Uncertainty estimate by $\mathbf{P}$

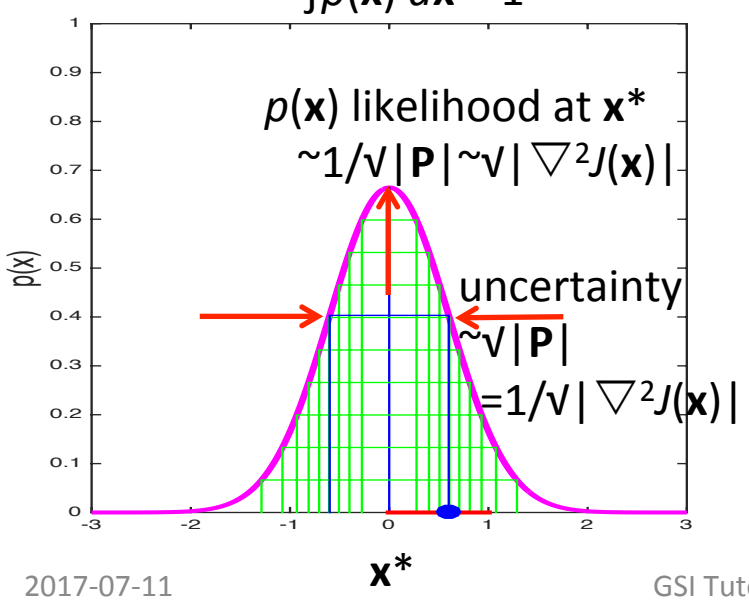
error covariance (NxN) matrix

$$\mathbf{P} = E[\mathbf{e}\mathbf{e}^T] = \begin{bmatrix} P_{11} & & P_{1N} \\ & \ddots & \\ P_{N1} & & P_{NN} \end{bmatrix}$$

$$\text{trace } \mathbf{P} = \sum_{n=1}^{N} P_{nn} = \text{size of total risk}$$

$$= \text{total variance } \sigma^2$$

$\int p(\mathbf{x})\, d\mathbf{x} = 1$



If Gaussian,

– $p(\mathbf{x})$ is defined by $\mathbf{x}^*$ and $\mathbf{P}$

$$p(\mathbf{x}) \sim N(\mathbf{x}^*, \mathbf{P}) \propto \exp\left[-\boxed{\frac{1}{2}(\mathbf{x}-\mathbf{x}^*)^T \mathbf{P}^{-1} (\mathbf{x}-\mathbf{x}^*)}\right]$$

$$= \exp\left[-\underline{J(\mathbf{x})}\right]$$

– Most likely $\mathbf{x}^*$ by $p(\mathbf{x})$, when $J(\mathbf{x})$ is min at $\mathbf{x}^*$

Probability in Practical DA: Background

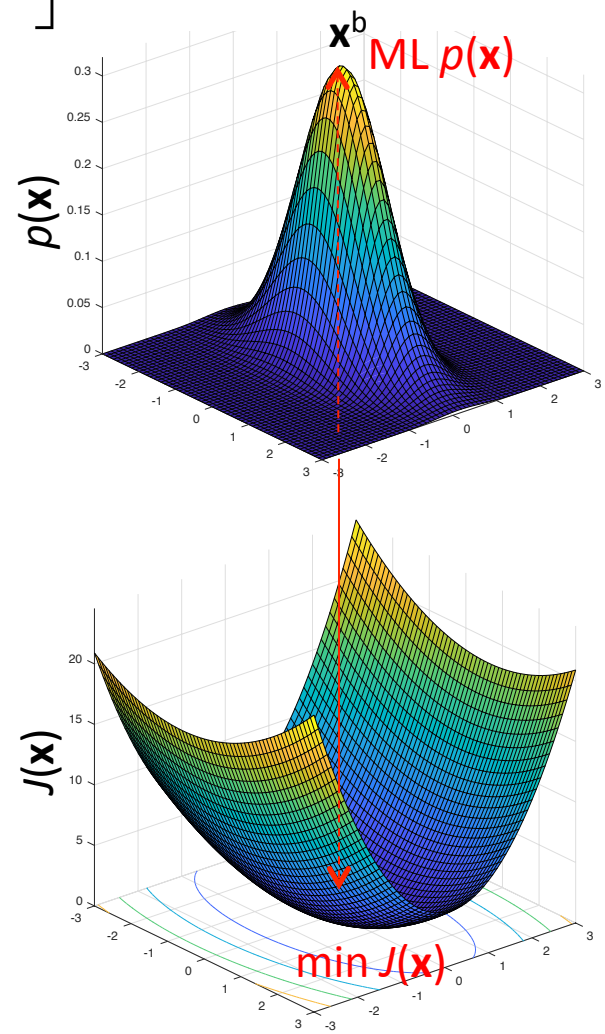
- Prior PDF

$$p(\mathbf{x}) \sim N(\mathbf{x}^{\mathrm{b}},\mathbf{B}) \propto \exp\left[-\frac{1}{2}(\mathbf{x}-\mathbf{x}^{\mathrm{b}})^T\ \mathbf{B}^{-1}\ (\mathbf{x}-\mathbf{x}^{\mathrm{b}})\right] = J^{\mathrm{b}}(\mathbf{x})$$

$\mathbf{x}^{\mathrm{b}}$: by model forecast

$\mathbf{B}$: provided by climatology(statistical)

or model forecast(dynamical)



- $J^{\mathrm{b}}(\mathbf{x})$: background cost function

$$J^{\mathrm{b}}(\mathbf{x}) = \frac{1}{2}(\mathbf{x}-\mathbf{x}^{\mathrm{b}})^T\ \mathbf{B}^{-1}\ (\mathbf{x}-\mathbf{x}^{\mathrm{b}})$$

Maximum Likelihood (ML) conditions = min $J^{\mathrm{b}}(\mathbf{x})$

» $\nabla J^{\mathrm{b}}(\mathbf{x}) = \mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}^{\mathrm{b}}) = \mathbf{0} \rightarrow \mathbf{x} = \mathbf{x}^{\mathrm{b}}$

» $\nabla^2 J^{\mathrm{b}}(\mathbf{x}) = \mathbf{B}^{-1}$= full rank & positive definite

Probability in Practical DA: Observations

- Observation likelihood $p(\mathbf{y}|\mathbf{x})$ =likelihood of being $\mathbf{y}$ given $\mathbf{x}$

$$p(\mathbf{y}\,|\,\mathbf{x}) \propto \exp\left[-\frac{1}{2}(\mathbf{y}^{\mathrm{o}}-\mathbf{h}(\mathbf{x}))^T\ (\mathbf{R})^{-1}\ (\mathbf{y}^{\mathrm{o}}-\mathbf{h}(\mathbf{x}))\right] = \exp\left[-J^{\mathrm{o}}(\mathbf{x})\right]$$

$\mathbf{y}^{\mathrm{o}}= \mathbf{y}^{\mathrm{t}}+ \mathbf{e}^{\mathrm{o}}$: obs with unbiased error $\mathbf{e}^{\mathrm{o}}$ assuming $\mathbf{y}^{\mathrm{t}}=\mathbf{h}(\mathbf{x}^{\mathrm{t}})$

$\mathbf{R}=E[\mathbf{e}^{\mathrm{o}}(\mathbf{e}^{\mathrm{o}})^{\mathrm{T}}]$: obs error covariance for $\mathbf{y}^{\mathrm{o}}$

- $J^{\mathrm{o}}(\mathbf{x})$: Observation cost function

$$J^{\mathrm{o}}(\mathbf{x}) = \frac{1}{2}(\mathbf{y}^{\mathrm{o}}-\mathbf{h}(\mathbf{x}))^T\ (\mathbf{R})^{-1}\ (\mathbf{y}^{\mathrm{o}}-\mathbf{h}(\mathbf{x}))$$

  - If $\mathbf{y}$ consists of L set of independent $\mathbf{y}_l$

$$J^{\mathrm{o}}(\mathbf{x}) = \sum_{l}^{L} J_l^{\mathrm{o}}(\mathbf{x})$$

$$J_l^{\mathrm{o}}(\mathbf{x}) = \frac{1}{2}(\mathbf{y}_l^{\mathrm{o}}-\mathbf{h}_l(\mathbf{x}))^T\ (\mathbf{R}_l)^{-1}\ (\mathbf{y}_l^{\mathrm{o}}-\mathbf{h}_l(\mathbf{x}))$$

corresponding to $p(\mathbf{y}|\mathbf{x})=p_1(\mathbf{y}|\mathbf{x})\ \ldots\ p_L(\mathbf{y}|\mathbf{x})$

$$\mathbf{y}^{\mathrm{o}} = \begin{pmatrix} \mathbf{y}_1^{\mathrm{o}} \\ \vdots \\ \mathbf{y}_L^{\mathrm{o}} \end{pmatrix},\quad \mathbf{h}(\mathbf{x}) = \begin{pmatrix} \mathbf{h}_1(\mathbf{x}) \\ \vdots \\ \mathbf{h}_1(\mathbf{x}) \end{pmatrix}$$

$$\mathbf{R} = \begin{pmatrix} \mathbf{R}_1 & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & \mathbf{R}_L \end{pmatrix}$$

Probability in Practical DA: Observations

- $\mathbf{x}^{ML}$ of $p(\mathbf{y}|\mathbf{x})$ as the weighted least square estimate

$$\min \quad J^o(\mathbf{x}) = \frac{1}{2}(\mathbf{y}^o - \mathbf{h}(\mathbf{x}))^T \ (\mathbf{R})^{-1} \ (\mathbf{y}^o - \mathbf{h}(\mathbf{x}))$$

  - Nonlinear $\mathbf{h}(\mathbf{x})$
    - $\nabla J^o(\mathbf{x}) = -\mathbf{H}^T\mathbf{R}^{-1}(\mathbf{y}^o - \mathbf{h}(\mathbf{x})) = \mathbf{0}$
    - $\nabla^2 J^o(\mathbf{x}) = \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}$

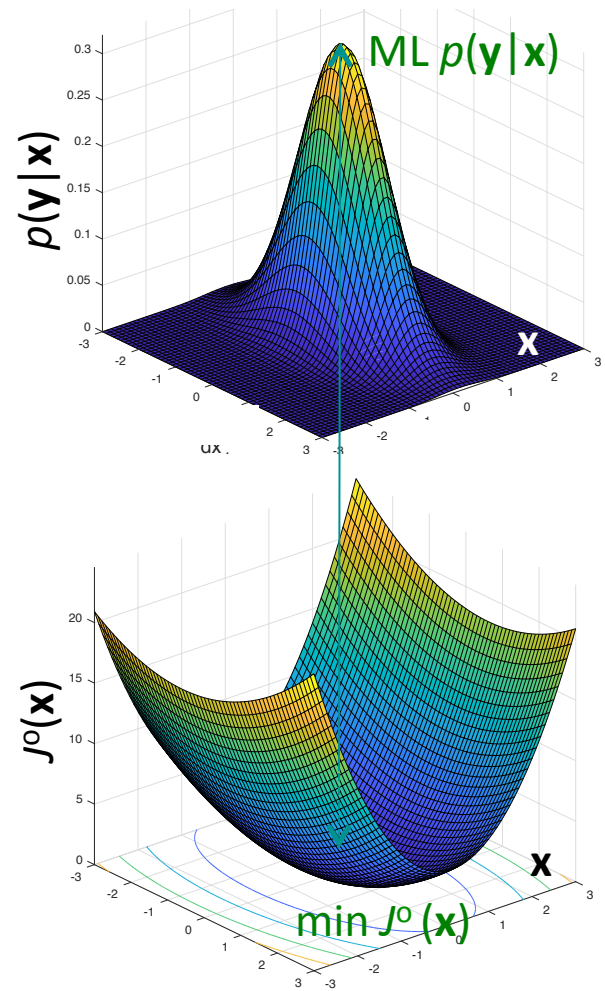
      = full rank & positive definite in **x** space

  - Linear $\mathbf{h}(\mathbf{x}) = \mathbf{H}\mathbf{x}$
    - $\nabla J^o(\mathbf{x}) = -\mathbf{H}^T\mathbf{R}^{-1}(\mathbf{y}^o - \mathbf{H}\mathbf{x}) = \mathbf{0}$

      $\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}\,\mathbf{x} = \mathbf{H}^T\mathbf{R}^{-1}\mathbf{y}^o$

      $\mathbf{x} = (\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\ \mathbf{H}^T\mathbf{R}^{-1}\mathbf{y}^o$
    - $\nabla^2 J^o(\mathbf{x}) = \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}$

      = full rank & positive definite in **x** space



Probability in Practical DA: Observations

- 2D linear interpolation example $\mathbf{x} = (x_1, x_2)^T$

$$\mathbf{y}^o = \mathbf{H}\mathbf{x} + \mathbf{e}^o$$

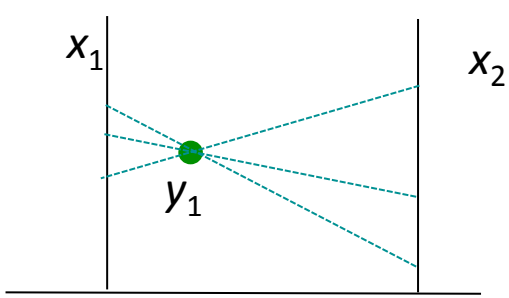
$$y_l = \mathbf{H}_l\mathbf{x} = (1-w_l)\, x_1 + w_l\, x$$

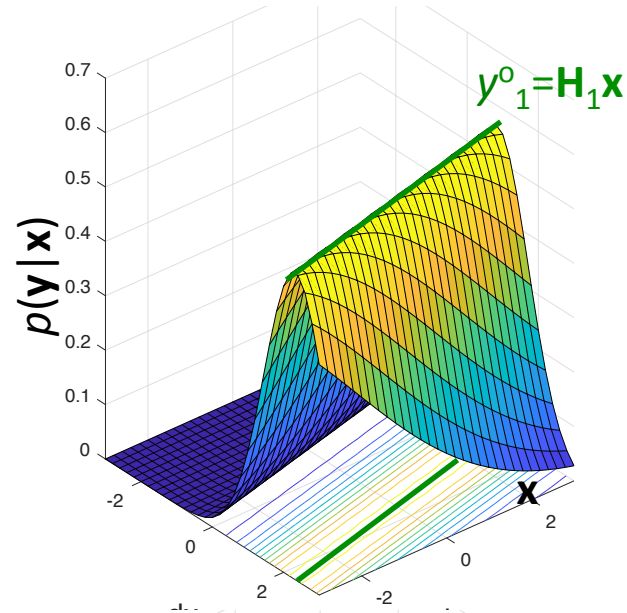
  - Single obs $y^o{}_1$:

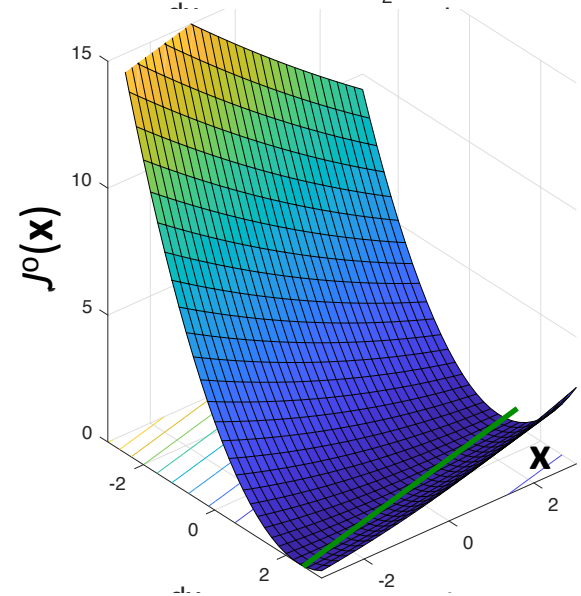
$$J^o(\mathbf{x}) = (y^o{}_1 - \mathbf{H}_1\mathbf{x})^2/2R_1$$

$$\nabla J^o(\mathbf{x}) = -\mathbf{H}_1{}^T(y^o{}_1 - \mathbf{H}_1\mathbf{x})/R_1 = \mathbf{0}$$

$$\nabla^2 J^o(\mathbf{x}) = \mathbf{H}_1{}^T\mathbf{H}_1 / R_1$$







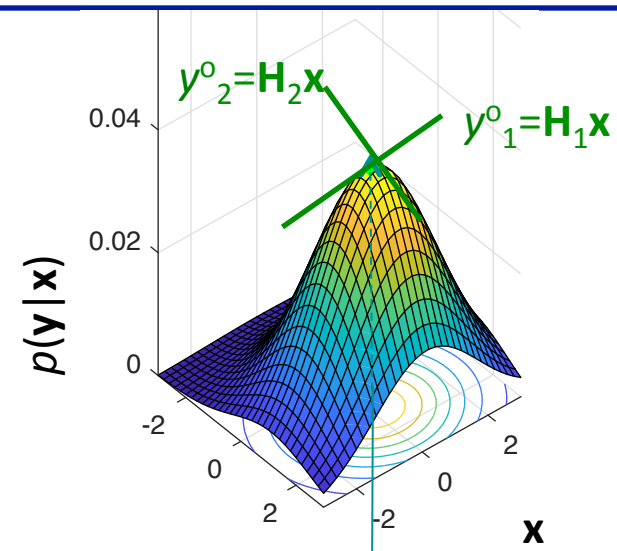
Probability in Practical DA: Observations

