Variance loss in ensemble-based error covariance evolution with advection transport

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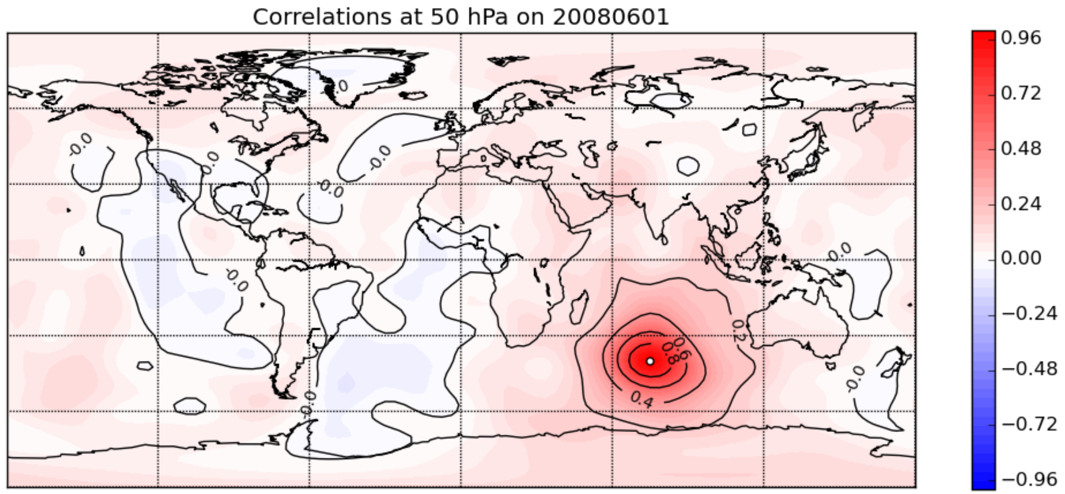
5th Annual International Symposium on Data Assimilation
Reading, UK, July 18, 2016

Motivation

Initial error correlation with *Nens* =500



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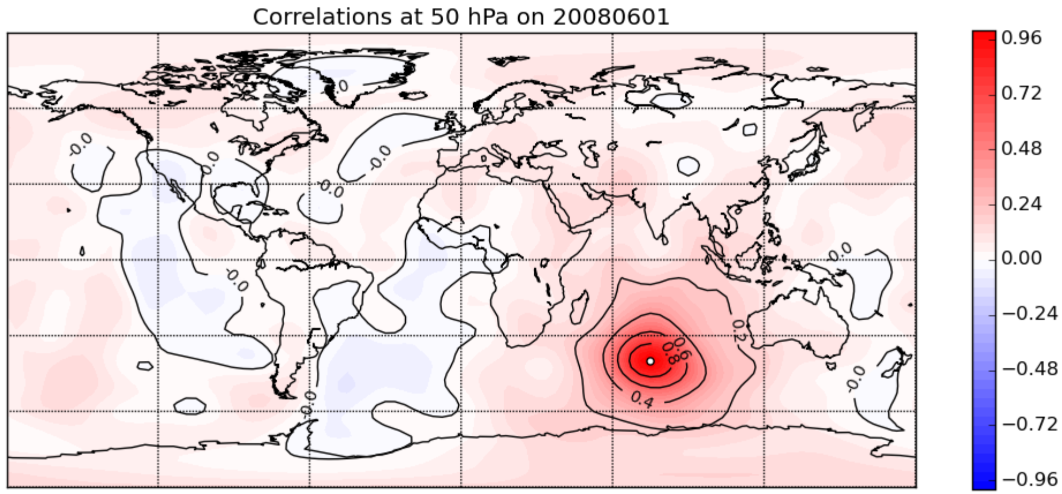
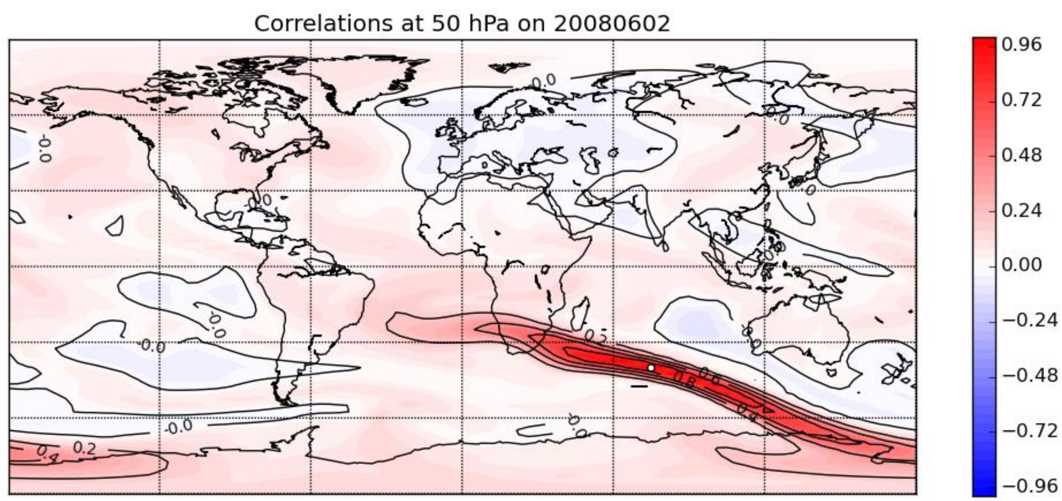


