Mathematics of Data Assimilation-
Complex Systems in Numerical Weather Prediction

Melina Freitag

Department of Mathematical Sciences
University of Bath

BICS meeting 'The Maths of Complex Systems'
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Outline

What is Data Assimilation?

Loose definition

Estimation and prediction (analysis) of an unknown, true state by combining observations and system dynamics (model output).

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- Navigation (collect observations and produce velocity corrections)
- Geophysics (values of some model parameter must be obtained from the observed data)
- Medical imaging

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- Medical imaging
- Numerical weather prediction

The atmosphere

- The atmosphere is a complex system!
- Mathematical modelling, observations and mathematical Data Assimilation help to understand this complex multi-scale system

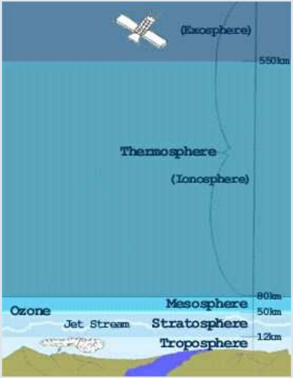

Figure: http://www.usoe.k12.ut.us

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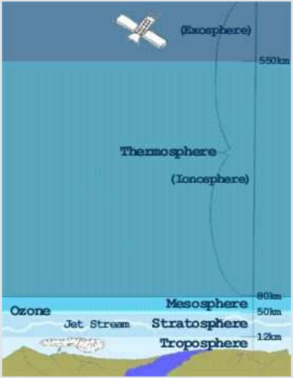

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⇒"Aspects of Ionosphere modelling" Nathan (see talk later this afternoon)

The weather (NWP)

Data Assimilation in NWP

Estimate the state of the atmosphere $\mathbf{x}_i$ at a certain time/certain times i.

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- Satellites
- Ships and buoys
- Surface stations
- Airplanes

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Assimilation algorithms

- used to find an (approximate) state of the atmosphere $\mathbf{x}_i$ at times i (usually $i = 0$)
- using this/these states a forecast for future states of the atmosphere can be obtained

Outline

Schematics of DA

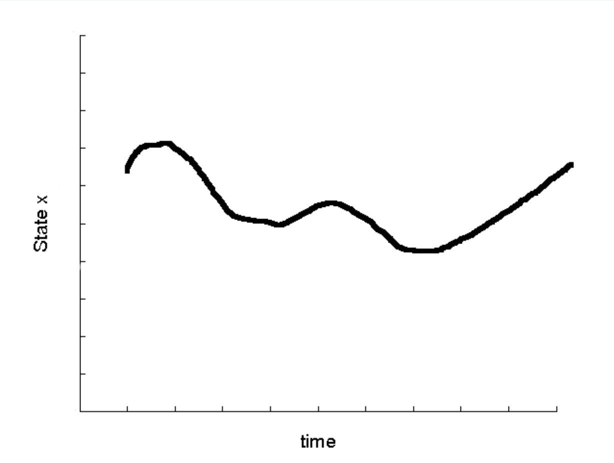

Figure: Background state $\mathbf{x}^B$

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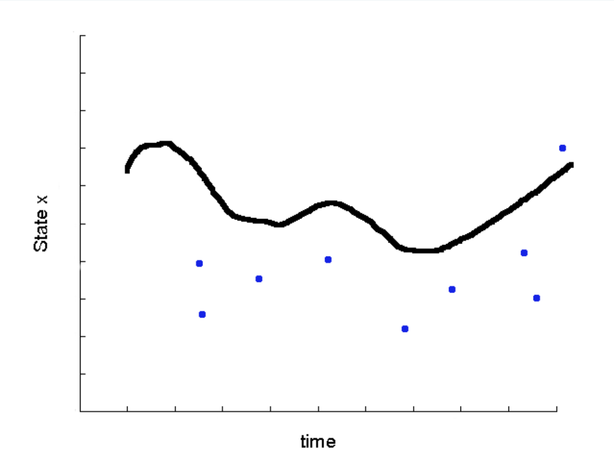