– Two obs: y^o_1 and y^o_2:

$$J^o(\mathbf{x}) = (y^o_1-\mathbf{H}_1\mathbf{x})^2/2R_1+(y^o_2-\mathbf{H}_2\mathbf{x})^2/2R_2$$

$$\nabla J^o(\mathbf{x}) = -\mathbf{H}_1^T(y^o_1-\mathbf{H}_1\mathbf{x})/R_1 - \mathbf{H}_2^T(y^o_2-\mathbf{H}_2\mathbf{x})/R_2 = \mathbf{0}$$

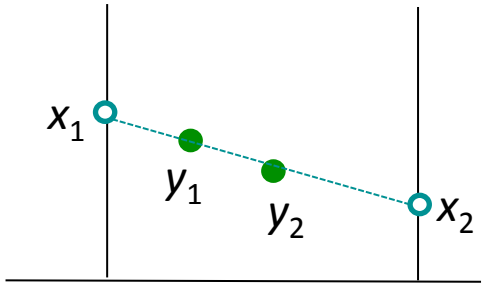
$$\nabla^2 J^o(\mathbf{x}) = \mathbf{H}_1^T\mathbf{H}_1/R_1 + \mathbf{H}_2^T\mathbf{H}_2/R_2$$

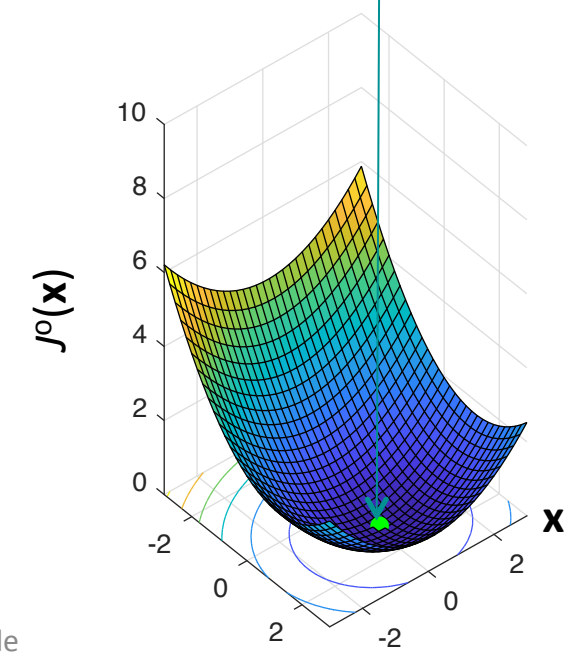


Unique $\mathbf{x}^{ML}$

» unless $w_1=w_2$

» regardless of R_1 & R_2





Probability in Practical DA: Observations

– L (>2) independent obs:

$$J^o(\mathbf{x}) = \Sigma_l^L (y^o_l - \mathbf{H}_l\mathbf{x})^2/2R_l$$

$$\nabla J^o(\mathbf{x}) = -\Sigma_l^L \mathbf{H}_l^T(y^o_l - \mathbf{H}_l\mathbf{x})/R_l = 0$$

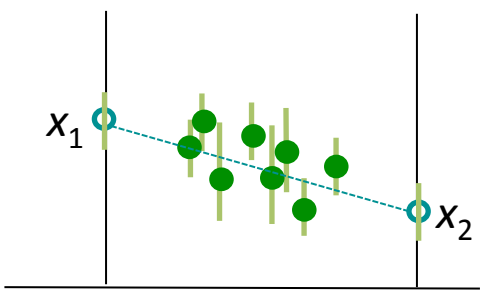
$$\nabla^2 J^o(\mathbf{x}) = \Sigma_l^L \mathbf{H}_l^T\mathbf{H}_l/R_l$$

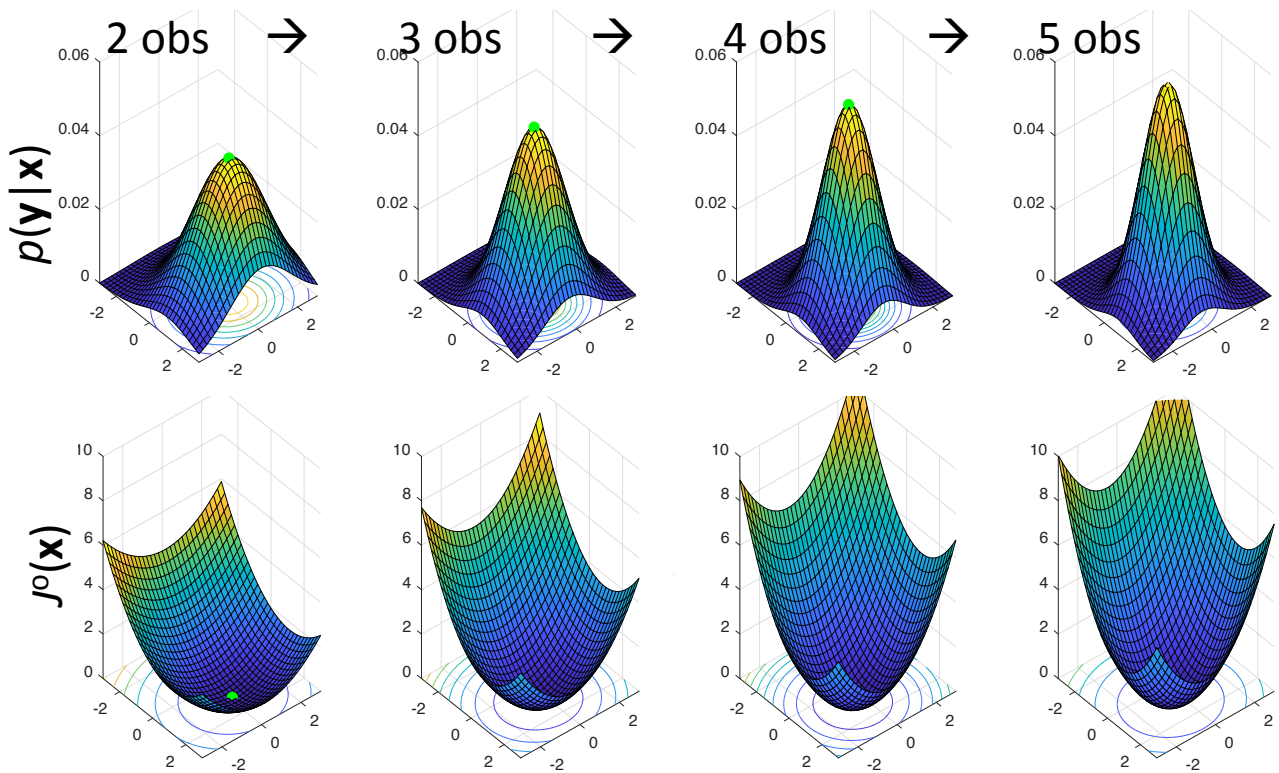
Adding more y^o_l

→ $|\nabla^2 J^o(\mathbf{x})| \uparrow$

→ $1/\sigma^2 \uparrow$ [likelihood ↑]

→ $\sigma^2 \downarrow$ [uncertainty ↓]





Two Practical Approaches to DA

Prior PDF
$p(\mathbf{x})$

Step 1. Model Forecast
Forecast→Background: $\mathbf{x}^b_k$
$\mathbf{x}_k = \mathbf{m}_{k,k-1}(\mathbf{x}_{k-1})$

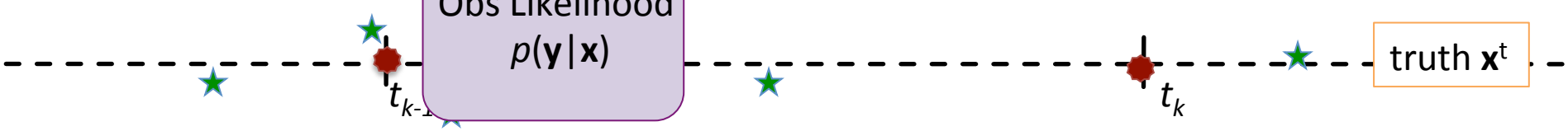
Uncertainty
$\mathbf{x}^a_k = \mathbf{x}^t_k + \mathbf{e}^a_k$

Step 2. Assimilation
$\mathbf{x}^b_k$ and $\mathbf{y}^o_k$ → analysis $\mathbf{x}^a_k$
$\mathbf{x}^a_k = \mathbf{x}^b_k + \Delta\mathbf{x}^a_k$

Observation
Measurement: $\mathbf{y}^o_{k'}$
$\mathbf{y}_{k'} = \mathbf{h}_{k'}(\mathbf{x}_{k'})$

Two equivalent approaches to $\mathbf{x}^a_k$
- Maximum likelihood (ML)→Var
- Minimum Variance (MV)→ OI/KF

Obs Likelihood
$p(\mathbf{y}|\mathbf{x})$



Outline of This Lecture

- Background
  - NWP as DA: framework & elements
  - Basic ideas of probability for estimation

- Practical Methods of DA
  - 3D methods using static **B**
    - 3DVar = Variational
    - OI = Optimal Interpolation
  - Towards 4D
    - FGAT = Asynchronized obs within one cycle
  - 4D methods using evolving **B**
    - 4DVar = Var along the model trajectory over a DA cycle
    - EKF/EnKF = Error evolution/explicit estimation of $\mathbf{B}_e$
    - 4DEnVar = Var analysis using $\mathbf{B}_e$
    - Hybrid 4DEnVar = Integration of 4DEnVar and 3DVar FGAT

duality

- Concluding Remarks

3D DA Schematics

Background
$p(\mathbf{x}) \sim N(\mathbf{x}^b, \mathbf{B})$
B : Static

Step 1. Model Forecast
Forecast→Background: $\mathbf{x}^b$
$\mathbf{x}_k = \mathbf{m}_{k,k-1}(\mathbf{x}_{k-1})$

Analysis
$\mathbf{x}^a_k = \mathbf{x}^t_k + \mathbf{e}^a_k$

$\mathbf{d} = \mathbf{y}^o - \mathbf{h}(\mathbf{x}^b)$

Step 2. Assimilation
$\mathbf{x}^b$ and $\mathbf{y}^o$ → analysis $\mathbf{x}^a$
$\mathbf{x}^a = \mathbf{x}^b + \Delta\mathbf{x}^a$

Observation
Measurement: $\mathbf{y}^o$
$\mathbf{y} = \mathbf{h}(\mathbf{x})$

Obs Likelihood
$p(\mathbf{y}|\mathbf{x}) \sim N(\mathbf{y}^o, \mathbf{R})$
R : Given

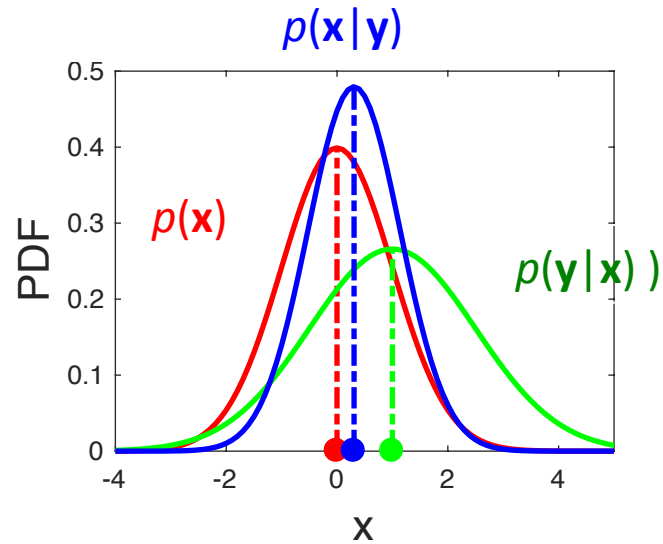
Two equivalent approaches to $\mathbf{x}^a_k$
- Maximum likelihood (ML)→Var
- Minimum Variance (MV)→ OI/KF

3D Method I: 3DVar

- Approach: ML $\mathbf{x}=\mathbf{x}^{\mathrm{b}}+\Delta\mathbf{x}$, s.t. $p(\mathbf{x}|\mathbf{y})$ is max given $p(\mathbf{x})$ & $p(\mathbf{y}|\mathbf{x})$ using Bayes theorem:

$$p(\mathbf{x}|\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{x})p(\mathbf{x})}{p(\mathbf{y})} \sim N(\mathbf{x}^{\mathrm{a}},\mathbf{A})$$

$$\propto \exp\left[-J^{\mathrm{o}}(\mathbf{x}) - J^{\mathrm{b}}(\mathbf{x})\right] = \exp\left[-J(\mathbf{x})\right]$$

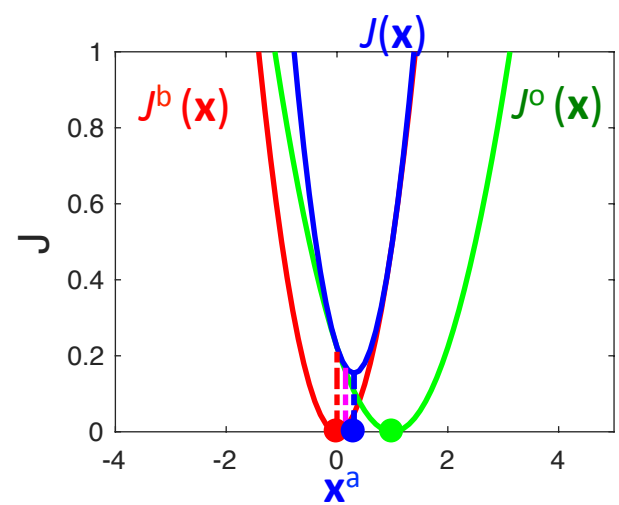


- 3DVar algorithms: Minimize

$$J(\mathbf{x}) = J^{\mathrm{b}}(\mathbf{x}) + J^{\mathrm{o}}(\mathbf{x})$$

$$J^{\mathrm{b}}(\mathbf{x}) = \frac{1}{2}(\mathbf{x}-\mathbf{x}^{\mathrm{b}})^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}^{\mathrm{b}})$$

$$J^{\mathrm{o}}(\mathbf{x}) = \frac{1}{2}(\mathbf{y}^{\mathrm{o}}-\mathbf{h}(\mathbf{x}))^T\ \mathbf{R}^{-1}\ (\mathbf{y}^{\mathrm{o}}-\mathbf{h}(\mathbf{x}))$$



3D Method I: 3DVar

Prior
$p(\mathbf{x}) \sim N(\mathbf{x}^b, \mathbf{B})$
B : Static

Step 1. Model Forecast
Forecast→Background: $\mathbf{x}^b$
$\mathbf{x}_k = \mathbf{m}_{k,k-1}(\mathbf{x}_{k-1})$

posterior
$p(\mathbf{x}|\mathbf{y}) \sim N(\mathbf{x}^a, \mathbf{A})$
A : Usually not computed

$\mathbf{d} = \mathbf{y}^o - \mathbf{h}(\mathbf{x}^b)$

Step 2. Assimilation
Integration of $\mathbf{x}^b$ and $\mathbf{y}^o$ → $\mathbf{x}^a$
$\mathbf{x}^a = \mathbf{x}^b + \Delta\mathbf{x}^a$

Observation
Measurement: $\mathbf{y}^o$
$\mathbf{y} = \mathbf{h}(\mathbf{x})$

Obs Likelihood
$p(\mathbf{y}|\mathbf{x}) \sim N(\mathbf{y}^o, \mathbf{R})$
R : Given