After one day



Motivation

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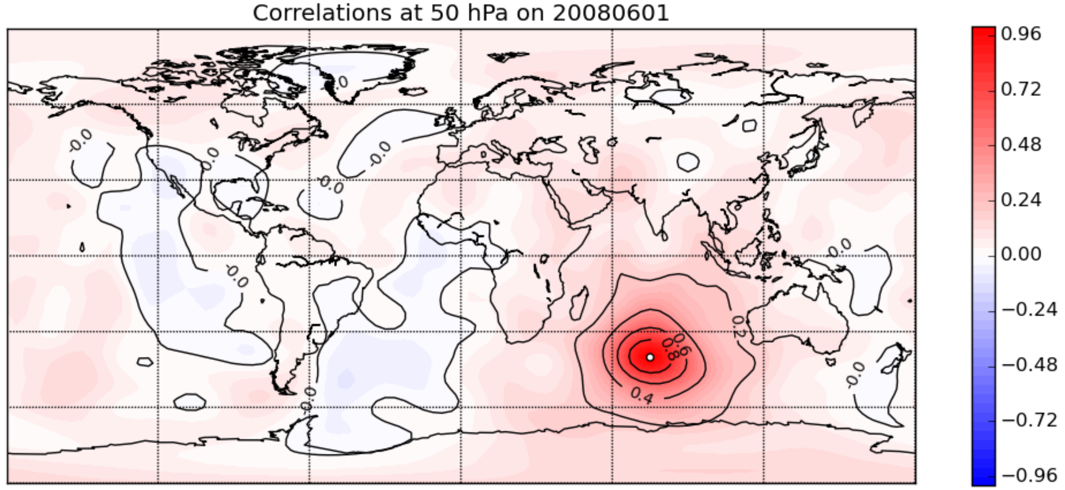