Figure: Observations $\mathbf{y}$

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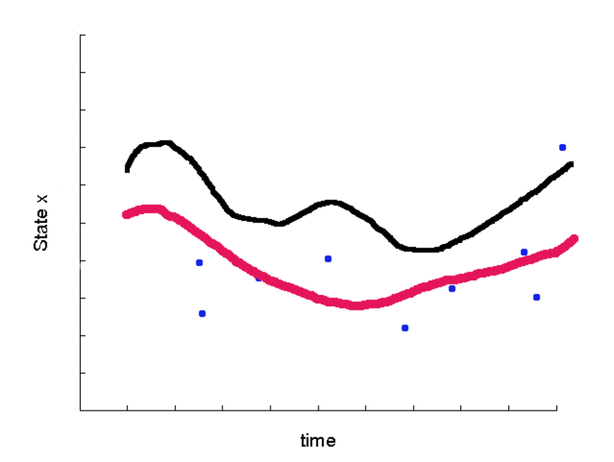

Figure: Analysis $\mathbf{x}^A$ (consistent with observations and model dynamics)

Data Assimilation in NWP

Underdeterminacy

- Size of the state vector $\mathbf{x}$: $432 \times 320 \times 50 \times 7 = \mathcal{O}(10^7)$
- Number of observations (size of $\mathbf{y}$): $\mathcal{O}(10^5 - 10^6)$
- Operator H (nonlinear!) maps from state space into observations space: $\mathbf{y} = H(\mathbf{x})$

Notation

- $\mathbf{x}^{\text{Truth}}$: True state
- $\mathbf{x}^{B}$: Background state (taken from previous forecast)
- $\mathbf{x}^{A}$: Analysis (estimation of the true state after the DA)

Outline

Data Assimilation in NWP

We are looking for the state of the atmosphere $\mathbf{x}_i$ at a certain time/certain times i.

Apriori information $\mathbf{x}^B$

- background state (usual previous forecast) has errors!

Models

- a model how the atmosphere evolves in time (imperfect)

$$\mathbf{x}_{i+1} = M(\mathbf{x}_i) + \text{error}$$

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Error variables

Modelling the errors

- background error $\varepsilon^B = \mathbf{x}^B - \mathbf{x}^{\text{Truth}}$ of average $\overline{\varepsilon}^B$ and covariance

$$\mathbf{B} = \overline{(\varepsilon^B - \overline{\varepsilon}^B)(\varepsilon^B - \overline{\varepsilon}^B)^T}$$

- observation error $\varepsilon^O = \mathbf{y} - H(\mathbf{x}^{\text{Truth}})$ of average $\overline{\varepsilon}^O$ and covariance

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Assumptions

- Linearised observation operator: $H(\mathbf{x}) - H(\mathbf{x}^B) = \mathbf{H}(\mathbf{x} - \mathbf{x}^B)$
- Nontrivial errors: $\mathbf{B}$, $\mathbf{R}$ are positive definite
- Unbiased errors: $\overline{\mathbf{x}^B - \mathbf{x}^{\text{Truth}}} = \overline{\mathbf{y} - H(\mathbf{x}^{\text{Truth}})} = 0$
- Uncorrelated errors: $\overline{(\mathbf{x}^B - \mathbf{x}^{\text{Truth}})(\mathbf{y} - H(\mathbf{x}^{\text{Truth}}))^T} = 0$

Optimal least-squares estimater

Cost function minimisation (3D-Var)

Solution of the variational optimisation problem $\mathbf{x}^A = \arg\min J(\mathbf{x})$ where

$$
\begin{aligned}
J(\mathbf{x}) &= (\mathbf{x}-\mathbf{x}^B)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}^B) + (\mathbf{y}-H(\mathbf{x}))^T\mathbf{R}^{-1}(\mathbf{y}-H(\mathbf{x})) \\
&= J_B(\mathbf{x}) + J_O(\mathbf{x})
\end{aligned}
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- $\mathbf{B}^{-1}$ expensive!

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Interpolation equations

$$\mathbf{x}^A = \mathbf{x}^B + \mathbf{K}(\mathbf{y} - H(\mathbf{x}^B)), \quad \text{where}$$
$$\mathbf{K} = \mathbf{B}\mathbf{H}^T(\mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{R})^{-1} \quad \mathbf{K}\ldots\text{gain matrix}$$

- expensive!