Minimization problem:

$$J(\Delta\mathbf{x}) = J^b(\Delta\mathbf{x}) + J^o(\Delta\mathbf{x})$$

$$J^b(\Delta\mathbf{x}) = \tfrac{1}{2}(\Delta\mathbf{x})^T \mathbf{B}^{-1}(\Delta\mathbf{x})$$

$$J^o(\Delta\mathbf{x}) = \tfrac{1}{2}(\mathbf{y}^o - \mathbf{h}(\mathbf{x}^b + \Delta\mathbf{x})^T \mathbf{R}^{-1}(\mathbf{y}^o - \mathbf{h}(\mathbf{x}^b + \Delta\mathbf{x}))$$

where

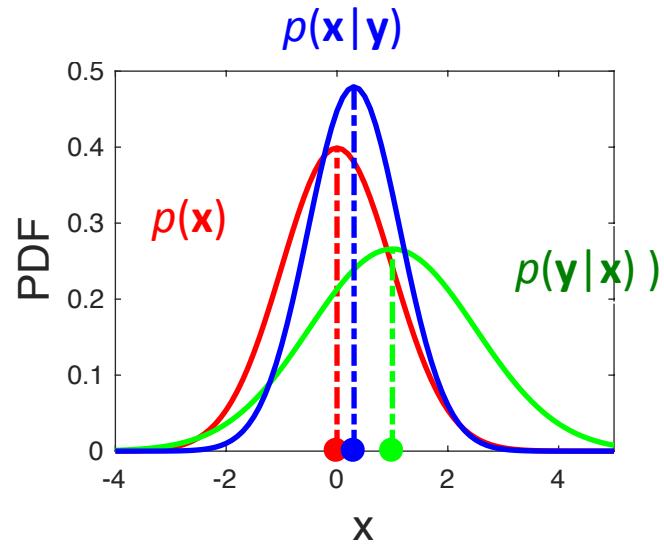
$$\Delta\mathbf{x} = \mathbf{x} - \mathbf{x}^b$$

3D Method I: Incremental 3DVar

- Approach: ML $\mathbf{x}=\mathbf{x}^b+\Delta\mathbf{x}$, s.t. $p(\mathbf{x}|\mathbf{y})$ is max given $p(\mathbf{x})$ & $p(\mathbf{y}|\mathbf{x})$ using Bayes theorem:

$$p(\mathbf{x}|\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{x})p(\mathbf{x})}{p(\mathbf{y})} \sim N(\mathbf{x}^a, \mathbf{A})$$

$$\propto \exp\left[-J^o(\mathbf{x}) - J^b(\mathbf{x})\right] = \exp\left[-J(\mathbf{x})\right]$$



- Linearized 3DVar algorithms by

$$\mathbf{y}^o - \mathbf{h}(\mathbf{x}^b + \Delta\mathbf{x}) \approx \mathbf{y}^o - \mathbf{h}(\mathbf{x}^b) - \left.\frac{\partial \mathbf{h}(\mathbf{x})}{\partial \mathbf{x}}\right|_{\mathbf{x}^b} \Delta\mathbf{x}$$

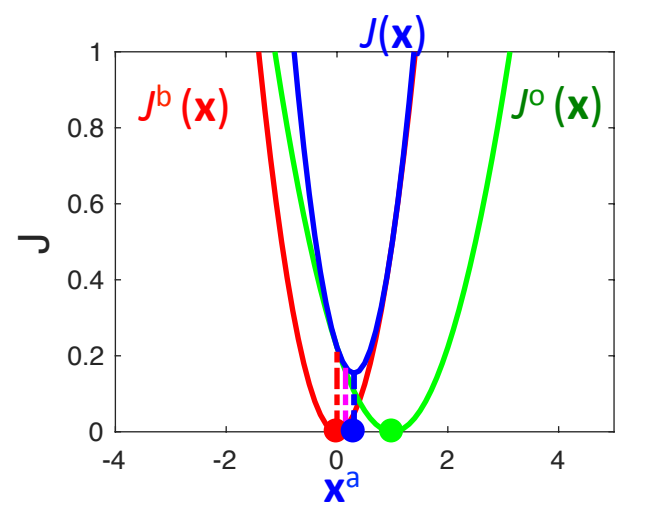
$$= \mathbf{d} \qquad\qquad - \mathbf{H}\Delta\mathbf{x}$$

minimize innovation

$$J(\Delta\mathbf{x}) = J^b(\Delta\mathbf{x}) + J^o(\Delta\mathbf{x})$$

$$J^b(\Delta\mathbf{x}) = \frac{1}{2}\Delta\mathbf{x}^T\mathbf{B}^{-1}\Delta\mathbf{x}$$

$$J^o(\Delta\mathbf{x}) = \frac{1}{2}(\mathbf{d} - \mathbf{H}\Delta\mathbf{x})^T\ \mathbf{R}^{-1}\ (\mathbf{d} - \mathbf{H}\Delta\mathbf{x})$$



3D Method I: Incremental 3DVar

[Use of the linearized $\mathbf{h}(\mathbf{x}^b+\Delta\mathbf{x})\approx\mathbf{h}(\mathbf{x}^b)+\mathbf{H}\Delta\mathbf{x}$ in 3DVar]

Prior
$p(\mathbf{x}) \sim N(\mathbf{x}^b, \mathbf{B})$
B : Static

Step 1. Model Forecast
Forecast→Background: $\mathbf{x}^b$
$\mathbf{x}_k=\mathbf{m}_{k,k-1}(\mathbf{x}_{k-1})$

posterior
$p(\mathbf{x}|\mathbf{y})\sim N(\mathbf{x}^a, \mathbf{A})$
A : Usually not computed

$\mathbf{d} = \mathbf{y}^o-\mathbf{h}(\mathbf{x}^b)$

Step 2. Assimilation
$\mathbf{x}^b$ and $\mathbf{y}^o$ → analysis $\mathbf{x}^a$
$\mathbf{x}^a = \mathbf{x}^b + \Delta\mathbf{x}^a$

Observation
Measurement: $\mathbf{y}^o$
$\mathbf{y}=\mathbf{h}(\mathbf{x})$

Obs Likelihood
$p(\mathbf{y}|\mathbf{x})\sim N(\mathbf{y}^o, \mathbf{R})$
R : Given

Minimization problem:

$$J(\Delta\mathbf{x}) = J^b(\Delta\mathbf{x}) + J^o(\Delta\mathbf{x})$$

$$J^b(\Delta\mathbf{x}) = \tfrac{1}{2}(\Delta\mathbf{x})^T \mathbf{B}^{-1}(\Delta\mathbf{x})$$

$$J^o(\Delta\mathbf{x}) = \tfrac{1}{2}(\mathbf{d}-\mathbf{H}\Delta\mathbf{x})^T \mathbf{R}^{-1}(\mathbf{d}-\mathbf{H}\Delta\mathbf{x})$$

Where

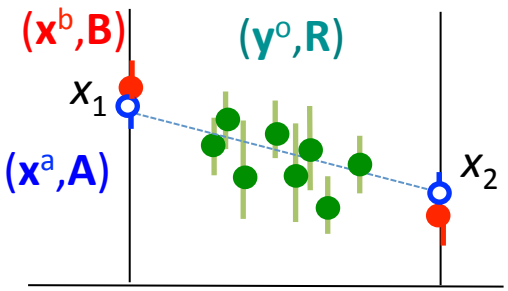
$$\mathbf{d} = \mathbf{y}^o - \mathbf{h}(\mathbf{x}^b) \qquad \mathbf{H} = \left.\frac{\partial\mathbf{h}(\mathbf{x})}{\partial\mathbf{x}}\right|_{\mathbf{x}^b}$$

3D Method I: Incremental 3DVar

- Interpretation
  - Background: one more set of independent "obs" ($\mathbf{x}^b$,$\mathbf{B}$)

$$p(\mathbf{x}|\mathbf{y}) \sim p_1(\mathbf{y}|\mathbf{x}) \ldots p_L(\mathbf{y}|\mathbf{x})\, p(\mathbf{x})$$

Analogy to 2D $p(\mathbf{y}|\mathbf{x})$



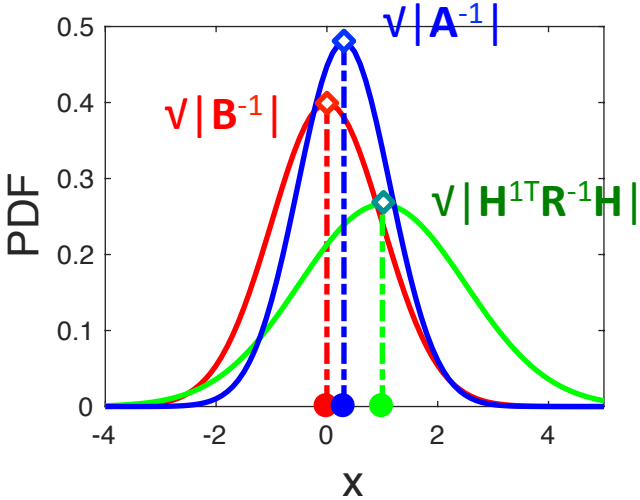
  - Analytical solution

$$J(\Delta\mathbf{x}) = \frac{1}{2}(\Delta\mathbf{x} - \Delta\mathbf{x}^a)^T \mathbf{A}^{-1}(\Delta\mathbf{x} - \Delta\mathbf{x}^a) + J(\Delta\mathbf{x}^a)$$

$$\Delta\mathbf{x}^a = \mathbf{A}\mathbf{H}^T\mathbf{R}^{-1}\mathbf{d}$$

$$\nabla^2 J(\Delta\mathbf{x}) = \mathbf{A}^{-1} = \mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}$$

By assimilation $\mathbf{y}^o$
>(Likelihood)^2 adds up
>(uncertainty) reduces



3D Method II. OI

- Approach: Analytically solve for $\mathbf{x}=\mathbf{x}^b+\Delta\mathbf{x}$ s.t. tr$\mathbf{P}$ is min given $p(\mathbf{x})$ & $p(\mathbf{y}|\mathbf{x})$ using Best Linear Unbiased Estimation (BLUE)= choose $\mathbf{G}^*$ and $\mathbf{K}^*$

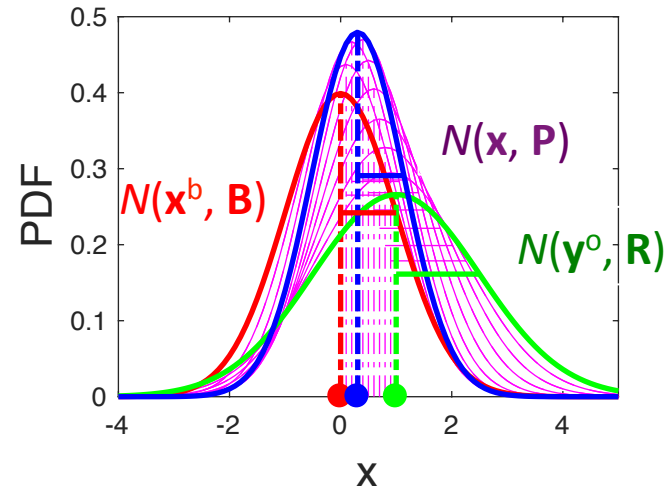
  (=Optimal Interpolation: OI)

  $$\mathbf{x} = \mathbf{G}^* \mathbf{x}^b + \mathbf{K}^* \mathbf{y}^o = \mathbf{x}^t + \boldsymbol{\varepsilon}$$

  $$\mathbf{P}=E[\boldsymbol{\varepsilon}(\boldsymbol{\varepsilon})^T]$$

  such that resulting $\mathbf{x}^{OI}=\mathbf{x}^b+\Delta\mathbf{x}^a$ has

  - No bias: $E[\boldsymbol{\varepsilon}]=\mathbf{0}$
  - MV (least risk) min: $tr\mathbf{P}=\Sigma_n^N P_{nn}$



- Algorithm (analytical solution)

  $$\Delta\mathbf{x}^a = \mathbf{K}\,\mathbf{d}$$

  $$\mathbf{K} = \mathbf{B}\mathbf{H}^T(\mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{R})^{-1}$$

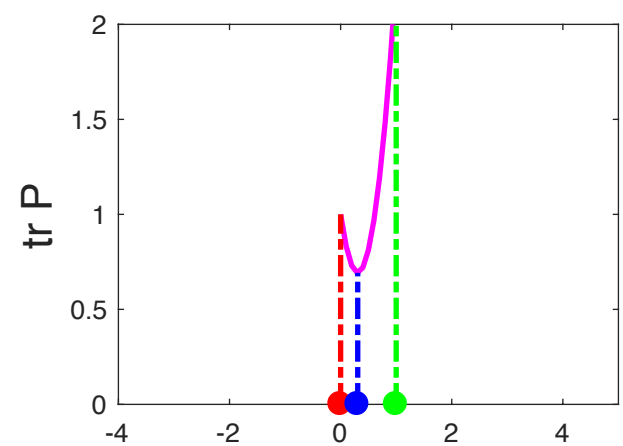
  where

  $$\mathbf{d} = \mathbf{y}^o - \mathbf{h}(\mathbf{x}^b)$$

  although not required

  $$\mathbf{A} = (\mathbf{I} - \mathbf{K}\,\mathbf{H})\mathbf{B} : \text{uncertainty} < \mathbf{B}$$

  $$[\,\mathbf{G} = (\mathbf{I} - \mathbf{K}\,\mathbf{H})]$$



3D Method II: OI

Prior
$p(\mathbf{x}) \sim N(\mathbf{x}^b, \mathbf{B})$
B : Static

Step 1. Model Forecast
Forecast→Background: $\mathbf{x}^b$
$\mathbf{x}_k = \mathbf{m}_{k,k-1}(\mathbf{x}_{k-1})$

posterior
$p(\mathbf{x}|\mathbf{y}) \sim N(\mathbf{x}^a, \mathbf{A})$
A : Usually not computed

$\mathbf{d} = \mathbf{y}^o - \mathbf{h}(\mathbf{x}^b)$

Step 2. Assimilation
$\mathbf{x}^b$ and $\mathbf{y}^o$ → analysis $\mathbf{x}^a$
$\mathbf{x}^a = \mathbf{x}^b + \Delta\mathbf{x}^a$

Observation
Measurement: $\mathbf{y}^o$
$\mathbf{y} = \mathbf{h}(\mathbf{x})$

$$\Delta\mathbf{x}^a = \mathbf{K}\,\mathbf{d}$$
$$\mathbf{K} = \mathbf{B}\mathbf{H}^T(\mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{R})^{-1}$$
$$\mathbf{d} = \mathbf{y}^o - \mathbf{h}(\mathbf{x}^b)$$

Obs Likelihood
$p(\mathbf{y}|\mathbf{x}) \sim N(\mathbf{y}^o, \mathbf{R})$
R : Given

Duality / Equivalance

If $p(\mathbf{x})$ and $p(\mathbf{y}|\mathbf{x})$ are Gaussian & $\mathbf{h}(\mathbf{x})$ is linear,

$$\mathbf{x}^{ML} = \mathbf{x}^{MV}$$

[Although not necessary in 3D: $\mathbf{A}^{ML}=\mathbf{A}^{MV}$]

Maximum likelihood (ML)

$$\Delta\mathbf{x}^{ML} = \mathbf{K}^{ML}\,\mathbf{d}$$

$$(\mathbf{A}^{ML})^{-1} = \mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}$$

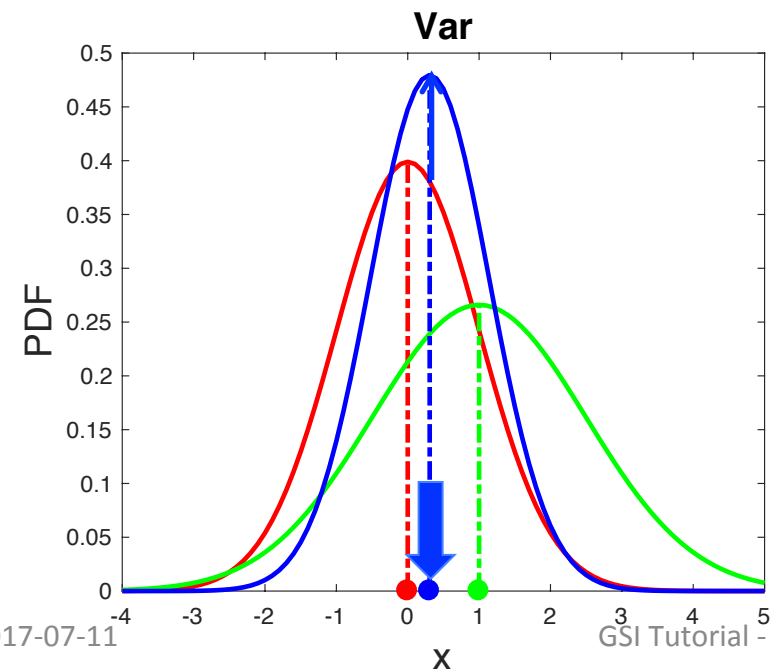
$$\mathbf{K}^{ML} = \mathbf{A}^{ML}\mathbf{H}^T\,\mathbf{R}^{-1}$$

