Accounting for Model Error in 4D-Var

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Outline

Data Assimilation

- The goal of data assimilation is to estimate the state of a system given all available information:
  - Observations of the system,
  - Theoretical knowledge of the system (model).
- Through cycling of the data assimilation system we introduce an auxiliary source of information: the background (*a priori* knowledge given the model and past observations).
- Uncertainty in the two main sources of information (observation and model) should be accounted for. What is the best estimate of the state of the system knowing these errors are present?
- Model error is difficult to take into account: in existing operational systems, it is hidden in the background error.

Model Error in Data Assimilation

For our purpose, the definition of model error is:

$$\eta_i = \mathbf{x}_i^t - \mathcal{M}(\mathbf{x}_{i-1}^t)$$

- This definition does not rely on any assumption.
- In real systems, the true state is unknown and model error cannot be computed.

- Model error has bias and random components.
- Model errors that vary on a timescale longer than an assimilation window will be called **systematic error**.
- Model errors that vary on a timescale shorter than an assimilation window will be called **random error**.

Outline

4D Variational Data Assimilation

Based on a maximum likelihood formulation, 4D-Var comprises the minimisation of:

$$\begin{aligned} J(\mathbf{x}) &= \frac{1}{2}[\mathcal{H}(\mathbf{x})-\mathbf{y}]^T\mathbf{R}^{-1}[\mathcal{H}(\mathbf{x})-\mathbf{y}] \\ &+ \frac{1}{2}(\mathbf{x}_0-\mathbf{x}_b)^T\mathbf{B}^{-1}(\mathbf{x}_0-\mathbf{x}_b)+\frac{1}{2}\mathcal{F}(\mathbf{x})^T\mathbf{C}^{-1}\mathcal{F}(\mathbf{x}) \end{aligned}$$

- $\mathbf{x}$ is the 4D state of the atmosphere over the assimilation window.
- $\mathcal{H}$ is a 4D observation operator, accounting for the time dimension.
- $\mathcal{F}$ represents the remaining theoretical knowledge after background information has been accounted for (balance, DFI...).
- Control variable reduces to $\mathbf{x}_0$ using the *perfect model* assumption:

$$\mathbf{x}_i = \mathcal{M}_i(\mathbf{x}_{i-1}).$$

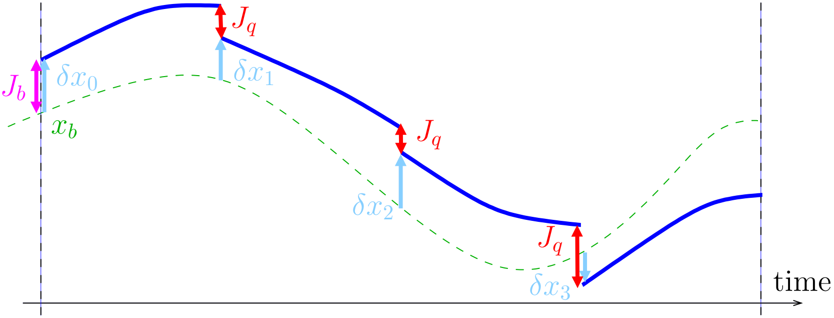
Weak Constraint 4D-Var

- For Gaussian temporally-uncorrelated model error, the weak constraint 4D-Var cost function is:

$$
\begin{aligned}
J(\mathbf{x}) &= \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_b) \\
&+ \frac{1}{2}\sum_{i=0}^{n}[\mathcal{H}_i(\mathbf{x}_i) - \mathbf{y}_i]^T \mathbf{R}_i^{-1}[\mathcal{H}_i(\mathbf{x}_i) - \mathbf{y}_i] \\
&+ \frac{1}{2}\sum_{i=1}^{n}[\mathbf{x}_i - \mathcal{M}_i(\mathbf{x}_{i-1})]^T \mathbf{Q}_i^{-1}[\mathbf{x}_i - \mathcal{M}_i(\mathbf{x}_{i-1})] + J_c
\end{aligned}
$$

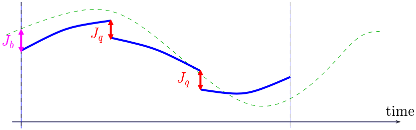
- Do not reduce the control variable using the model and retain the 4D nature of the control variable.
- Account for the fact that the model contains some information but is not exact by adding a model error term to the cost function.
- If model error is correlated in time, the model error term contains additional cross-correlation blocks.