Four-dimensional variational assimilation (4D-Var)

Minimise the cost function

$$J(\mathbf{x}_0) = (\mathbf{x}_0 - \mathbf{x}^B)^T \mathbf{B}^{-1} (\mathbf{x}_0 - \mathbf{x}^B) + \sum_{i=0}^{n} (\mathbf{y}_i - H_i(\mathbf{x}_i))^T \mathbf{R}_i^{-1} (\mathbf{y}_i - H_i(\mathbf{x}_i))$$

subject to model dynamics $\mathbf{x}_i = M_{0\rightarrow i}\mathbf{x}_0$

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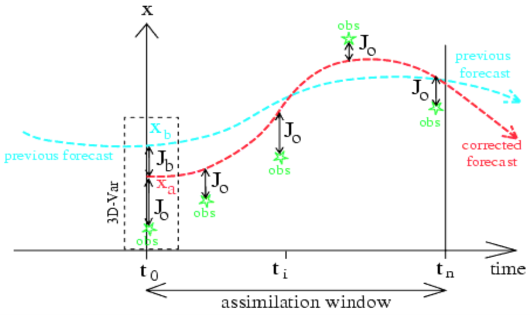
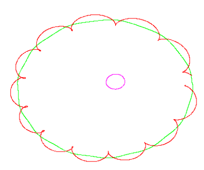


Figure: Copyright:ECMWF

Example - Three-Body Problem

Motion of three bodies in a plane, two position ($\mathbf{q}$) and two momentum ($\mathbf{p}$) coordinates for each body $\alpha = 1, 2, 3$



Equations of motion

$$
\begin{aligned}
H(\mathbf{q}, \mathbf{p}) &= \frac{1}{2} \sum_{\alpha} \frac{|\mathbf{p}_\alpha|^2}{m_\alpha} - \sum \sum_{\alpha < \beta} \frac{m_\alpha m_\beta}{|\mathbf{q}_\alpha - \mathbf{q}_\beta|} \\
\frac{d\mathbf{q}_\alpha}{dt} &= \frac{\partial H}{\partial \mathbf{p}_\alpha} \\
\frac{d\mathbf{p}_\alpha}{dt} &= -\frac{\partial H}{\partial \mathbf{q}_\alpha}
\end{aligned}
$$

Example - Three-Body problem

- solver: partitioned Runge-Kutta scheme with time step $h = 0.001$
- observations are taken as noise from the truth trajectory
- background is given from a perturbed initial condition
- assimilation window is taken 300 time steps
- minimisation of cost function J using a Gauss-Newton method

$$\nabla J(\mathbf{x}_0) = 0$$

$$\nabla\nabla J(\mathbf{x}_0^j)\Delta\mathbf{x}_0^j = -\nabla J(\mathbf{x}_0^j), \quad \mathbf{x}_0^{j+1} = \mathbf{x}_0^j + \Delta\mathbf{x}_0^j$$