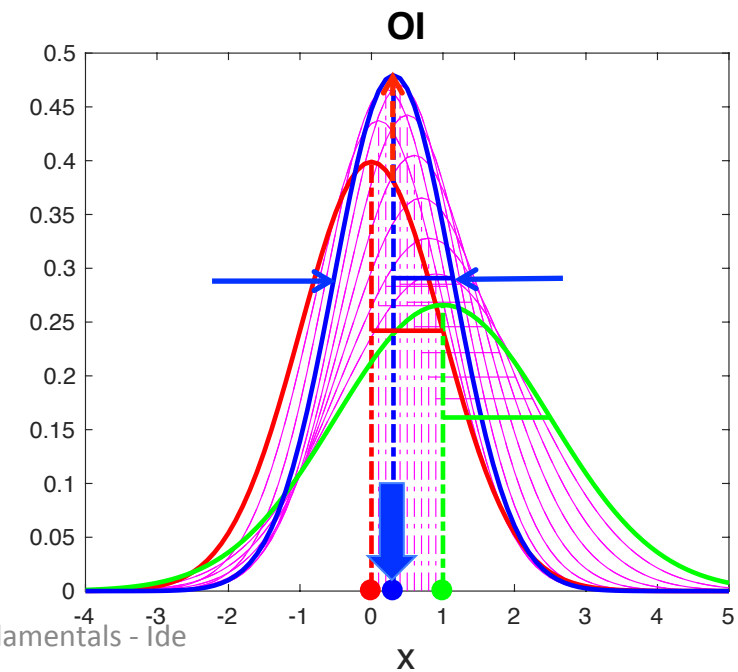
Minimum Variance (MV)

$$\Delta\mathbf{x}^{MV} = \mathbf{K}^{MV}\,\mathbf{d}$$

$$\mathbf{A}^{MV} = (\mathbf{I} - \mathbf{K}^{MV}\,\mathbf{H})\,\mathbf{B}$$

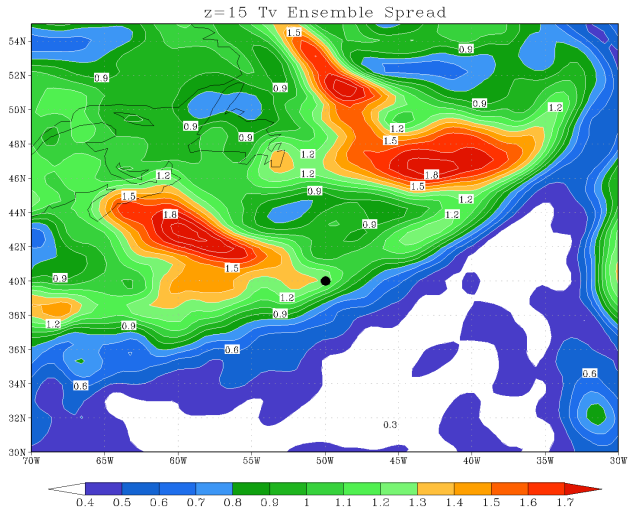
$$\mathbf{K}^{MV} = \mathbf{B}\mathbf{H}^T\,(\mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{R})^{-1}$$

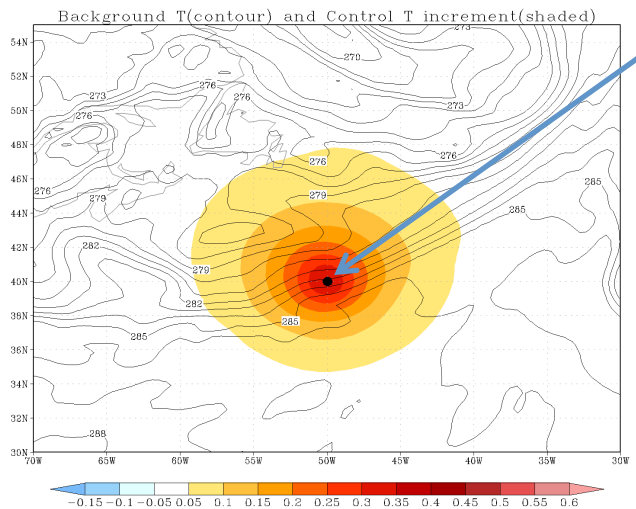




Impact of **B**

- GSI Example





y position

3DVar
[=OI]

$$\begin{pmatrix} \Delta x_1^{\mathrm{OI}} \\ \vdots \\ \Delta x_I^{\mathrm{OI}} \\ \vdots \\ \Delta x_N^{\mathrm{OI}} \end{pmatrix} = \begin{pmatrix} B_{1I} \\ \vdots \\ B_{II} \\ \vdots \\ B_{NI} \end{pmatrix} (R + B_{II})^{-1} \; (y^{\mathrm{o}} - x^{b})$$

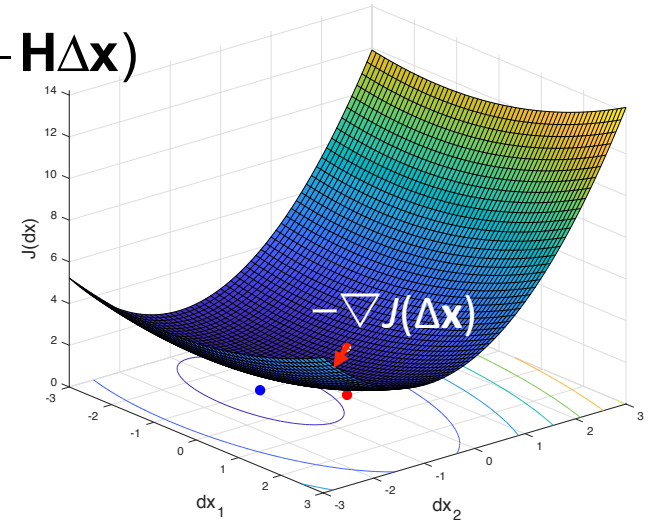
Obs. info in **d** propagates $\Delta\mathbf{x}^{\mathrm{OI}}$ through **B**
→ **B** impacts $\Delta\mathbf{x}^{\mathrm{OI}}$

Single 850mb Tv observation (1K O-F, 1K error) – Courtesy of D. Kleist

3DVar: Computational Aspects

- Initial "guess": $\Delta\mathbf{x}=\mathbf{0}$ [$\mathbf{x}=\mathbf{x}^b$], find $\Delta\mathbf{x}^a$ that minimizes

$$J(\Delta\mathbf{x}) = \frac{1}{2}\Delta\mathbf{x}^T\mathbf{B}^{-1}\Delta\mathbf{x} + \frac{1}{2}(\mathbf{d}-\mathbf{H}\Delta\mathbf{x})^T\ \mathbf{R}^{-1}\ (\mathbf{d}-\mathbf{H}\Delta\mathbf{x})$$



- Mathematical conditions for min
  - $\nabla J(\Delta\mathbf{x}) = \mathbf{0}$ where

$$\nabla J(\Delta\mathbf{x}) = \mathbf{B}^{-1}\Delta\mathbf{x} + \mathbf{H}^T\ \mathbf{R}^{-1}\ (\mathbf{d}-\mathbf{H}\Delta\mathbf{x})$$

  - $\nabla^2 J(\Delta\mathbf{x})$ = semi-positive definite

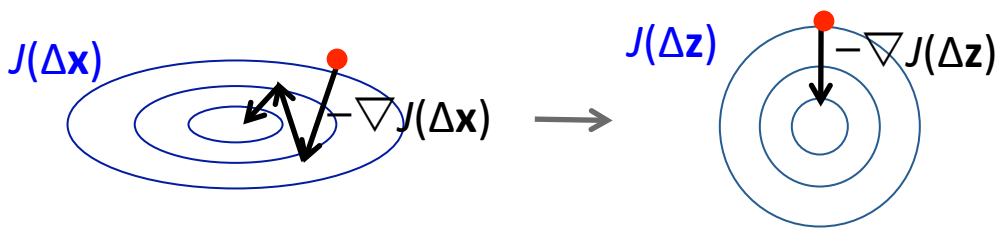
$$\nabla^2 J(\Delta\mathbf{x}) = \mathbf{B}^{-1} + \mathbf{H}^T\ \mathbf{R}^{-1}\mathbf{H} = \mathbf{A}^{-1}$$

- Computational algorithms for optimization, e.g.,
  - Conjugate gradient (GSI default)
  - Quasi-Newton method

  requiring (at the minimum)
  - TLM $\mathbf{H} = \left.\frac{\partial \mathbf{h}(\mathbf{x})}{\partial \mathbf{x}}\right|_{\mathbf{x}^b}$: $\mathbf{x} \rightarrow \mathbf{y}$
  - ADJ $\mathbf{H}^T = \left(\left.\frac{\partial \mathbf{h}(\mathbf{x})}{\partial \mathbf{x}}\right|_{\mathbf{x}^b}\right)^T$: $\mathbf{y} \rightarrow \mathbf{x}$

3DVar: Computational Aspects

- Pre-conditioning
  - Change of variable: $\Delta\mathbf{x}$ to $\Delta\mathbf{z}$ so that $-\nabla J(\Delta\mathbf{z})$ points to $\Delta\mathbf{z}^a$



  - (Un)isometry around the minimum $\mathbf{x}^a$: Controlled by $\nabla^2 J(\mathbf{x}) = \mathbf{A}^{-1}$

$$J(\Delta\mathbf{x}) = \frac{1}{2}(\Delta\mathbf{x} - \Delta\mathbf{x}^a)^T \mathbf{A}^{-1}(\Delta\mathbf{x} - \Delta\mathbf{x}^a) + J(\Delta\mathbf{x}^a)$$

    - Ideal preconditioning: $\Delta\mathbf{x}=\mathbf{A}^{1/2}\Delta\mathbf{z}$

$$J(\Delta\mathbf{z}) = \frac{1}{2}(\Delta\mathbf{z} - \Delta\mathbf{z}^a)^T (\Delta\mathbf{z} - \Delta\mathbf{z}^a) + J(\Delta\mathbf{x}^a)$$

    - GSI preconditioning: $\Delta\mathbf{x}=\mathbf{B}\,\mathbf{z}$ from practical reasons

$$J(\mathbf{z}) = \frac{1}{2}(\mathbf{z} - \mathbf{z}^a)^T \mathbf{B}(\mathbf{z} - \mathbf{z}^a) + J^o(\mathbf{B}\mathbf{z})$$

3DVar: Computational Aspects

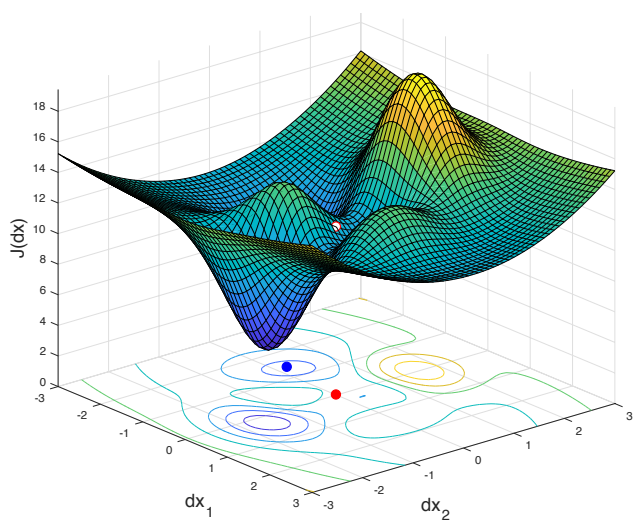
- Outer-Inner loop for nonlinear $\mathbf{h}(\mathbf{x})$
  - Incremental 3DVar: $\mathbf{d}$, $\mathbf{H}$, & $\mathbf{H}^T$ are evaluated at $\mathbf{x}^b$
  - Scheme

    > Outer loop for the initialization ($\mathbf{d}$, $\mathbf{H}$, & $\mathbf{H}^T$) of inner loop using "$\mathbf{x}^b$"

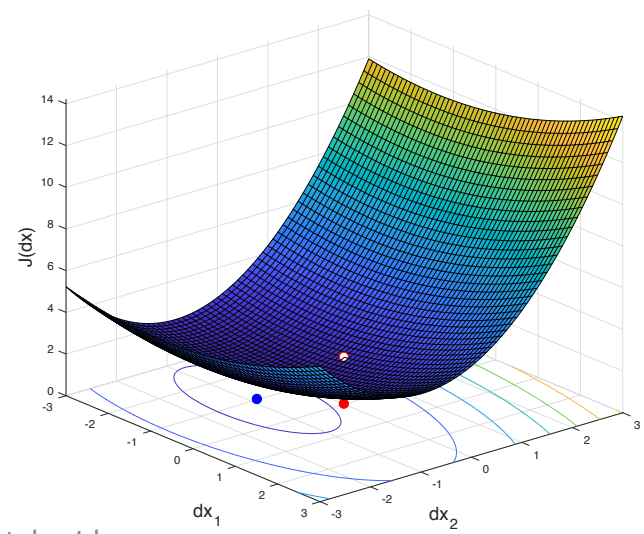
    » Inner loop to solve for "$\Delta\mathbf{x}^a$" incremental 3DVar

new $\mathbf{x}^b$
$= \text{old } \mathbf{x}^b + \Delta\mathbf{x}^a$

3DVar $J(\Delta\mathbf{x})$
Highly nonlinear $\mathbf{h}(\mathbf{x}^b+\Delta\mathbf{x})$



Incremental 3DVar $J(\Delta\mathbf{x})$
Linearized $\mathbf{h}(\mathbf{x}^b+\Delta\mathbf{x}) = \mathbf{h}(\mathbf{x}^b)+ \mathbf{H}\Delta\mathbf{x}$
& $\mathbf{d} = \mathbf{y}^o - \mathbf{h}(\mathbf{x}^b)$



3DVar: Advantages & Flexibility of $J(\Delta\mathbf{x})$

- Quadratic form of $J(\Delta\mathbf{x})$ due to Gaussian assumption can be relaxed
  - Variational quality control (QC) for observations

- Additional terms: $J(\Delta\mathbf{x}) = J^{b}(\Delta\mathbf{x}) + J^{o}(\Delta\mathbf{x}) + J^{c}(\Delta\mathbf{x}) + J^{bc}(\Delta\mathbf{x})$
  - Strong/weak constraints to reduce unwanted fast moving waves
  - Bias correction based on $\mathbf{d} = \mathbf{y}^{o} - \mathbf{h}(\mathbf{x}^{b})$

- Localization based on **B**
  - Spatial localization is in **x** space
  - Variable localization (including variable transform) to suppress unphysical correlation, i.e.,

$$\Delta\mathbf{x} = \Delta\mathbf{x}^{\text{balanced}} + \Delta\mathbf{x}^{\text{unbalanced}} \Leftrightarrow \Delta\mathbf{w} = \begin{pmatrix} \Delta\mathbf{x}^{\text{balanced}} \\ \Delta\mathbf{x}^{\text{unlalanced}} \end{pmatrix} \;\&\; \mathbf{B}_{\mathbf{w}} = \begin{pmatrix} \mathbf{B}^{bb} & \cancelto{0}{\mathbf{B}^{bu}} \\ \cancel{\mathbf{B}^{ub}} & \mathbf{B}^{uu} \end{pmatrix}$$

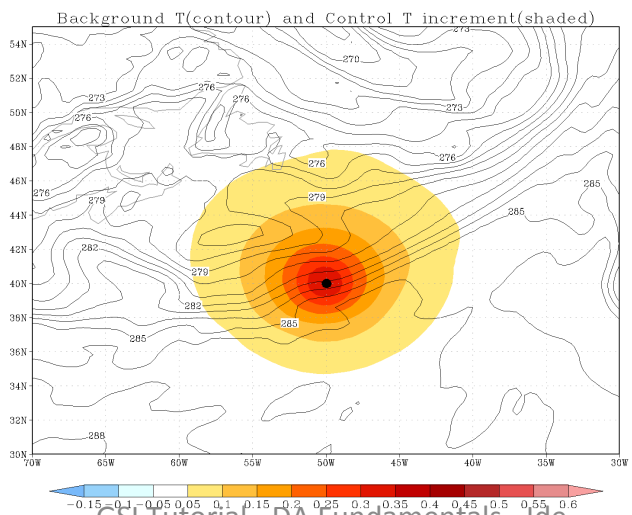
- This lecture (on fundamentals) focuses on the simplest form of $J(\Delta\mathbf{x})$
- See other lectures on useful and important details that make GSI work