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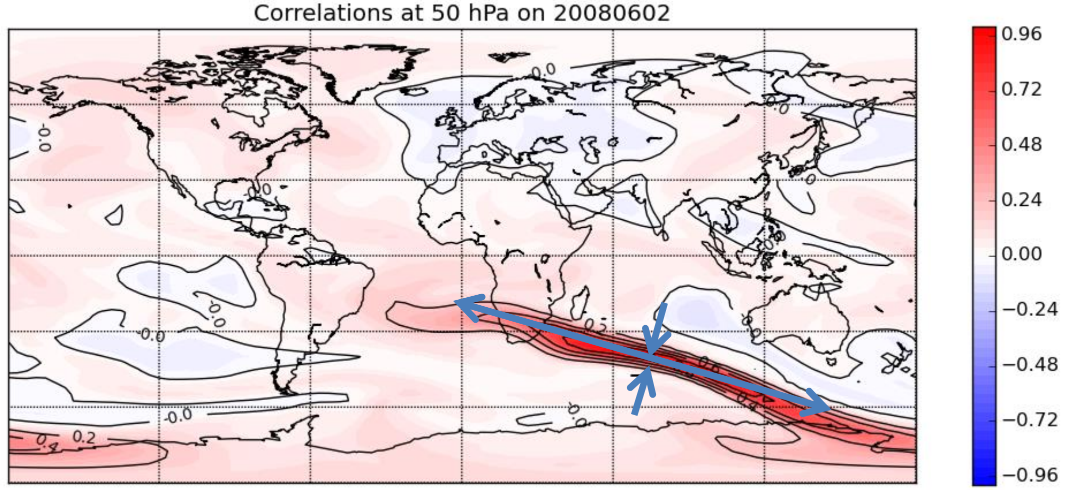
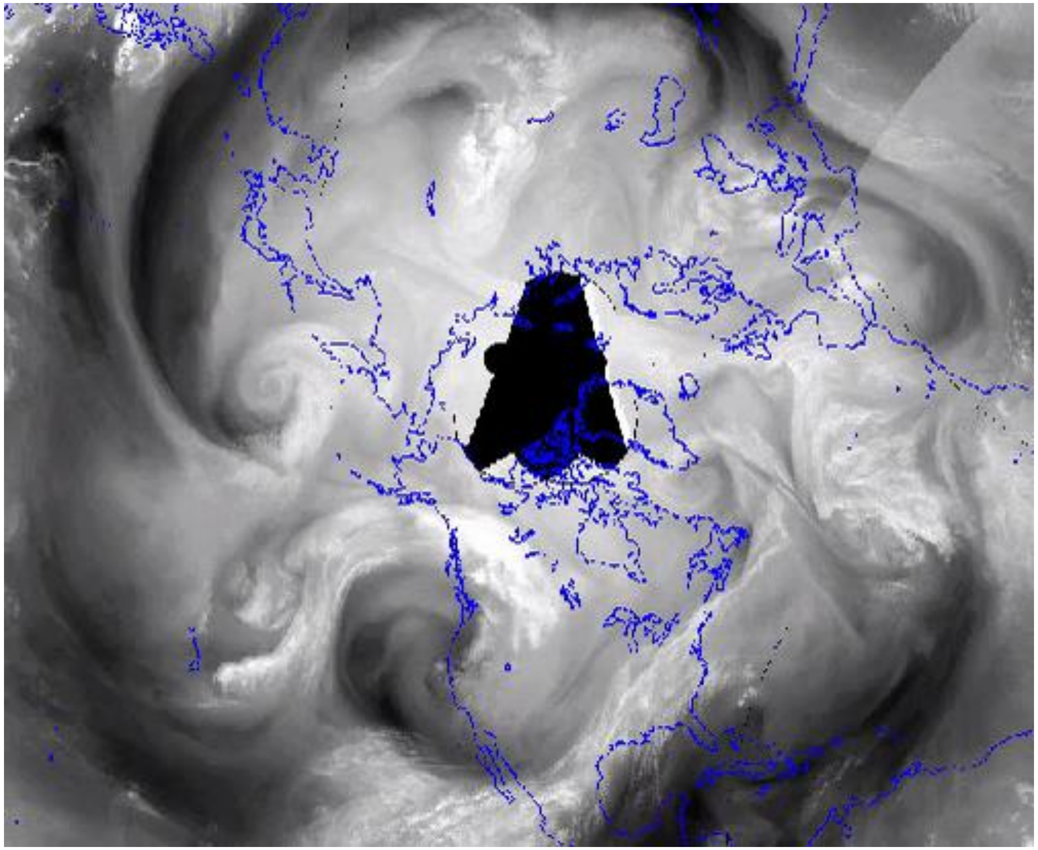


- Shear strain by winds introduces a downscale (and also upscale) of the tracer variance
- Large body of literature that discusses this in Eulerian and Lagrangian models, in Turbulence theory, and it is seen in observations (e.g. laminea in ozone profiles, streamers in the water vapor channel)



- Here we examine the implications this have on error covariance propagation
- And we recall that there is **no observation update** in this study

Transport of mass

$$\frac{\partial q}{\partial t} + \mathbf{V} \cdot \nabla q = 0$$

covariance matrix – discrete space

discrete model time stepping – state vector $\mathbf{q}$ for each ensemble member i

$$\mathbf{q}_i(t + \Delta t) = M \ \mathbf{q}_i(t) \qquad i = 1, \ldots, N_{ens}$$