- subsequent forecast is take 5000 time steps

Example- Three-Body problem

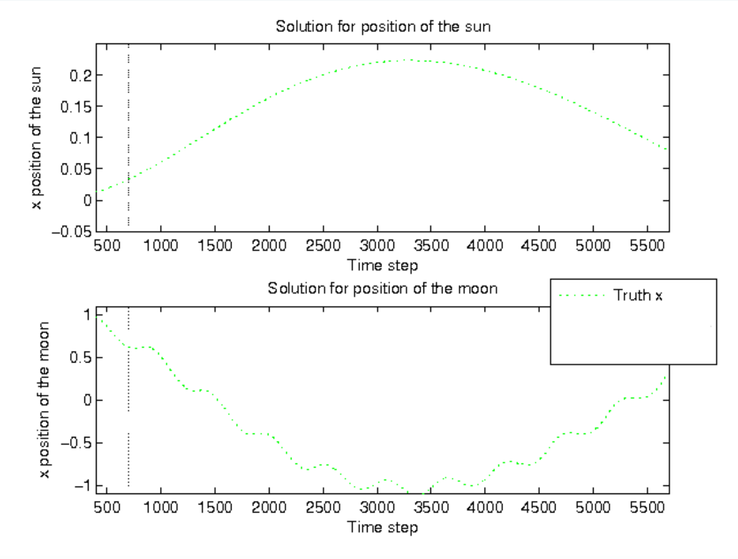


Figure: Truth trajectory

Example- Three-Body problem

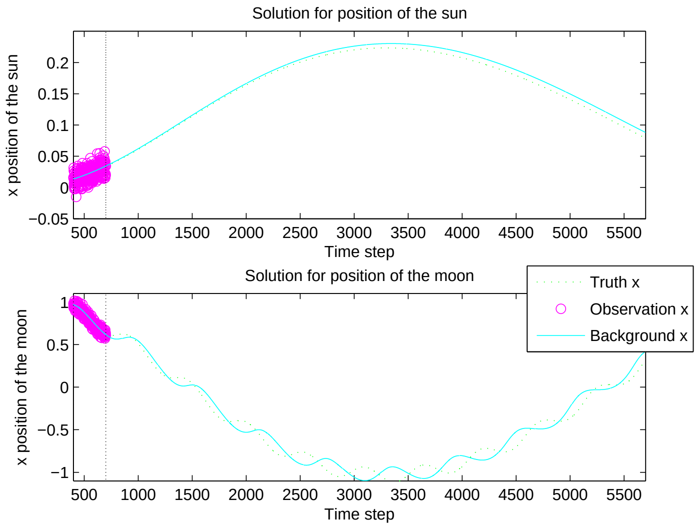


Figure: Truth trajectory with observations and background

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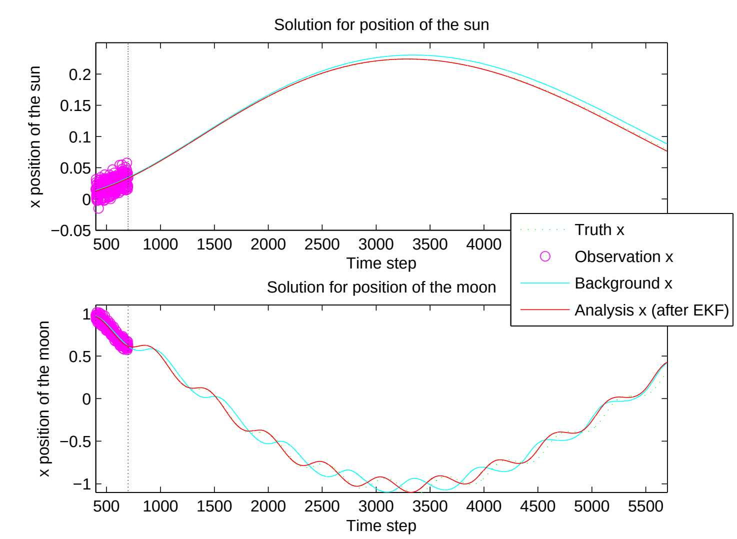

Figure: Analysis

Example- Three-Body problem

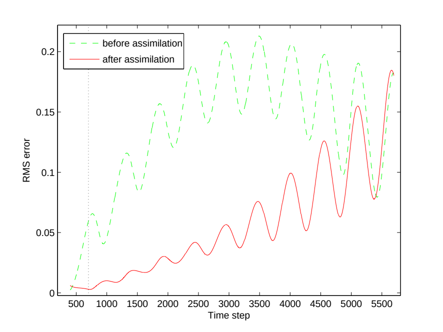

Figure: RMS error

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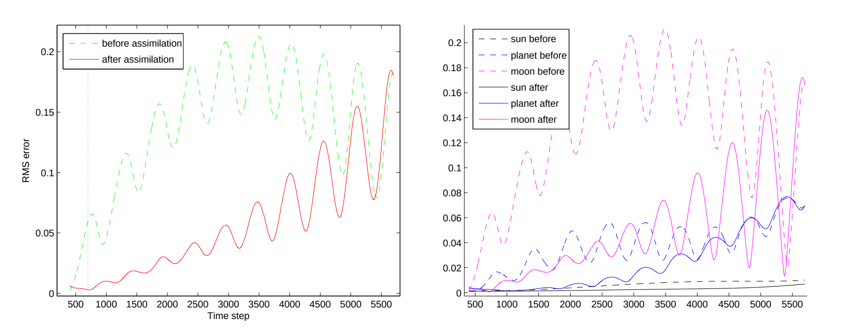