Challenges of 3D Methods

- Modeling of static **B**
  - NMC Method: Parrish and Derber, 1992
  - Large dimensions
    - Parameterization
    - Preconditioning
    - Localization: space & variable
  - Mostly homogenous (with little flow dependence)

    → 3D to 4D

$\Delta\mathbf{x}^a$ by single obs



3DVar
[=OI]

Courtesy of D. Kleist

Outline of This Lecture

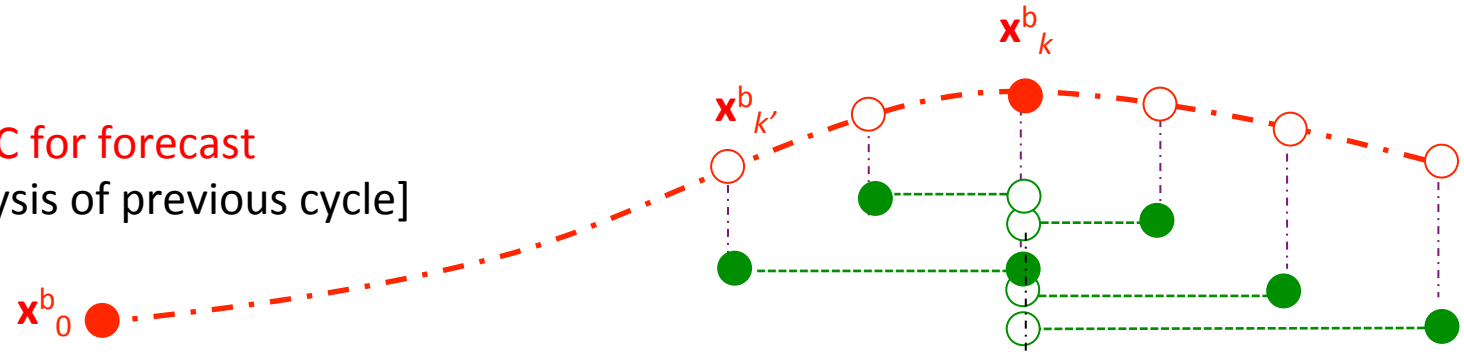
- Background
  - NWP as DA: framework & elements
  - Basic ideas of probability for estimation

- Practical Methods of DA
  - 3D methods using static **B**
    - 3DVar = Variational
    - OI = Optimal Interpolation
  - Towards 4D
    - FGAT = Asynchronized obs within one cycle
  - 4D methods using evolving **B**
    - 4DVar = Var along the model trajectory over a DA cycle
    - EKF/EnKF = Error evolution/explicit estimation of $\mathbf{B}_e$
    - 4DEnVar = Var analysis using $\mathbf{B}_e$
    - Hybrid 4DEnVar = Integration of 4DEnVar and 3DVar FGAT

duality

- Concluding Remarks

3D Method with 4D Asynchronous Observations at $t_{k'}$



Unknown $\mathbf{x}^t$

- 3D methods with FGAT:

  [First Guess at Appropriate Time]

$$\begin{pmatrix} \mathbf{d}^*_1 \\ \vdots \\ \mathbf{d}^*_K \end{pmatrix} = \begin{pmatrix} \mathbf{y}^o_1 - \mathbf{h}_1(\mathbf{x}^b_1) \\ \vdots \\ \mathbf{y}^o_K - \mathbf{h}_K(\mathbf{x}^b_K) \end{pmatrix}$$

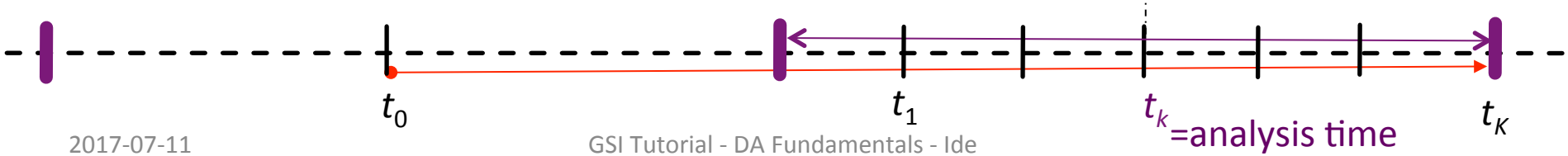
$$J^o(\Delta\mathbf{x}) = \tfrac{1}{2}\Sigma_{k'}(\mathbf{d}^*_{k'} - \mathbf{H}_{k'}\Delta\mathbf{x})^T \mathbf{R}_{k'}^{-1}(\mathbf{d}^*_{k'} - \mathbf{H}_{k'}\Delta\mathbf{x})$$

- 3D method (conventional)

  [$\mathbf{x}^b$ at t_k only]

$$\begin{pmatrix} \mathbf{d}_1 \\ \vdots \\ \mathbf{d}_K \end{pmatrix} = \begin{pmatrix} \mathbf{y}^o_1 - \mathbf{h}_1(\mathbf{x}^b_k) \\ \vdots \\ \mathbf{y}^o_K - \mathbf{h}_K(\mathbf{x}^b_k) \end{pmatrix}$$

$$J^o(\Delta\mathbf{x}) = \tfrac{1}{2}\Sigma_{k'}(\mathbf{d}_{k'} - \mathbf{H}_{k'}\Delta\mathbf{x})^T \mathbf{R}_{k'}^{-1}(\mathbf{d}_{k'} - \mathbf{H}_{k'}\Delta\mathbf{x})$$



3D Method: Incremental 3DVar FGAT

[Use of the linearized $\mathbf{h}(\mathbf{x}^b+\Delta\mathbf{x})\approx\mathbf{h}(\mathbf{x}^b)+\mathbf{H}\Delta\mathbf{x}$ in 3DVar]

Prior
$p(\mathbf{x}) \sim N(\mathbf{x}^b, \mathbf{B})$
B : Static

Step 1. Model Forecast
Forecast→Background: $\mathbf{x}^b_k$
$\mathbf{x}^b_{k'}=\mathbf{m}_{k',k'-1}(\mathbf{x}^b_{k'-1})$

$\mathbf{d}_{k'} = \mathbf{y}^o_{k'} - \mathbf{h}_{k'}(\mathbf{x}^b_{k'})$

Observation
Measurement: $\mathbf{y}^o_{k'}$
$\mathbf{y}_{k'}=\mathbf{h}_{k'}(\mathbf{x}_{k'})$

Obs Likelihood
$p(\mathbf{y}_{k'}|\mathbf{x}_{k'}) \sim N(\mathbf{y}^o_{k'}, \mathbf{R}_{k'})$
R : Given

posterior
$p(\mathbf{x}|\mathbf{y}) \sim N(\mathbf{x}^a, \mathbf{A})$
A : Usually not computed

Step 2. Assimilation
$\mathbf{x}^b$ and $\mathbf{y}^o$ → analysis $\mathbf{x}^a$
$\mathbf{x}^a = \mathbf{x}^b + \Delta\mathbf{x}^a$

$$J(\Delta\mathbf{x}) = J^b(\Delta\mathbf{x}) + J^o(\Delta\mathbf{x})$$
$$J^b(\Delta\mathbf{x}) = \tfrac{1}{2}(\Delta\mathbf{x})^T \mathbf{B}^{-1}(\Delta\mathbf{x})$$
$$J^o(\Delta\mathbf{x}) = \tfrac{1}{2}\Sigma_{k'}(\mathbf{d}^*_{k'}-\mathbf{H}_{k'}\Delta\mathbf{x})^T \mathbf{R}_{k'}^{-1}(\mathbf{d}^*_{k'}-\mathbf{H}_{k'}\Delta\mathbf{x})$$
$$\mathbf{d}^*_{k'} = \mathbf{y}^o_{k'} - \mathbf{h}_{k'}(\mathbf{x}^b_{k'})$$

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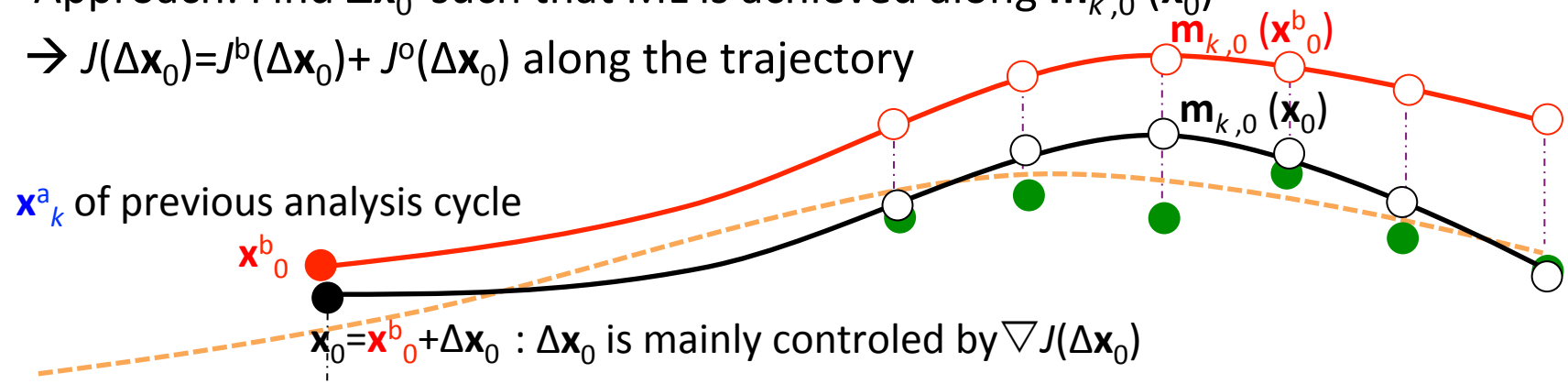
duality

- Concluding Remarks

4D Method I: 4DVar

- Approach: Find $\Delta\mathbf{x}_0$ such that ML is achieved along $\mathbf{m}_{k,0}(\mathbf{x}_0)$

  → $J(\Delta\mathbf{x}_0)=J^b(\Delta\mathbf{x}_0)+J^o(\Delta\mathbf{x}_0)$ along the trajectory



$\mathbf{x}_0=\mathbf{x}^b_0+\Delta\mathbf{x}_0$: $\Delta\mathbf{x}_0$ is mainly controled by $\nabla J(\Delta\mathbf{x}_0)$

$$p(\mathbf{x}_0)\sim N(\mathbf{x}^b_0,\mathbf{B}_0)\propto \exp\left[-J^b(\Delta\mathbf{x})\right]$$

$$J^b(\Delta\mathbf{x}_0)=\frac{1}{2}(\Delta\mathbf{x}_0)^T\ (\mathbf{B}_0)^{-1}\ \Delta\mathbf{x}_0$$

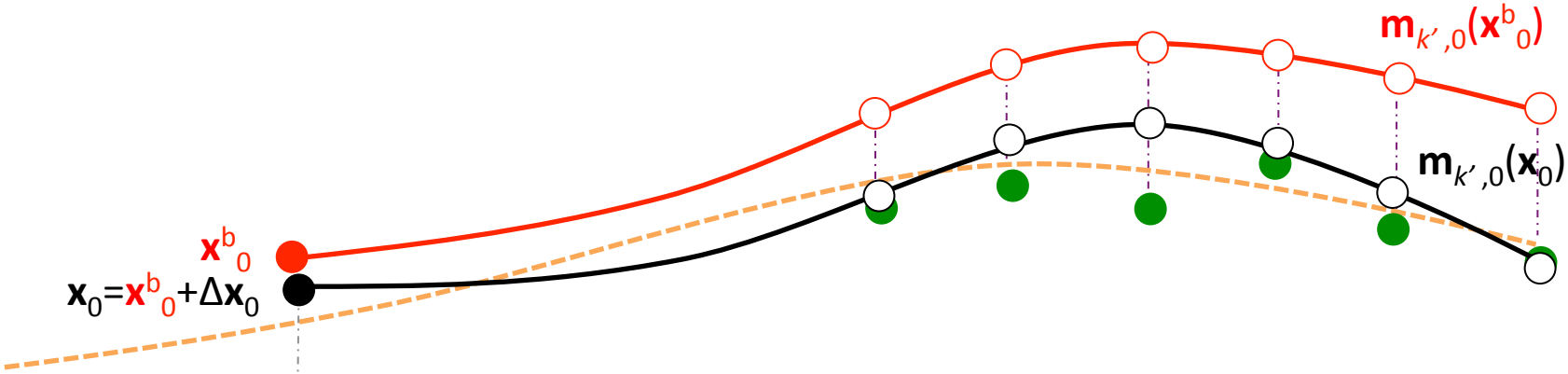
$$p(\mathbf{y}\,|\,\mathbf{x}_0)=\prod_{k'=1}^{K}p(\mathbf{y}_{k'}\,|\,\mathbf{x}_0)\propto \exp\left[-\sum_{k'=1}^{K}J^o_{k'}(\Delta\mathbf{x}_0)\right]$$

$$J^o(\Delta\mathbf{x}_0)=\sum_{k'=1}^{K}\frac{1}{2}(\mathbf{y}^o_{k'}-\mathbf{h}_{k'}(\mathbf{m}_{k',0}(\mathbf{x}^b_0+\Delta\mathbf{x}_0))^T\ (\mathbf{R}_{k'})^{-1}\ (\mathbf{y}^o_{k'}-\mathbf{h}_{k'}(\mathbf{m}_{k',0}(\mathbf{x}^b_0+\Delta\mathbf{x}_0))$$

To address 4Dness, model forecast must be explicitly included in DA

4D Method I: 4DVar

- Computational challenges: each iteration requires



- Nonlinear model forecast $\mathbf{x}_{k'}=\mathbf{m}_{k',0}(\mathbf{x}^b_0+\Delta\mathbf{x}_0)$ to compute $\mathbf{y}^o_{k'}-\mathbf{h}_{k'}(\mathbf{x}_{k'})$

expensive

$$J^o(\Delta\mathbf{x}_0)=\sum_{k'=1}^{K}\frac{1}{2}(\mathbf{y}^o_{k'}-\mathbf{h}_{k'}(\mathbf{m}_{k',0}(\mathbf{x}^b_0+\Delta\mathbf{x}_0))^T\ (\mathbf{R}_{k'})^{-1}\ (\mathbf{y}^o_{k'}-\mathbf{h}_{k'}(\mathbf{m}_{k',0}(\mathbf{x}^b_0+\Delta\mathbf{x}_0))$$

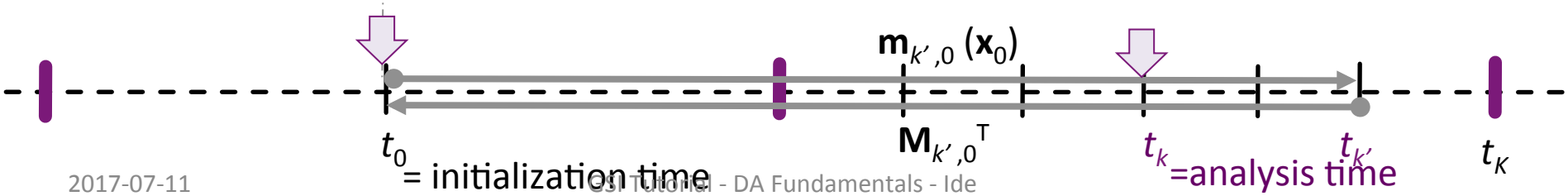
- Model ADJ: $\mathbf{M}_{k',0}^T$ to bring $\mathbf{y}^o_{k'}-\mathbf{h}_{k'}(\mathbf{x}_{k'})$ back to t_0

complex

$$\nabla J^o(\Delta\mathbf{x}_0)=\sum_{k'=1}^{K}\mathbf{M}_{k',0}^T\ \mathbf{H}_{k'}^T(\mathbf{R}_{k'})^{-1}\ (\mathbf{y}^o_{k'}-\mathbf{h}_{k'}(\mathbf{m}_{k',0}(\mathbf{x}^b_0+\Delta\mathbf{x}_0))$$

TLM $\mathbf{M}_{k',0}=\partial\mathbf{m}_{k',0}(\mathbf{x}_0)/\partial\mathbf{x}_0$: $\Delta\mathbf{x}_0 \rightarrow \Delta\mathbf{x}_{k'}$