4D State Control Variable



- Model integrations within each time-step (or sub-window) are independent:
  - Information is not propagated across sub-windows by TL/AD models,
  - Natural parallel implementation.
- Similar to having several 4D-Var cycles coupled and optimised together.

Weak Constraint 4D-Var: Sliding Window



(1) Weak constraint 4D-Var

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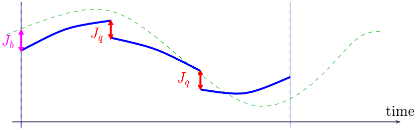

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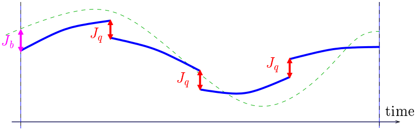
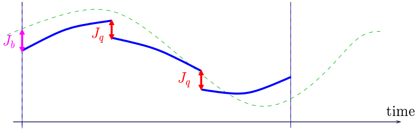


(2) Extended window

Weak Constraint 4D-Var: Sliding Window



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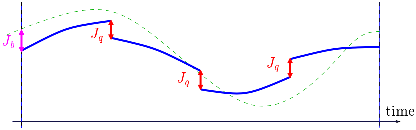
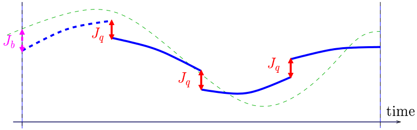
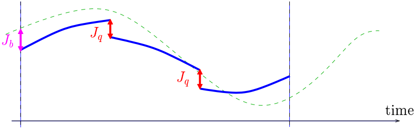


(2) Extended window



(3) Initial term has converged

Weak Constraint 4D-Var: Sliding Window



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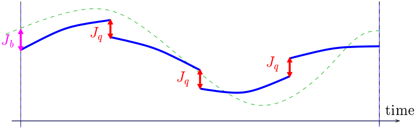

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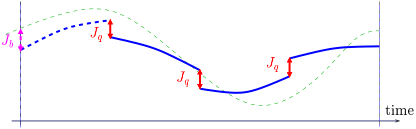

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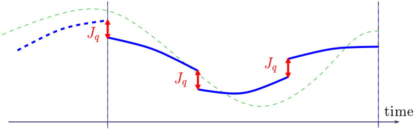
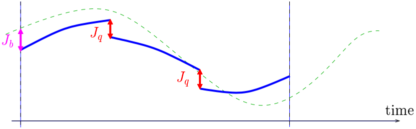


(4) Assimilation window is moved forward

Weak Constraint 4D-Var: Sliding Window



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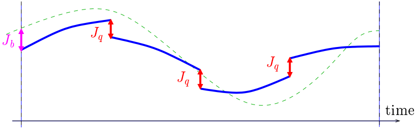

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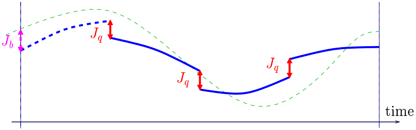

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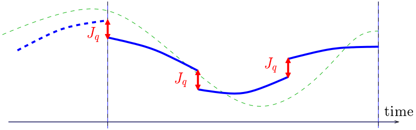


(4) Assimilation window is moved forward

- This implementation is an approximation of weak contraint 4D-Var with an assimilation window that extends indefinitely in the past...
- ...which is equivalent to a (full rank) Kalman smoother that has been running indefinitely.