Figure: RMS error

The Kalman Filter Algorithm

- Sequential data assimilation
- covariance matrices are updated at each step $\mathbf{P}^F$, $\mathbf{P}^A$

State and error covariance forecast

$$
\begin{aligned}
\text{State forecast} \quad \mathbf{x}_{i+1}^F &= \mathbf{M}_{i+1,i}\mathbf{x}_i^A \\
\text{Error covariance forecast} \quad \mathbf{P}_{i+1}^F &= \mathbf{M}_{i+1,i}\mathbf{P}_i^A\mathbf{M}_{i+1,i}^T + \mathbf{Q}_i
\end{aligned}
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State and error covariance analysis

$$\begin{aligned} \text{Kalman gain} \quad \mathbf{K}_i &= \mathbf{P}_i^F\mathbf{H}_i^T(\mathbf{H}_i\mathbf{P}_i^F\mathbf{H}_i^T + \mathbf{R}_i)^{-1} \\ \text{State analysis} \quad \mathbf{x}_i^A &= \mathbf{x}_i^F + \mathbf{K}_i(\mathbf{y}_i - \mathbf{H}_i\mathbf{x}_i^F) \\ \text{Error covariance of analysis} \quad \mathbf{P}_i^A &= (\mathbf{I} - \mathbf{K}_i\mathbf{H}_i)\mathbf{P}_i^F \end{aligned}$$

Example - Three-Body Problem

- same setup as before
- Compare using $\mathbf{B} = \mathbf{I}$ with using a flow-dependent matrix $\mathbf{B}$ which was generated by a Kalman Filter before the assimilation starts (see G. Inverarity (2007))

Example - Three-Body Problem

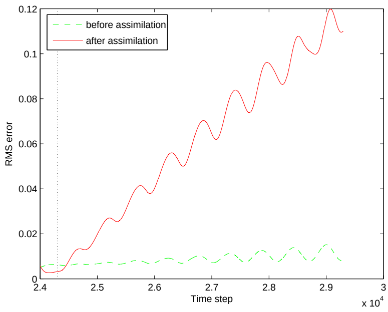

Figure: 4D-Var with $\mathbf{B} = \mathbf{I}$

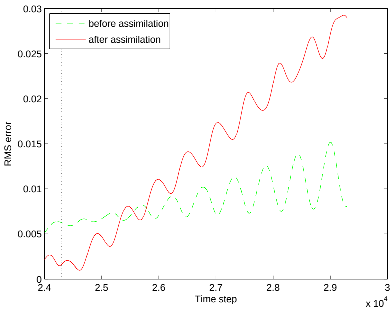

Figure: 4D-Var with $\mathbf{B} = \mathbf{P}^A$

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  - $\mathbf{B}$ needs to be modeled and diagonalised since $\mathbf{B}^{-1}$ too expensive to compute (”control variable transform”)

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  - errors non-Gaussian, data have biases
  - forward model operator M is not exact and also non-linear and system dynamics are chaotic
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- model error not included

Outline

Model error and perturbation error

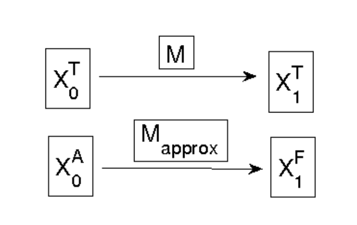
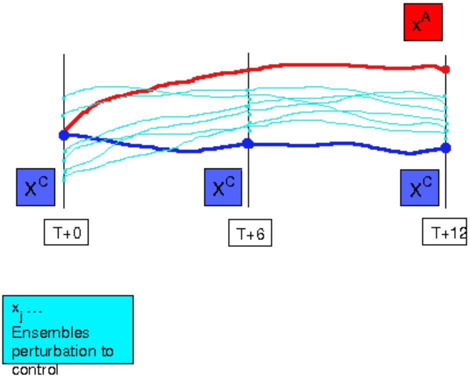