ADJ $\mathbf{M}_{k',0}^T$: $\Delta\mathbf{x}_{k'} \rightarrow \Delta\mathbf{x}_0$



4D Method I: 4DVar

Challenging

Prior
$p(\mathbf{x}_0) \sim N(\mathbf{x}^b_0, \mathbf{B}_0)$
$\mathbf{B}_0$: Static

Step 1. Model Forecast
Forecast→Background: $\mathbf{x}^b_k$
$\mathbf{x}^b_{k'} = \mathbf{m}_{k',k'-1}(\mathbf{x}^b_{k'-1})$

posterior
$p(\mathbf{x}_k|\mathbf{y}) \sim N(\mathbf{x}^a_k, \mathbf{A}_k)$
$\mathbf{A}_k$: Usually not computed

Step 2. Assimilation
$\mathbf{x}^b_{k'}$ and $\mathbf{y}^o_{k'}$ → analysis $\mathbf{x}^a_0$
$\mathbf{x}^a_k = \mathbf{m}_{k,k-1}(\mathbf{x}^b_0 + \Delta\mathbf{x}^a_0)$

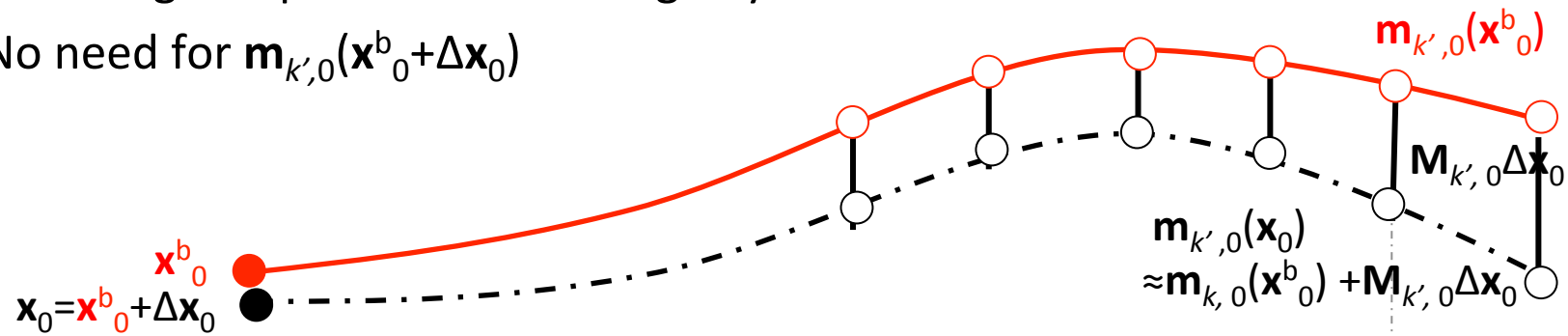
Observation
Measurement: $\mathbf{y}^o_{k'}$
$\mathbf{y}_{k'} = \mathbf{h}_{k'}(\mathbf{x}_{k'})$

Obs Likelihood
$p(\mathbf{y}_{k'}|\mathbf{x}_{k'}) \sim N(\mathbf{y}^o_{k'}, \mathbf{R}_{k'})$
$\mathbf{R}$: Given

$$J(\Delta\mathbf{x}_0) = J^b(\Delta\mathbf{x}_0) + J^o(\Delta\mathbf{x}_0)$$
$$J^b(\Delta\mathbf{x}_0) = \tfrac{1}{2}(\Delta\mathbf{x}_0)^T \mathbf{B}_0^{-1}\Delta\mathbf{x}_0$$
$$J^o(\Delta\mathbf{x}_0) = \Sigma_{k'}\tfrac{1}{2}(\mathbf{y}^o_{k'} - \mathbf{h}_{k'}(\mathbf{m}_{k',0}(\mathbf{x}^b_0 + \Delta\mathbf{x}_0)))^T \mathbf{R}_{k'}^{-1}(\mathbf{y}^o_{k'} - \mathbf{h}_{k'}(\mathbf{m}_{k',0}(\mathbf{x}^b_0 + \Delta\mathbf{x}_0)))$$

4D Method I: Incremental 4DVar

- Addressing computational challenge by linearized model
  = No need for $\mathbf{m}_{k',0}(\mathbf{x}^b{}_0+\Delta\mathbf{x}_0)$



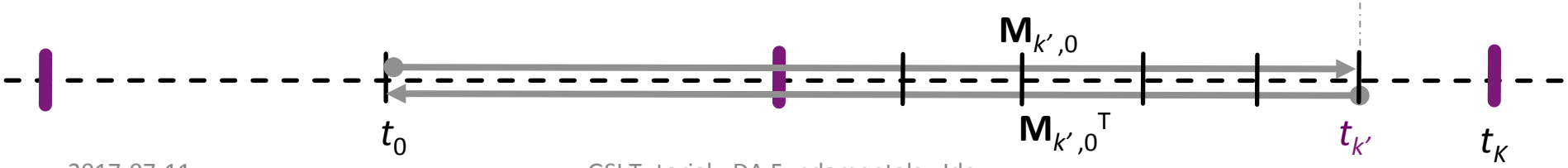
- Trajectory: $\mathbf{m}_{k',0}(\mathbf{x}^b{}_0+\Delta\mathbf{x}_0) = \mathbf{m}_{k',0}(\mathbf{x}^b{}_0)+\Delta\mathbf{x}_{k'} \approx\mathbf{m}_{k',0}(\mathbf{x}^b{}_0) + \mathbf{M}_{k',0}\Delta\mathbf{x}_0 \; [+\mathbf{w}_{k',0}]$
- Increment: $\Delta\mathbf{x}_{k'} \approx \mathbf{M}_{k',0}\Delta\mathbf{x}_0 \; [+\mathbf{w}_{k',0}]$

Process noise

- Discrepancy: $\mathbf{y}^o{}_{k'} - \mathbf{h}_{k'}(\mathbf{m}_{k',0}(\mathbf{x}^b{}_0+\Delta\mathbf{x}_0)) \approx \mathbf{y}^o{}_{k'} - \mathbf{h}_{k'}(\mathbf{m}_{k',0}(\mathbf{x}^b{}_0)) - \mathbf{H}_{k'}\mathbf{M}_{k',0}\Delta\mathbf{x}_0$

- Obs cost func: $$J^o(\Delta\mathbf{x}_0)=\sum_{k'=1}^{K}\frac{1}{2}(\mathbf{d}_{k'}-\mathbf{H}_{k'}\mathbf{M}_{k',0}\Delta\mathbf{x}_0)^T\,(\mathbf{R}_{k'})^{-1}\,(\mathbf{d}_{k'}-\mathbf{H}_{k'}\mathbf{M}_{k',0}\Delta\mathbf{x}_0)$$

$$\nabla J^o(\Delta\mathbf{x}_0)=\sum_{k'=1}^{K}\mathbf{M}_{k',0}{}^T\mathbf{H}_{k'}{}^T\,(\mathbf{R}_{k'})^{-1}\,(\mathbf{d}_{k'}-\mathbf{H}_{k'}\mathbf{M}_{k',0}\Delta\mathbf{x}_0)$$



4D Method I: Incremental 4DVar

Challenging

$\mathbf{x}^a_k$ only, not $\mathbf{A}_k$

Prior
$p(\mathbf{x}_0) \sim N(\mathbf{x}^b_0, \mathbf{B}_0)$
$\mathbf{B}_0$: Static

Step 1. Model Forecast
Forecast→Background: $\mathbf{x}^b_k$
$\mathbf{x}^b_{k'} = \mathbf{m}_{k',k'-1}(\mathbf{x}^b_{k'-1})$

posterior
$p(\mathbf{x}_k|\mathbf{y}) \sim N(\mathbf{x}^a_k, \mathbf{A}_k)$
$\mathbf{A}_k = \mathbf{M}_{k,0}(\nabla^2 J(\Delta\mathbf{x}_0))^{-1}\ \mathbf{M}_{k,0}^T$

$\mathbf{d}_{k'} = \mathbf{y}^o_{k'} - \mathbf{h}_{k'}(\mathbf{x}^b_{k'})$

Step 2. Assimilation
$\mathbf{x}^b_{k'}$ and $\mathbf{y}^o_{k'}$ → analysis $\mathbf{x}^a_0$
$\mathbf{x}^a_k = \mathbf{x}^b_k + \mathbf{M}_{k,0}\ \Delta\mathbf{x}^a_0$

Observation
Measurement: $\mathbf{y}^o_{k'}$
$\mathbf{y}_{k'} = \mathbf{h}_{k'}(\mathbf{x}_{k'})$

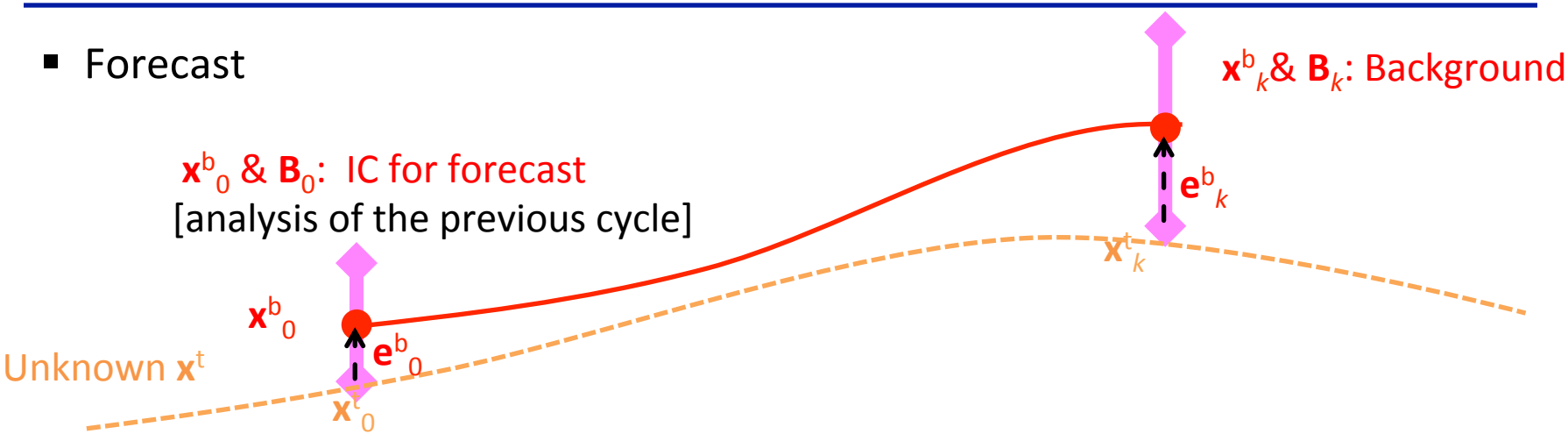
Obs Likelihood
$p(\mathbf{y}_{k'}|\mathbf{x}_{k'}) \sim N(\mathbf{y}^o_{k'}, \mathbf{R}_{k'})$
$\mathbf{R}_{k'}$: Given

$$J(\Delta\mathbf{x}_0) = J^b(\Delta\mathbf{x}_0) + J^o(\Delta\mathbf{x}_0)$$
$$J^b(\Delta\mathbf{x}_0) = \tfrac{1}{2}(\Delta\mathbf{x}_0)^T\ \mathbf{B}_0^{-1}\Delta\mathbf{x}_0$$
$$J^o(\Delta\mathbf{x}_0) = \Sigma_{k'}\tfrac{1}{2}\ (\mathbf{d}_{k'} - \mathbf{H}_{k'}\mathbf{M}_{k',0}\,\Delta\mathbf{x}_0))^T\ \mathbf{R}_k^{-1}(\mathbf{d}_{k'} - \mathbf{H}_{k'}\,\mathbf{M}_{k',0}\,\Delta\mathbf{x}_0))$$

with Outer-Inner loop

4D Uncertainty Propagation by TLM and ADJ

- Forecast



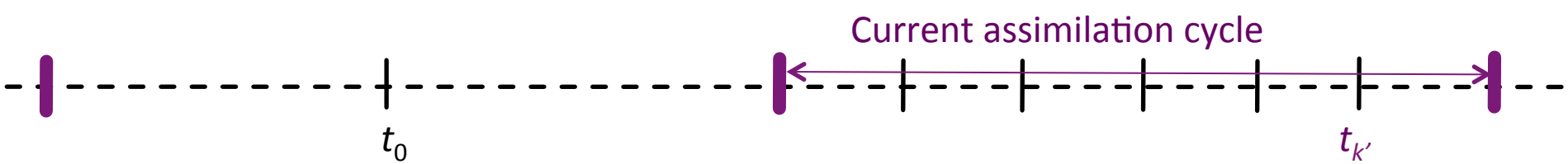
- State: $\mathbf{x}^b_k = \mathbf{m}_{k,0}(\mathbf{x}^b_0)$

$$\mathbf{x}^t_k + \mathbf{e}^b_k = \mathbf{m}_{k,0}(\mathbf{x}^t_0+\mathbf{e}^b_0) \approx \mathbf{m}_{k,0}(\mathbf{x}^t_0) + \mathbf{M}_{k,0}\mathbf{e}^b_0 \quad [+\mathbf{w}_{k,0}]$$

- Error : $\mathbf{e}^b_k \approx \mathbf{M}_{k,0}\mathbf{e}^b_0 \quad [+\mathbf{w}_{k,k-1}]$ Process noise

$$\mathbf{B}_k = \mathbf{M}_{k,0}\mathbf{B}_0\mathbf{M}_{k,0}^T \quad [+\mathbf{Q}_{k,0}] \qquad \mathbf{Q}_{k,0} = E[\mathbf{w}_{k,0}(\mathbf{w}_{k,0})^T]$$

- Analysis by MV with $\mathbf{B}_k$



4D Method IIa: EKF without FGAT

Challenging

IC ($\mathbf{x}^b_0$, $\mathbf{B}_0$)
← ($\mathbf{x}^a_k$, $\mathbf{A}_k$) of previous cycle

Step 1. Model Forecast

Forecast→Background: $\mathbf{x}^b$

$$\mathbf{x}^b_k = \mathbf{m}_{k,0}(\mathbf{x}^b_0)$$

$$\mathbf{B}_k = \mathbf{M}_{k,0}\mathbf{B}_0\,\mathbf{M}_{k,0}^T + \mathbf{Q}_{k,0}$$

$$\mathbf{d}_k = \mathbf{y}^o_{k;} - \mathbf{h}_{k'}(\mathbf{x}^b_k)$$

Observation

Measurement: $\mathbf{y}^o_{k'}$

$$\mathbf{y}_{k'} = \mathbf{h}(\mathbf{x}_{k'})$$

Step 2. Assimilation

Integration of $\mathbf{x}^b_k$ and $\mathbf{y}^o_k$

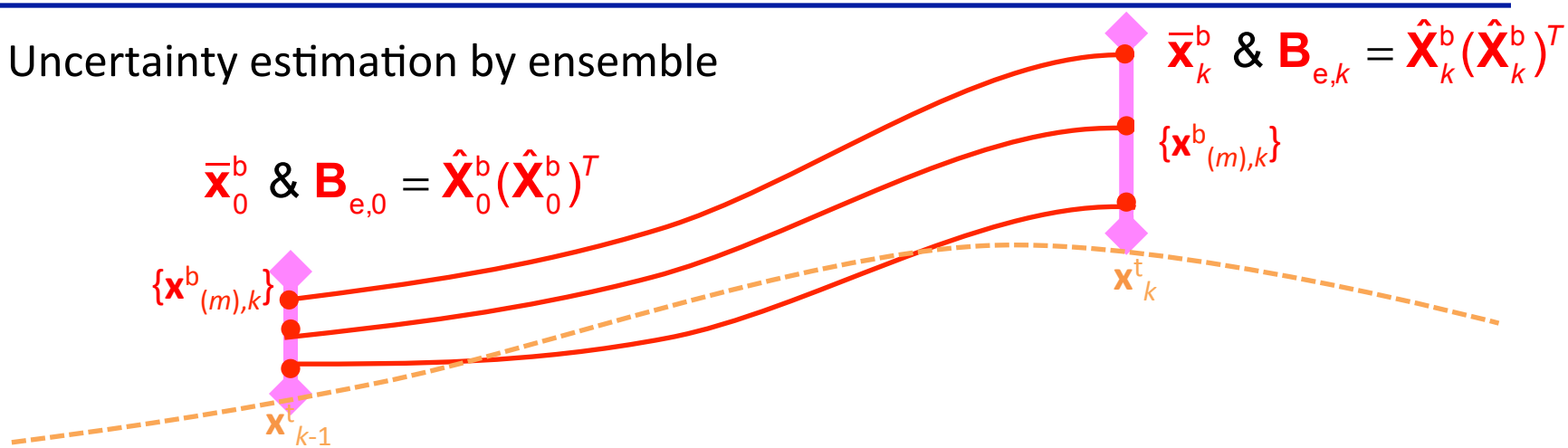
$$\mathbf{x}^a_k = \mathbf{x}^b_k + \mathbf{K}_k\,\mathbf{d}_k$$

$$\mathbf{A}_k = (\mathbf{I} - \mathbf{K}_k\mathbf{H}_k)\mathbf{B}_k$$

$$\mathbf{K}_k = \mathbf{B}_k\mathbf{H}_k^T\,(\mathbf{H}_k\mathbf{B}_k\mathbf{H}_k^T + \mathbf{R}_k)^{-1}$$