Outline

4D-Var with Model Error Forcing

- In practice, weak constraint 4D-Var is still difficult to implement.
- We make a change of variable:

$$
\begin{aligned}
J(\mathbf{x}_0, \eta) &= \frac{1}{2}\sum_{i=0}^{n}[\mathcal{H}(\mathbf{x}_i) - \mathbf{y}_i]^T \mathbf{R}_i^{-1}[\mathcal{H}(\mathbf{x}_i) - \mathbf{y}_i] \\
&+ \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_b) + \frac{1}{2}\sum_{i=1}^{n}\eta_i^T \mathbf{Q}_i^{-1}\eta_i
\end{aligned}
$$

$$
\text{with } \mathbf{x}_i = \mathcal{M}_i(\mathbf{x}_{i-1}) + \eta_i
$$

- η_i represents model error in a time step,
- η_i has the same dimension as a 3D state.

4D-Var with Constant Model Error Forcing

- We also make approximations:

$$
\begin{aligned}
J(\mathbf{x}_0, \eta) &= \frac{1}{2}\sum_{i=0}^{n}[\mathcal{H}(\mathbf{x}_i) - \mathbf{y}_i]^T \mathbf{R}_i^{-1}[\mathcal{H}(\mathbf{x}_i) - \mathbf{y}_i] \\
&+ \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_b) + \frac{1}{2}\eta^T \mathbf{Q}^{-1}\eta
\end{aligned}
$$

$$
\text{with } \mathbf{x}_i = \mathcal{M}_i(\mathbf{x}_{i-1}) + \eta
$$

- η represents model error in a time step,
- η has the same dimension as a 3D state.

Weak Constraints 4D-Var with Cycling Term

- For random model error, the 4D-Var cost function is:

$$
\begin{aligned}
J(\mathbf{x}_0,\eta) &= \frac{1}{2}\sum_{i=0}^{n}[\mathcal{H}(\mathbf{x}_i)-\mathbf{y}_i]^T\mathbf{R}_i^{-1}[\mathcal{H}(\mathbf{x}_i)-\mathbf{y}_i] \\
&+ \frac{1}{2}(\mathbf{x}_0-\mathbf{x}_b)^T\mathbf{B}^{-1}(\mathbf{x}_0-\mathbf{x}_b)+\frac{1}{2}\eta^T\mathbf{Q}^{-1}\eta
\end{aligned}
$$

- For systematic model error, we use:

$$
\begin{aligned}
J(\mathbf{x}_0,\eta) &= \frac{1}{2}\sum_{i=0}^{n}[\mathcal{H}(\mathbf{x}_i)-\mathbf{y}_i]^T\mathbf{R}_i^{-1}[\mathcal{H}(\mathbf{x}_i)-\mathbf{y}_i] \\
&+ \frac{1}{2}(\mathbf{x}_0-\mathbf{x}_b)^T\mathbf{B}^{-1}(\mathbf{x}_0-\mathbf{x}_b)+\frac{1}{2}(\eta-\eta_b)^T\mathbf{Q}^{-1}(\eta-\eta_b)
\end{aligned}
$$

- Test case: can we address the model bias in the stratosphere?

Outline

Model Error Covariance Matrix

- An easy choice is $\mathbf{Q} = \alpha\mathbf{B}$.
- If $\mathbf{Q}$ and $\mathbf{B}$ are proportional, $\delta\mathbf{x}_0$ and η are constrained in the same directions, may be with different relative amplitudes.
- They both predominantly retrieve the same information.