Figure: One assimilation window (6 hours)

$$
\begin{aligned}
\mathbf{x}_1^F - \mathbf{x}_1^{\text{Truth}} &= M_{\text{appr}}(\mathbf{x}_0^A) - M(\mathbf{x}_0^{\text{Truth}}) \\
&= \underbrace{M_{\text{appr}}(\mathbf{x}_0^A) - M_{\text{appr}}(\mathbf{x}_0^{\text{Truth}})}_{\text{Perturbation error}} + \underbrace{M_{\text{appr}}(\mathbf{x}_0^{\text{Truth}}) - M(\mathbf{x}_0^{\text{Truth}})}_{\text{Model error}}
\end{aligned}
$$

Model error and perturbation error



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Model error

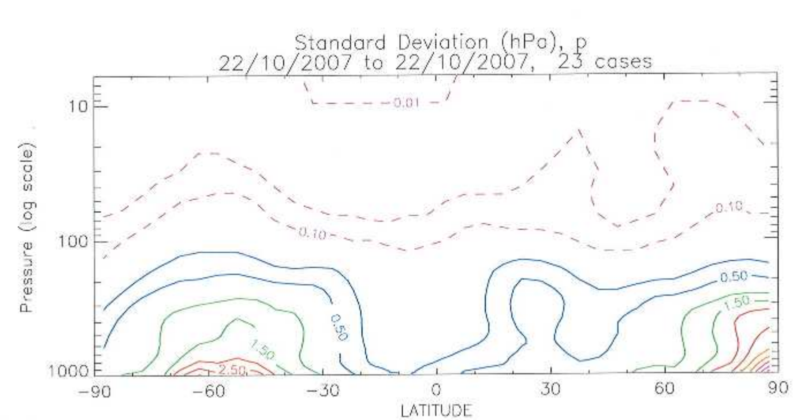

Figure: Perturbation error after 7 hours (Copyright: MetOffice)

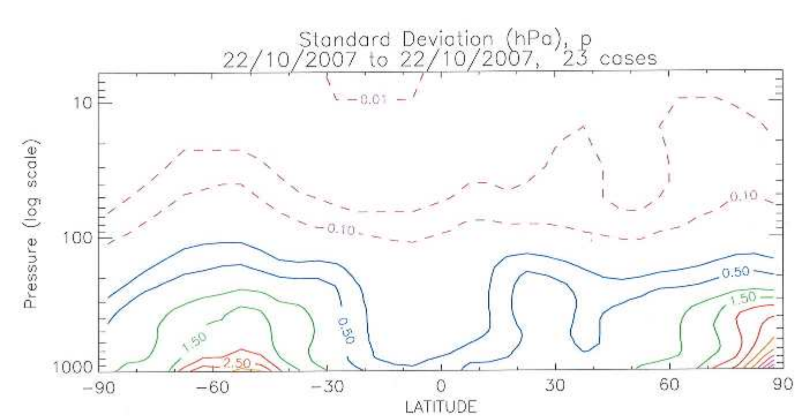

Figure: Perturbation error after 12 hours (Copyright: MetOffice)

Model error

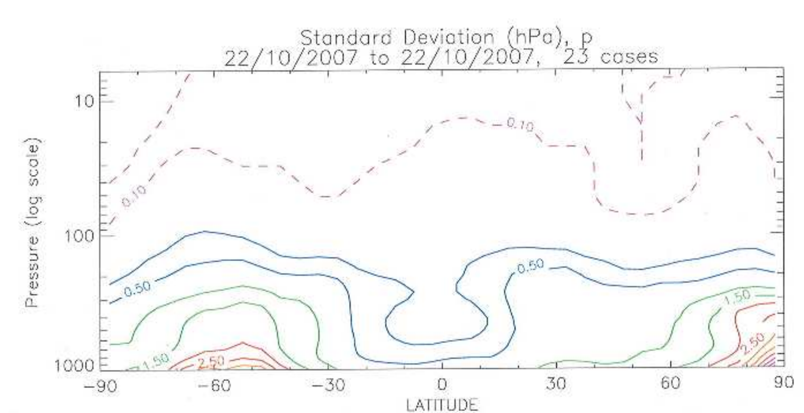

Figure: Model error after 12 hours (Copyright: MetOffice)

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- include several time scales (to model the atmosphere)

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- Theme D: Numerical methods for multi-scale modelling