4D Error/Uncertainty Propagation by Ensemble $\mathbf{X}=\{\mathbf{x}_{(m)}\}$

- Uncertainty estimation by ensemble

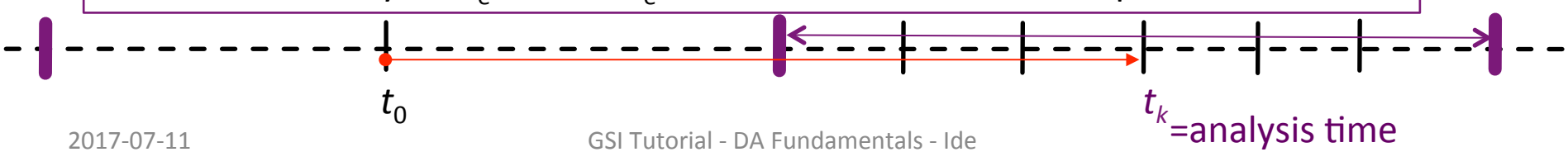


State estimate: $\bar{\mathbf{x}} = \frac{1}{M}\sum_{m=1}^{M}\mathbf{x}_{(m)}$ $\qquad \bar{\mathbf{y}} = \frac{1}{M}\sum_{m=1}^{M}\mathbf{y}_{(m)}; \quad \mathbf{y}_{(m)} = \mathbf{h}(\mathbf{x}_{(m)})$

Error covariance: $\mathbf{B}_{\mathrm{e}} = \hat{\mathbf{X}}^{\mathrm{b}}(\hat{\mathbf{X}}^{\mathrm{b}})^{T}$ $\qquad \mathbf{H}\mathbf{B}_{\mathrm{e}}\mathbf{H}^{T} \approx \hat{\mathbf{Y}}^{\mathrm{b}}(\hat{\mathbf{Y}}^{\mathrm{b}})^{T}$

$$\hat{\mathbf{X}}_{\mathrm{e}} = \frac{1}{\sqrt{M-1}}\{\mathbf{x}_{(m)} - \bar{\mathbf{x}}\} \qquad \hat{\mathbf{Y}} = \frac{1}{\sqrt{M-1}}\{\mathbf{y}_{(m)} - \bar{\mathbf{y}}\}$$

No need for $\mathbf{M}$ or $\mathbf{M}^{\mathrm{T}}$ to propagate $\mathbf{B}_{\mathrm{e},0}$ & Computationally feasible for small M
→ Rank deficiency in $\mathbf{B}_{\mathrm{e}}$ and $\mathbf{H}\mathbf{B}_{\mathrm{e}}\mathbf{H}^{\mathrm{T}}$ → need for localization $\rho_{\circ}$



4D Method IIb: EnKF without FGAT

- Localization $\rho\circ$ in obs space
- Inflation (explicit or implicit)

Step 1. Ensemble Forecast

$\{\mathbf{x}^b_{k(m)}\}$

$\mathbf{x}^b_{k(m)}=\mathbf{m}_{k,0}(\mathbf{x}^b_{0(m)})$

Step 2. Assimilation

$\{\mathbf{x}^b_{k(m)}\}$ and $\mathbf{y}^o_k \rightarrow \{\mathbf{x}^a_{k(m)}\}$

$$\bar{\mathbf{x}}^a_k = \bar{\mathbf{x}}^b_k + \hat{\mathbf{K}}_k \mathbf{d}_k$$

$$\mathbf{A}_{e,k} = (\mathbf{I} - \hat{\mathbf{K}}_k \mathbf{H}_k)\mathbf{B}_{e,k}$$

$$\hat{\mathbf{K}}_k = \rho \circ \hat{\mathbf{X}}_k \hat{\mathbf{Y}}_k (\rho \circ \hat{\mathbf{Y}}_k \hat{\mathbf{Y}}_k + \mathbf{R}_k)^{-1}$$

Observation

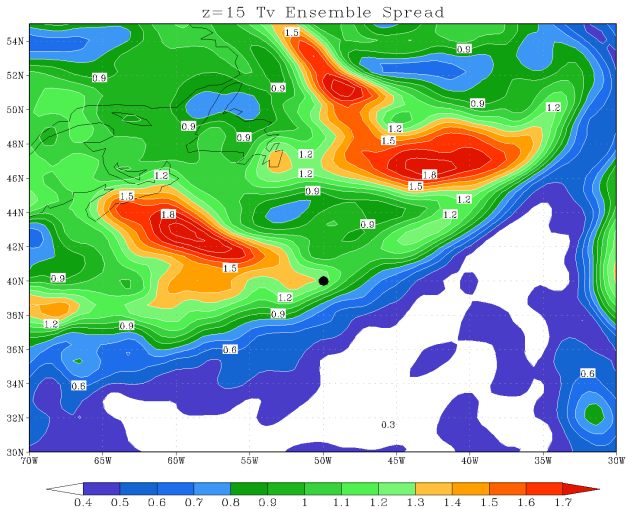
Measurement: $\mathbf{y}^o_{k'}$

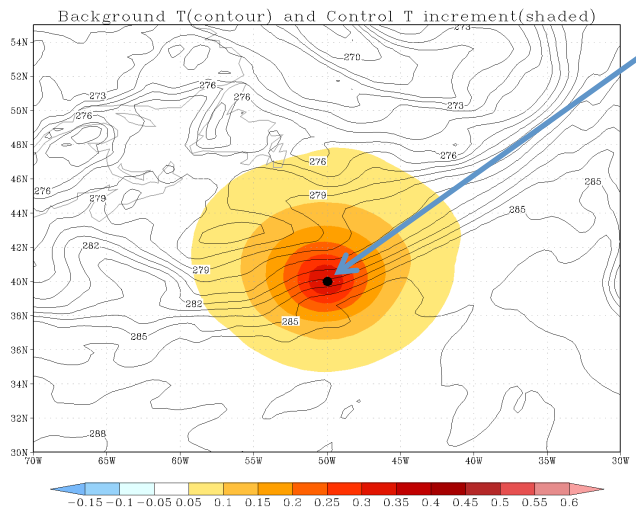
$\mathbf{y}_{k'}=\mathbf{h}(\mathbf{x}_{k'})$

- EnKF never computes $\mathbf{A}_e$ or $\mathbf{B}_e$ themselves
- $\{\mathbf{x}^{a.b}_{k(m)}\}$ satisfies ensemble approximation to EKF
  [Infinitely many possible choices of $\mathbf{X}^{a,b}_k$ exist]
  - Ensemble Square Root Filter (EnSRF)
  - Local Ensemble Transform Kalman Filter (LETKF)
  - Many variatnts

Impact of **B**

- GSI Example

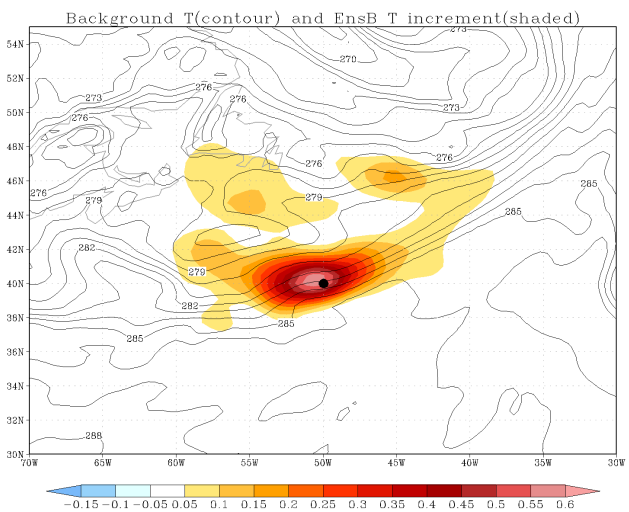




y position

3DVar
[=OI]
B=**B**$_c$

EnVar
B=**B**$_e$



$$\begin{pmatrix} \Delta x_1^a \\ \vdots \\ \Delta x_I^a \\ \vdots \\ \Delta x_N^a \end{pmatrix} = \begin{pmatrix} B_{1I} \\ \vdots \\ B_{II} \\ \vdots \\ B_{NI} \end{pmatrix} (R + B_{II})^{-1} \; (y^o - x^b)$$

Obs. info in **d** propagates Δ**x**^{a} through **B**
→ **B** impacts quality of Δ**x**^{a}

Single 850mb Tv observation (1K O-F, 1K error) – Courtesy of D. Kleist

4D Method III: 4D Ensemble Var (Incremental)

- Motivation:
  - 4DEnKF increment spans over ensemble space at each grid point

$$\Delta\mathbf{x} = \mathbf{K}\mathbf{d} = \hat{\mathbf{X}}^{\mathrm{b}}\boldsymbol{\alpha}$$

$\boldsymbol{\alpha}$: for ensemble members concatenated over the grid

  - 4D TLM and ADJ can be replaced by ensemble approximations

$$\mathbf{M}_{k',0}\Delta\mathbf{x}_0 = \mathbf{M}_{k',0}\hat{\mathbf{X}}_0\boldsymbol{\alpha} \approx \hat{\mathbf{X}}_{k'}\boldsymbol{\alpha}$$

$$\mathbf{H}_{k'}\mathbf{M}_{k',0}\Delta\mathbf{x}_0 = \mathbf{H}_{k'}\mathbf{M}_{k',0}\hat{\mathbf{X}}_0\boldsymbol{\alpha} \approx \mathbf{H}_{k'}\hat{\mathbf{X}}_{k'}\boldsymbol{\alpha} \approx \hat{\mathbf{Y}}_{k'}\boldsymbol{\alpha}$$

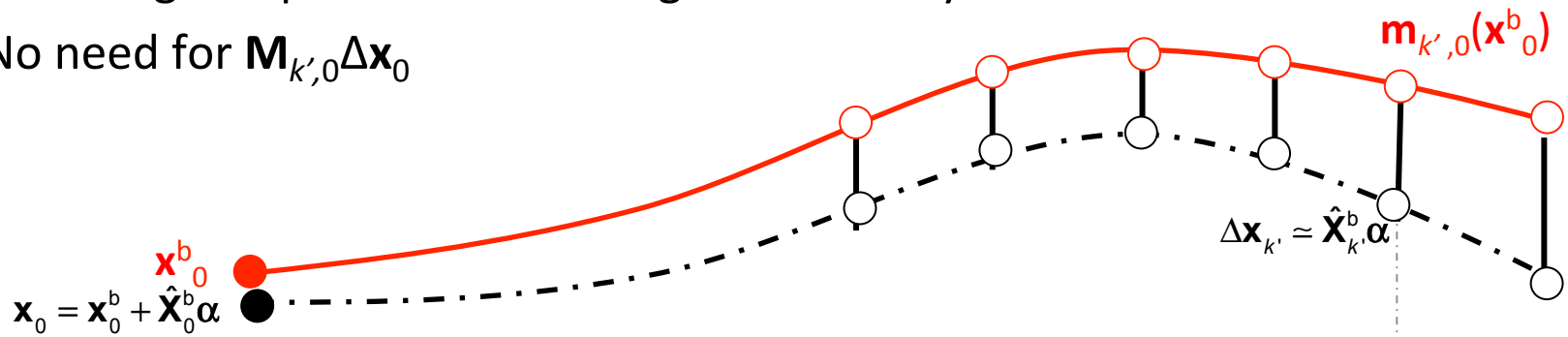
$\boldsymbol{\alpha}$: constant along the trajectory over the cycle

  - Var uses **x**-space localization **L**

$$\mathbf{B}_{\mathrm{e}} = (\hat{\mathbf{X}}^{\mathrm{b}})^T \circ \mathbf{L} \circ \hat{\mathbf{X}}^{\mathrm{b}}$$

4D Method: Incremental 4DEnVar

- Addressing computational challenge in 4DVar by ensemble
  = No need for $\mathbf{M}_{k',0}\Delta\mathbf{x}_0$



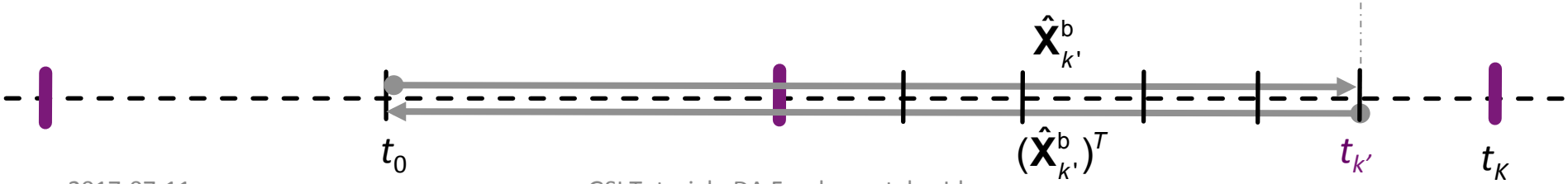
Loc in **x**-space

- Background

$$J^b(\alpha)\left[=\frac{1}{2}\Delta\mathbf{x}^T\mathbf{B}^{-1}\Delta\mathbf{x}\right]=\frac{1}{2}(\hat{\mathbf{X}}^b\alpha)^T\ [(\hat{\mathbf{X}}^b)^T\mathbf{L}\hat{\mathbf{X}}^b]^{-1}\ (\hat{\mathbf{X}}^b\alpha)\approx\boxed{\frac{1}{2}\alpha^T\mathbf{L}^{-1}\alpha}$$

- Observation

$$J^o(\alpha)=\sum_{k'=1}^{K}\frac{1}{2}(\mathbf{d}_{k'}-\hat{\mathbf{Y}}_{k'}\alpha)^T\ (\mathbf{R}_{k'})^{-1}\ (\mathbf{d}_{k'}-\hat{\mathbf{Y}}_{k'}\alpha)$$



4D Method: 4DEnVar

Step 1. Ensemble Forecast

$\{\mathbf{x}^b_{k'(m)}\}$

$\mathbf{x}^b_{k'(m)} = \mathbf{m}_{k',0}(\mathbf{x}^b_{0(m)})$

- Loc **L** in **x**-space
- Parallel run of EnKF is necessary for ensemble spread
  ↔4DLETKF (Loc in **y**-space)

Step 2. Assimilation

$\{\mathbf{x}^b_{k'(m)}\}$ and $\mathbf{y}^o_k \rightarrow \bar{\mathbf{x}}^a_k$

$$\bar{\mathbf{x}}^a_k = \bar{\mathbf{x}}^b_k + \hat{\mathbf{X}}_k \alpha$$

Observation

Measurement: $\mathbf{y}^o_{k'}$

$\mathbf{y}_{k'} = \mathbf{h}(\mathbf{x}_{k'})$

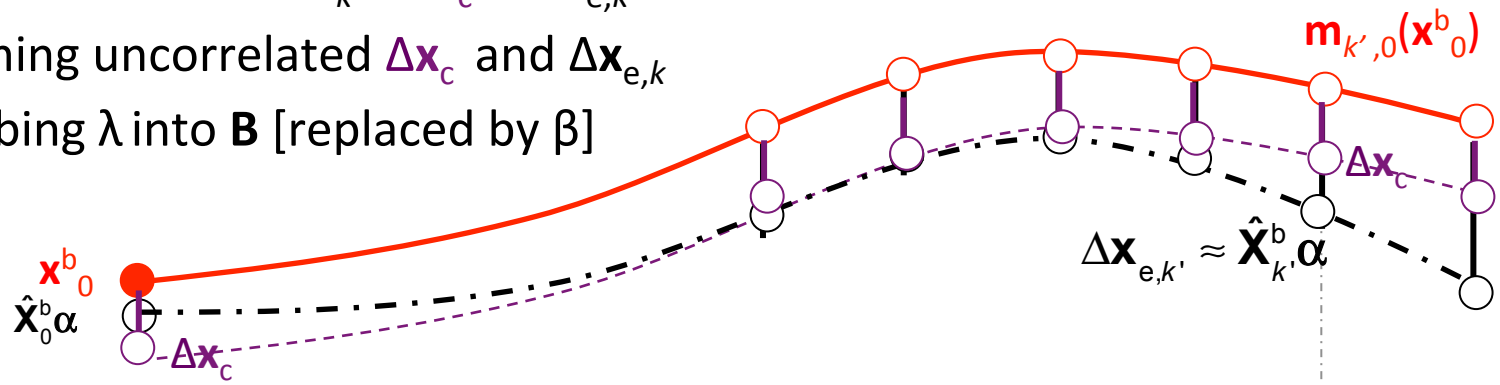
$$J(\boldsymbol{\alpha}) = J^b(\boldsymbol{\alpha}) + J^o(\boldsymbol{\alpha})$$

$$J^b(\boldsymbol{\alpha}) = \tfrac{1}{2}\boldsymbol{\alpha}^T \mathbf{L}^{-1}\boldsymbol{\alpha}$$

$$J^o(\boldsymbol{\alpha}) = \Sigma_{k'} \tfrac{1}{2} (\mathbf{d}_{k'} - \hat{\mathbf{Y}}_{k'}\boldsymbol{\alpha}))^T \mathbf{R}_{k'}^{-1}(\mathbf{d}_{k'} - \hat{\mathbf{Y}}_{k'}\boldsymbol{\alpha}))$$