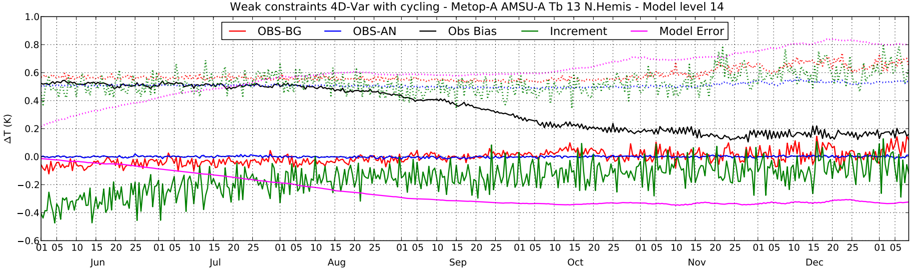
- $\mathbf{B}$ can be estimated from an ensemble of 4D-Var assimilations.
- Considering the forecasts run from the 4D-Var members:
  - At a given step, each model state is supposed to represent the same *true* atmospheric state,
  - The tendencies from each of these model states should represent possible evolutions of the atmosphere from that same *true* atmospheric state,
  - The differences between these tendencies can be interpreted as possible uncertainties in the model or realisations of *model error*.
- $\mathbf{Q}$ can be estimated by applying the statistical model used for $\mathbf{B}$ to tendencies instead of analysis increments.
- $\mathbf{Q}$ has narrower correlations and smaller amplitudes than $\mathbf{B}$.

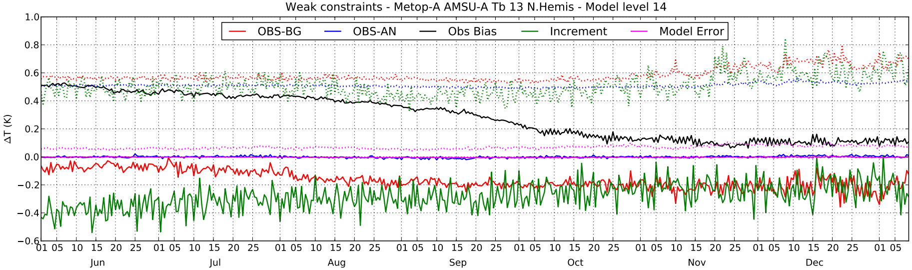
Model Error Covariance Matrix

- Currently, tendency differences between integrations of the members of an ensemble are used as a proxy for samples of model error.
- Statistics of model drift (currently being tested).
- Use results from stochastic representation of uncertainties in EPS.
- It is possible to derive an estimate of $\mathbf{HQH}^T$ from cross-covariances between observation departures produced from pairs of analyses with different length windows (R. Todling).
- Is it possible to extract model error information using the relation $\mathbf{P}^f = \mathbf{MP}^a\mathbf{M}^T + \mathbf{Q}$?
- Model error is correlated in time: $\mathbf{Q}$ should account for time correlations.
- How can we account for flow dependence?

Outline

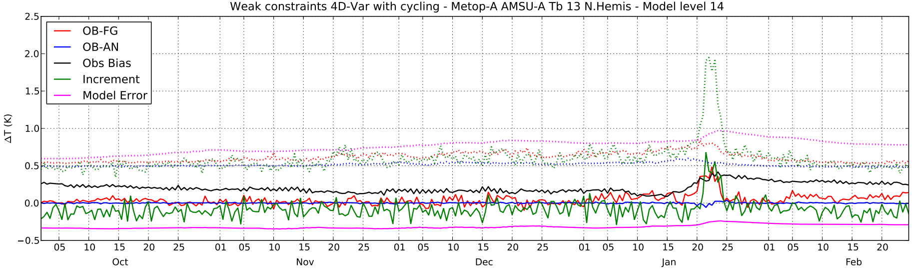
Weak Constraints 4D-Var with Cycling Term

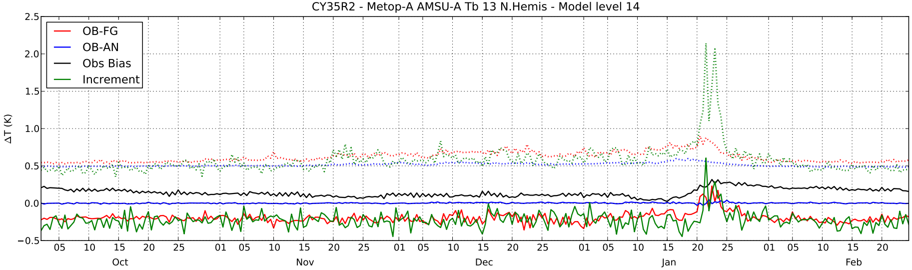




The short term forecast is improved with the model error cycling.
Weak constraints 4D-Var can correct for seasonal bias (partially).