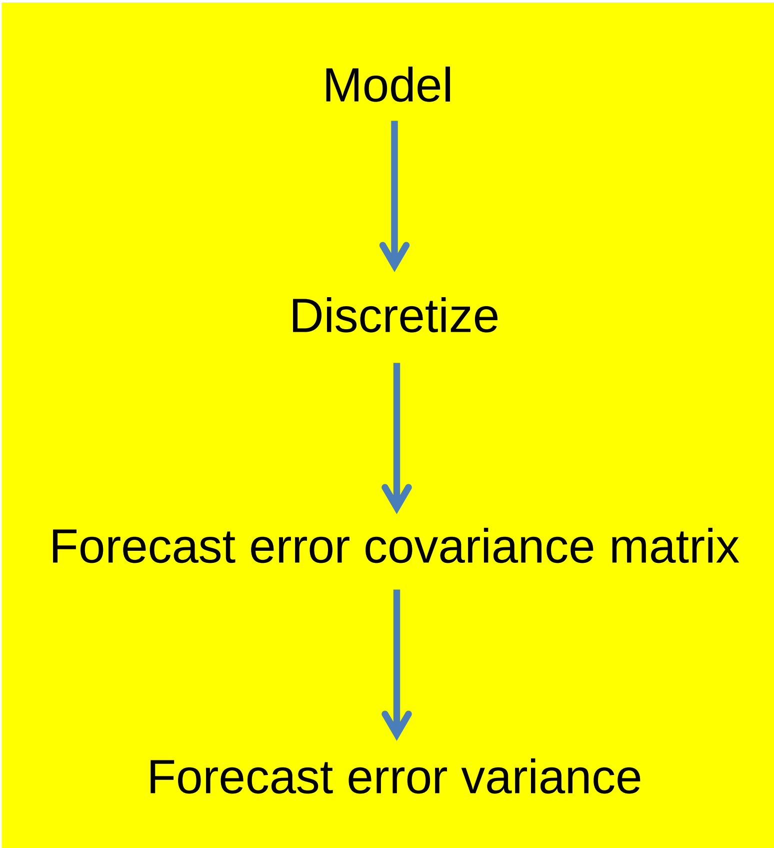
ensemble matrix

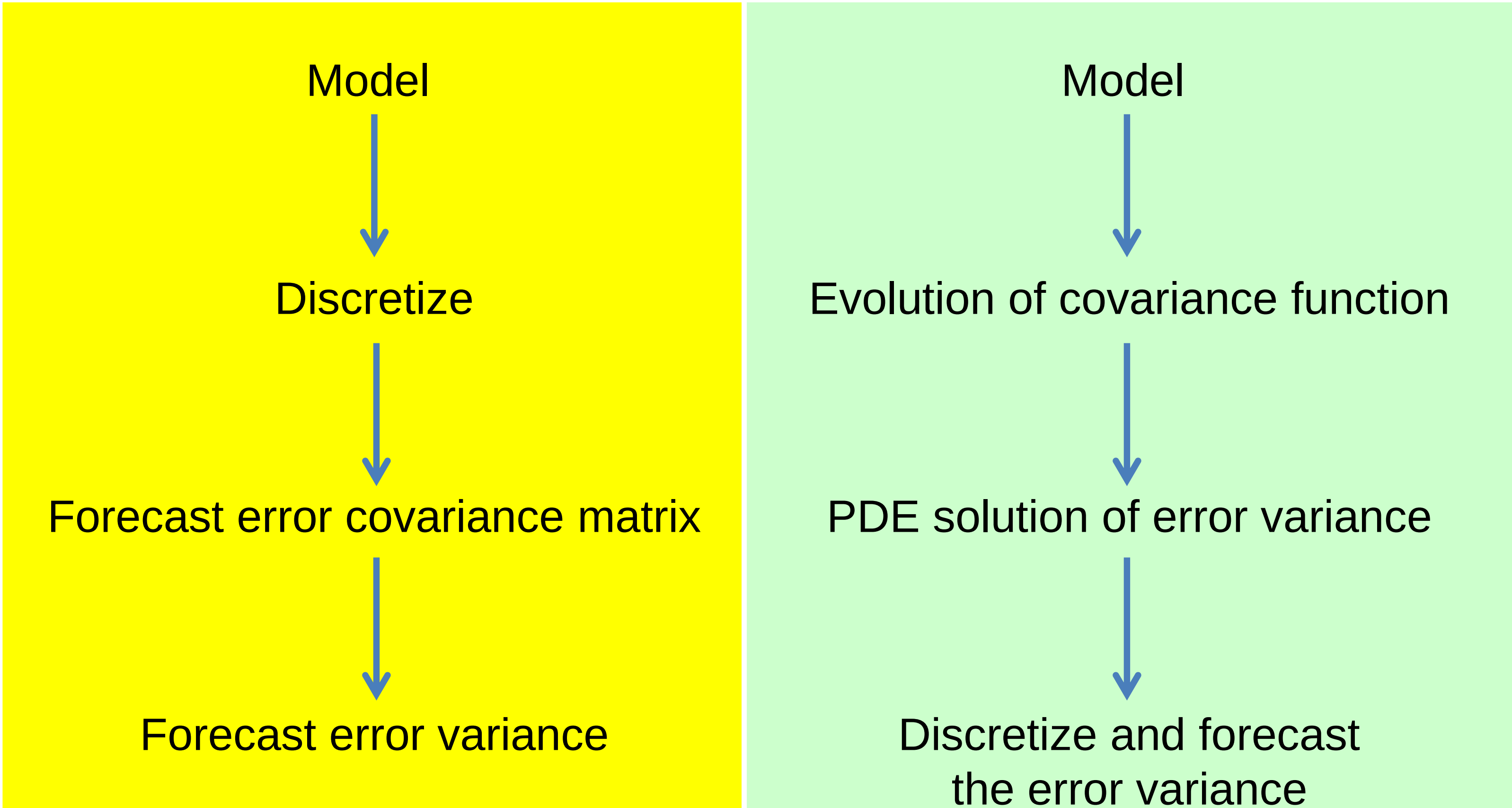
$$\tilde{\mathbf{Q}} = [\tilde{\mathbf{q}}_{\mathbf{1}}, \ \ldots \ , \tilde{\mathbf{q}}_{Nens} \ ]$$