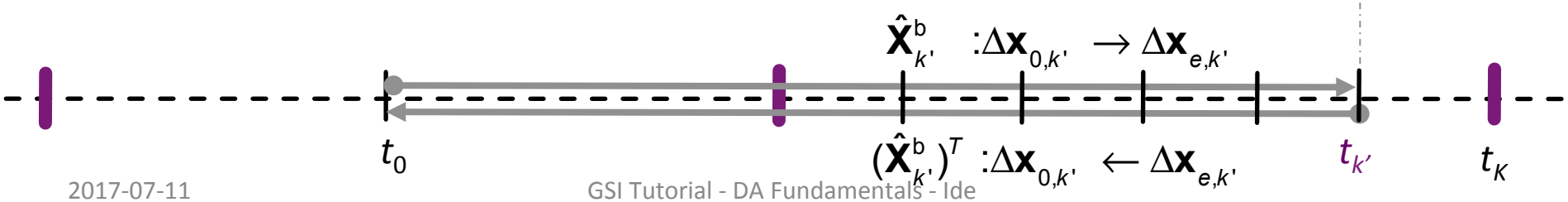
4D Method: Incremental 4DEnVar

- Hybrid in increment: $\Delta\mathbf{x}_k = \Delta\mathbf{x}_c + \Delta\mathbf{x}_{e,k}$
  - Assuming uncorrelated $\Delta\mathbf{x}_c$ and $\Delta\mathbf{x}_{e,k}$
  - absorbing λ into **B** [replaced by β]



- Cost function: $J(\Delta\mathbf{x}_c,\alpha) = J^b(\Delta\mathbf{x}_c,\alpha) + J^o(\Delta\mathbf{x}_c,\alpha)$
  - Background $J^b(\Delta\mathbf{x}_c,\alpha) = \beta_c \frac{1}{2}(\Delta\mathbf{x}_c)^T\ (\mathbf{B}_c)^{-1}\ \Delta\mathbf{x}_0 + \beta_{en}\frac{1}{2}\alpha^T\mathbf{L}^{-1}\alpha$
  - Obs $J^o(\Delta\mathbf{x}_c,\alpha) = \sum_{k'=1}^{K}\frac{1}{2}[\mathbf{d}_{k'} - \mathbf{H}_{k'}(\Delta\mathbf{x}_c + \hat{\mathbf{X}}_{k'}\alpha)]^T\ (\mathbf{R}_{k'})^{-1}\ [\mathbf{d}_{k'} - \mathbf{H}_{k'}(\Delta\mathbf{x}_c + \hat{\mathbf{X}}_{k'}\alpha)]$

(β_c, β_e): weight coefficients for climatology and ensemble Background



4D Method: Hybrid 4DEnVar

Operational GSI

Assimilation cycle

- Localization **L** in model space
- Parallel run of EnKF is necessary for ensemble spread

Step 1. Ensemble Forecast

Forecast→Background: $\mathbf{x}^b_k$

$\mathbf{x}^b_{k(m)}=\mathbf{m}_{k,0}(\mathbf{x}^b_{0(m)})$

Step 2. Assimilation

Integration of $\mathbf{x}^b$ and $\mathbf{y}^o$ →$\mathbf{x}^a$

$$\mathbf{x}^a_k = \mathbf{x}^b_k + (\Delta\mathbf{x}_c + \hat{\mathbf{X}}_k\alpha)$$

Observation

Measurement: $\mathbf{y}^o_{k'}$

$\mathbf{y}_{k'}=\mathbf{h}(\mathbf{x}_{k'})$

$$J(\Delta\mathbf{x}_c,\boldsymbol{\alpha}) = J^b(\Delta\mathbf{x}_c,\boldsymbol{\alpha}) + J^o(\Delta\mathbf{x}_c,\boldsymbol{\alpha})$$

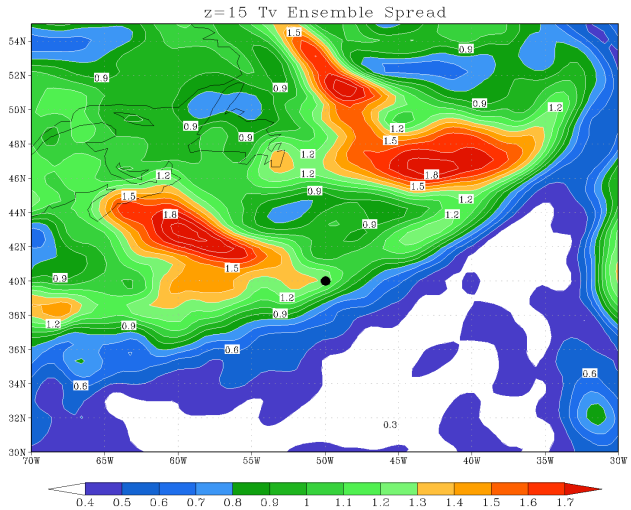
$$J^b(\Delta\mathbf{x}_c,\boldsymbol{\alpha}) = \beta_c ½\Delta\mathbf{x}_c^T\,\mathbf{B}_c^{-1}\Delta\mathbf{x}_c + \beta_e ½\boldsymbol{\alpha}^T\,\mathbf{L}^{-1}\boldsymbol{\alpha}$$

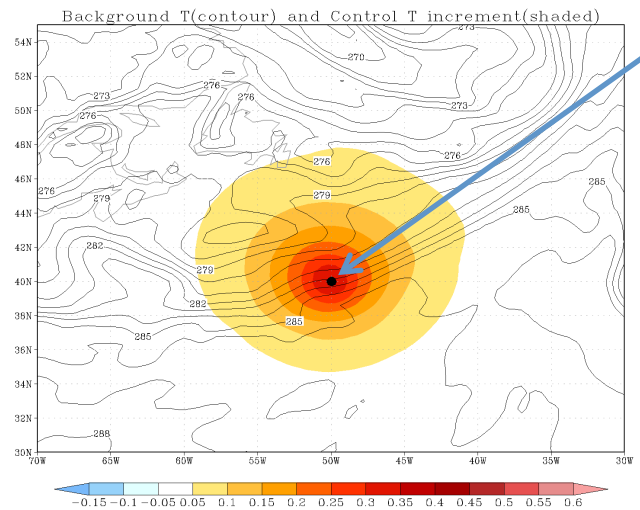
$$J^o(\Delta\mathbf{x}_c,\boldsymbol{\alpha}) = \Sigma_{k'} ½\,[\mathbf{d}_{k'}-\mathbf{H}_{k'}(\Delta\mathbf{x}_c + \mathbf{X}_{k'}\,\boldsymbol{\alpha})]^T\,\mathbf{R}_{k'}^{-1}\,[\mathbf{d}_{k'}-\mathbf{H}_{k'}(\Delta\mathbf{x}_c + \mathbf{X}_{k'}\,\boldsymbol{\alpha})]$$

Can run double/multi-resolution

Impact of B

- GSI Example





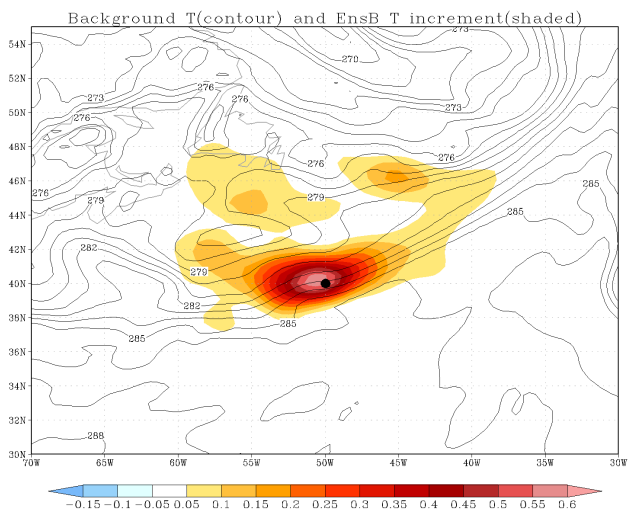
x_I *position*

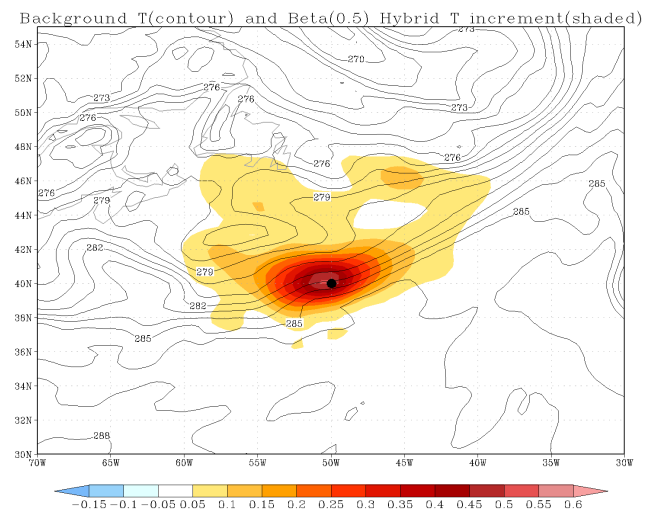
3DVAR

β_e=0
β_c=1

EnVar

β_e=1
β_c=0



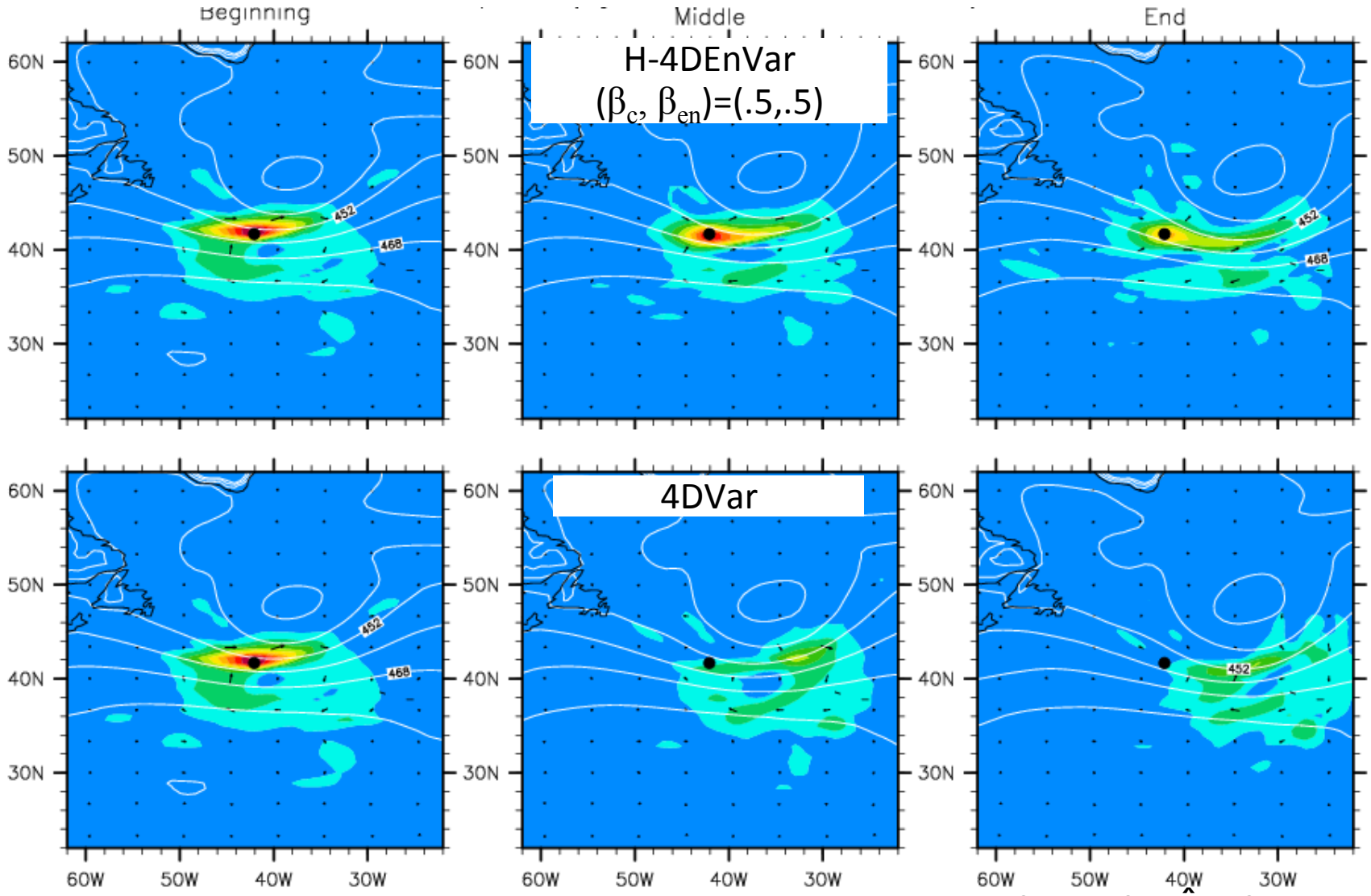


Hybrid

B_e=1/2
β_c=1/2

Single 850mb Tv observation (1K O-F, 1K error) – Courtesy of D. Kleist

Consideration: Issue with Static $\mathbf{B}_c$



Courtesy: A. Lorenc et al. 2016, MWR

$$\Delta\mathbf{x}_k^a = \Delta\mathbf{x}_c^a + \hat{\mathbf{X}}_k \alpha^a$$

Summary

	Advantages	**Challenges**
3DVar (OI) + FGAT	Full rank $\mathbf{B}_c$ Synchronized $\mathbf{d}_k$	Static $\mathbf{B}_c$ (no dynamic propagation) No **A** update in general
4DVar	Dynamic **B** propagation	No **A** update in general Expensive & Complex
EKF	Dynamic $\mathbf{B}_{EKF}$ and $\mathbf{A}_{EKF}$ Explicit evaluation of $\mathbf{A}_{EKF}$	Expensive & Complex
EnKF	Dynamic $\mathbf{B}_e$ and $\mathbf{A}_e$ Explicit evaluation of $\mathbf{A}_e$	Rank deficiency on $\mathbf{B}_e$ and $\mathbf{A}_e$ **y**-space localization on $\mathbf{B}_e$
EnVar	Dynamic $\mathbf{B}_e$ and $\mathbf{A}_e$ by EnKF **x**-space localization on $\mathbf{B}_e$	Parallel run of EnKF is required
Hybrid	$\begin{cases} \Delta\mathbf{x}_k = \lambda_c \Delta\mathbf{x}_c + \lambda_e \Delta\mathbf{x}_{e,k} \\ \mathbf{B}_k = \gamma_c \mathbf{B}_c + \gamma_e \mathbf{B}_{e,k} \end{cases}$ [equivalence by $\lambda^2=\gamma$]	$\Delta\mathbf{x}_c$ is 3D

Concluding Remarks

- NWP is extremely challenging from a wide range of reasons.
- DA methods attack NWP problem through the attempt to optimally estimate the state and uncertainty.
- Current operational GSI uses Hybrid 4DEnVar, a method that combines and integrates the preceding methods.
- Operational GSI is really a complex DA system with much more details than presented in this lecture. These details really matter as you will hear this week.
- Enjoy the Tutorial!