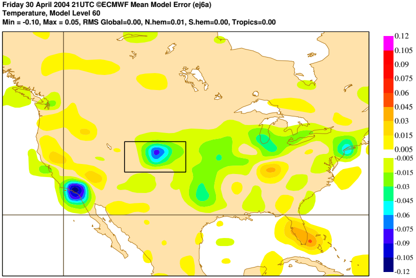
Observation Error or Model Error?

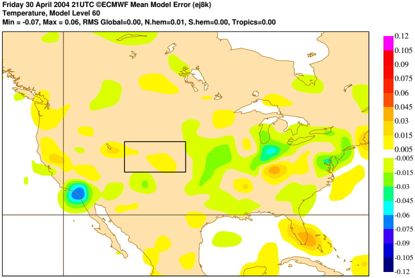




Observation error bias correction can compensate for model error.

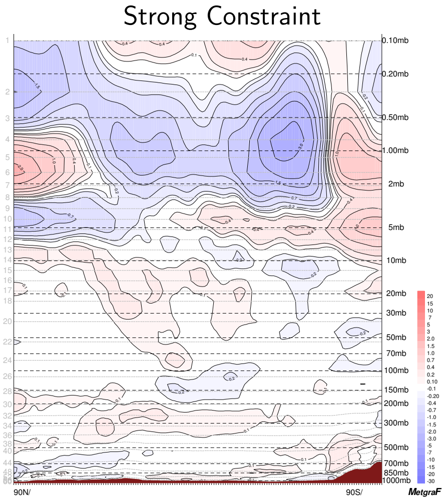
Model Error or Observation Error?





- The only significant source of observations in the box is aircraft data (Denver airport).
- Removing aircraft data in the box eliminates the spurious forcing.

Is it model error?



The work on model error has helped identify other sources of error in the system (balance term).

Outline

Status and Developments in Weak Constraints 4D-Var

- We only had a glimpse at the systematic component of model error.
- In the current formulation of weak constraints 4D-Var (model error forcing):
  - Background term to address systematic error,
  - 24h assimilation window,
  - Interactions with variational observation bias correction,
  - Extend model error to the troposphere and to other variables (humidity).
- Weak constraint 4D-Var with a 4D state control variable:
  - Four dimensional problem with a coupling term between sub-windows and can be interpreted as a smoother over assimilation cycles.
  - Can we extend the incremental formulation?
  - 4D-Var scales well up to 1,000s of processors, it has to scale to 10,000s of processors in the future. Can we combine the benefits of treating sub-windows in parallel with efficient preconditioning?

Weak Constraints 4D-Var

- Weak Constraints 4D-Var allows the perfect model assumption to be removed and the use of longer assimilation windows.
  - How much benefit can we expect from long window 4D-Var?
- Weak Constraints 4D-Var requires knowledge of the statistical properties of model error (covariance matrix).
  - The forecast model is such an important component of the forecasting system. It is surprising how little we know about its error characteristics.
  - The statistical description of model error is one of the main current challenges in data assimilation (and other applications).
- Data assimilation is where the model is systematically confronted with reality (through the observations).
- In particular, weak constraints 4D-Var provides feedback for model error representations.
  - All sources of model error are diagnosed: convection but also other physical parametrisations, interactions between them, numerical schemes, bugs...
  - Other sources of error can be entangled with model error in a real system: observations, data assimilation system...