where $\tilde{\mathbf{q}}_i = \mathbf{q}_i - \overline{\mathbf{q}}$ are departure from the mean

ensemble error covariance matrix

$$\mathbf{P}^e(t) = \frac{\tilde{\mathbf{Q}} \ \tilde{\mathbf{Q}}^T}{N_{ens} - 1} = \frac{1}{N_{ens} - 1} \sum_{i=1}^{Nens} \tilde{\mathbf{q}}_i \ \tilde{\mathbf{q}}_i^T$$


Model
Discretize
Forecast error covariance matrix
Forecast error variance


Model
Discretize
Forecast error covariance matrix
Forecast error variance
Model
Evolution of covariance function
PDE solution of error variance
Discretize and forecast
the error variance

Covariance function and their evolution

Covariance function defined for a pair of points $\mathbf{x}_1 \in R^3, \mathbf{x}_2 \in R^3$

$$P(\mathbf{x}_1, \mathbf{x}_2, t) = \mathbf{E}[\tilde{q}(\mathbf{x}_1, t)\ \tilde{q}(\mathbf{x}_2, t)]$$

is a $R^3 \times R^3$ dimensional function of space

- continuous function of space
- no spatial discretization

Evolution of covariance function

- with a linear model – no higher moment closure
- and here, an analytical solution can be obtained

Evolve an ensemble of mass fields

each member i obeys the transport equation, and so are their perturbations

$$\frac{\partial \tilde{q}_i}{\partial t} + \mathbf{V} \cdot \nabla \tilde{q}_i = 0$$

ensemble covariance function

$$P^e(\mathbf{x}_1, \mathbf{x}_2, t) = \frac{1}{N_{ens} - 1} \sum_{i=1}^{Nens} \tilde{q}_i(\mathbf{x}_1, t)\ \tilde{q}_i(\mathbf{x}_2, t)$$

Evolution of covariance function

$$\frac{\partial P^e}{\partial t} = \frac{1}{N_{ens}-1} \sum \left\{ \frac{\partial \tilde{q}_i(\mathbf{x}_1,t)}{\partial t}\, \tilde{q}_i(\mathbf{x}_2,t) + \tilde{q}_i(\mathbf{x}_1,t)\, \frac{\partial \tilde{q}_i(\mathbf{x}_2,t)}{\partial t} \right\}$$

with

$$\frac{\partial \tilde{q}_i(\mathbf{x}_1,t)}{\partial t} = -\mathbf{V}(\mathbf{x}_1,t)\cdot\nabla_{\mathbf{x}_1} \tilde{q}_i(\mathbf{x}_1,t)$$

$$\frac{\partial \tilde{q}_i(\mathbf{x}_2,t)}{\partial t} = -\mathbf{V}(\mathbf{x}_2,t)\cdot\nabla_{\mathbf{x}_2} \tilde{q}_i(\mathbf{x}_2,t)$$

we get (as in Cohn 1993)

$$\boxed{\frac{\partial P^e}{\partial t} + \mathbf{V}(\mathbf{x}_1,t)\cdot\nabla_{\mathbf{x}_1} P^e + \mathbf{V}(\mathbf{x}_2,t)\cdot\nabla_{\mathbf{x}_2} P^e = 0}$$

solution using the method of characteristics

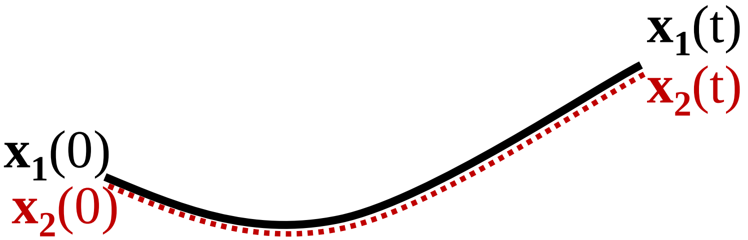
$$\frac{d\mathbf{x}_1}{dt} = \mathbf{V}(\mathbf{x}_1,t) \Rightarrow \mathbf{x}_1(t) = \mathbf{x}(t;\mathbf{x}_1(0)) \qquad \frac{d\mathbf{x}_2}{dt} = \mathbf{V}(\mathbf{x}_2,t) \Rightarrow \mathbf{x}_2(t) = \mathbf{x}(t;\mathbf{x}_2(0))$$

Then $P^e(\mathbf{x}_1,\mathbf{x}_2,t) = \mathrm{P}^e(t)$ is a function of time only

$$\boxed{\frac{d\,\mathrm{P}^e}{dt} = 0}$$

Solution : variance function equation

- for $\mathbf{x}_1(0) = \mathbf{x}_2(0)$ then the characteristics remain coincident $\mathbf{x}_1(t) = \mathbf{x}_2(t)$



- the covariance at the same point (i.e. the variance)

$$P^e(\mathbf{x}_1, \mathbf{x}_1, t) = V^e(\mathbf{x}, t) = \mathrm{V}^e(t) \qquad \frac{d\mathbf{x}}{dt} = \mathbf{V}(\mathbf{x}, t)$$

is constant along the characteristics (or along the flow)

$$\boxed{\frac{d\,\mathrm{V}^e}{dt} = \frac{\partial V^e}{\partial t} + \mathbf{V}(\mathbf{x}, t)\cdot\nabla V^e = 0}$$

How does it relate to an EnKF ?

We start with

$$\frac{\partial P}{\partial t} + L(\mathbf{x}_1)P + L(\mathbf{x}_2)P = 0 \qquad \text{..............(1)}$$

- discretize in space, and
- solve the evolution by operator splitting (first-order), on $\mathbf{x}_1$ and then on $\mathbf{x}_2$

We can show that this is equivalent to solving the covariance matrices as

$$\begin{aligned}\mathbf{P}(t+\Delta t) &= M\left(M\ \mathbf{P}(t)\right)^T = M\ \mathbf{P}(t)\,M^T \\ &= M\ \mathbf{X}(t)\left(M\ \mathbf{X}(t)\right)^T \qquad \text{......(2)}\end{aligned}$$

where M is the solution operator of

$$\frac{\partial q}{\partial t} + L(\mathbf{x})\,q = 0$$

Lets compare the advection of variance with the variance of the EnKF

Compare

- ❑ A – the numerical solution of advection of variance

  first obtain an analytical solution for variance then discretize

- ❑ B – the variance (diagonal of $\mathbf{P}^e$) from an ensemble of model transport

  first discretize the model then obtain the variance

both using the same transport model

- 3D transport model, flux form PPM (piece-wise parabolic) used for stratospheric transport and assimilation (BASCOE, Skachko et, 2014)
- resolution 3.75° longitude by 2.5° latitude on 37 levels
- using ERA-Interim meteorology

An ensemble of N_{ens} = 20 is generated with a homogeneous isotropic correlation model with L = 800 km

- initial variance used as initial condition for variance transport

Lets compare the advection of variance with the variance of the EnKF

Compare

- ❑ A – the numerical solution of advection of variance

  first obtain an analytical solution for variance then discretize

Model

↓

Evolution of covariance function

↓

PDE solution of error variance

↓

Discretize and forecast the error variance

Lets compare the advection of variance with the variance of the EnKF

Compare

- ❑ B – the variance (diagonal of $\mathbf{P}^e$) from an ensemble of model transport

  first discretize the model then obtain the variance

Model

↓

Discretize

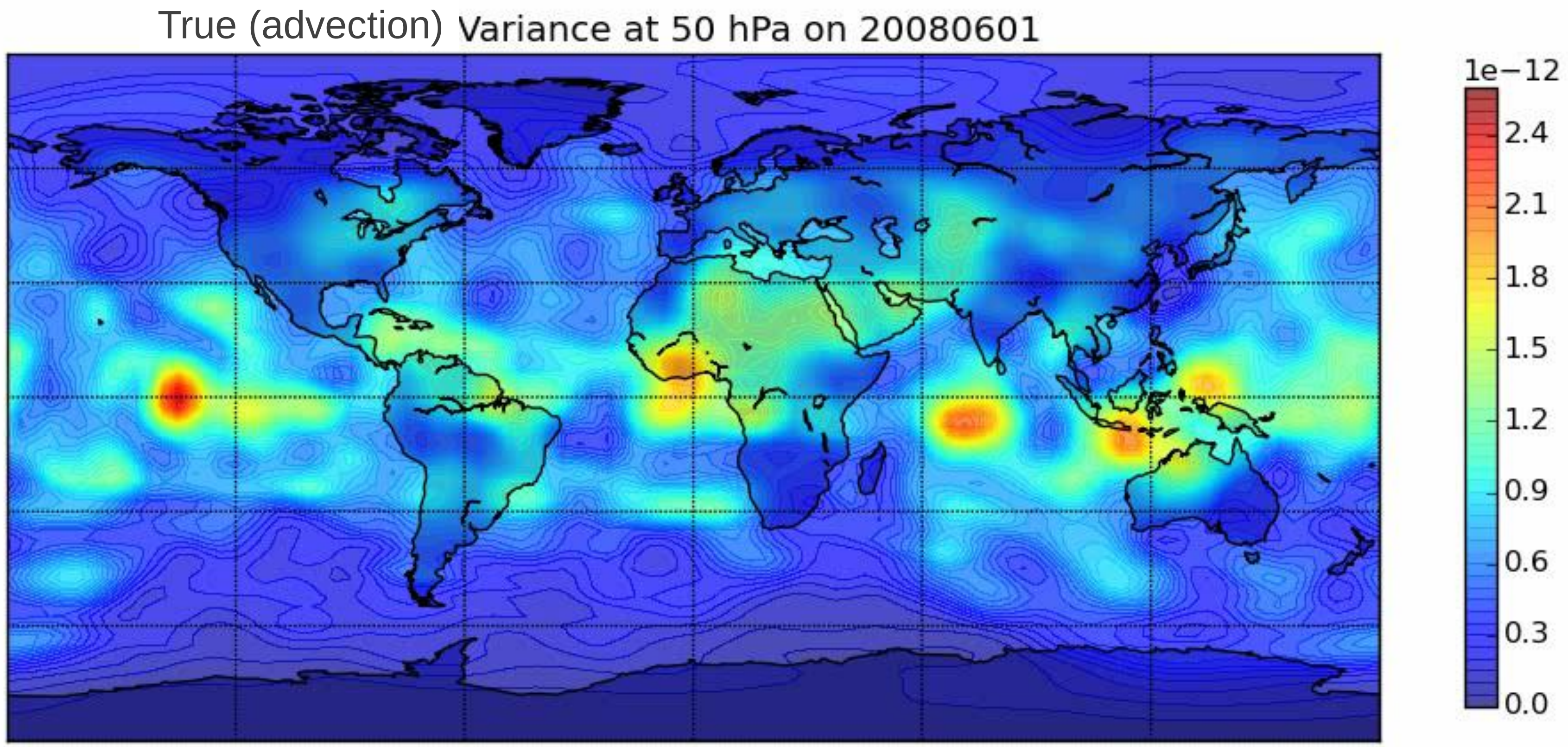
↓

Forecast error covariance matrix

↓

Forecast error variance

A - advection transport of variance



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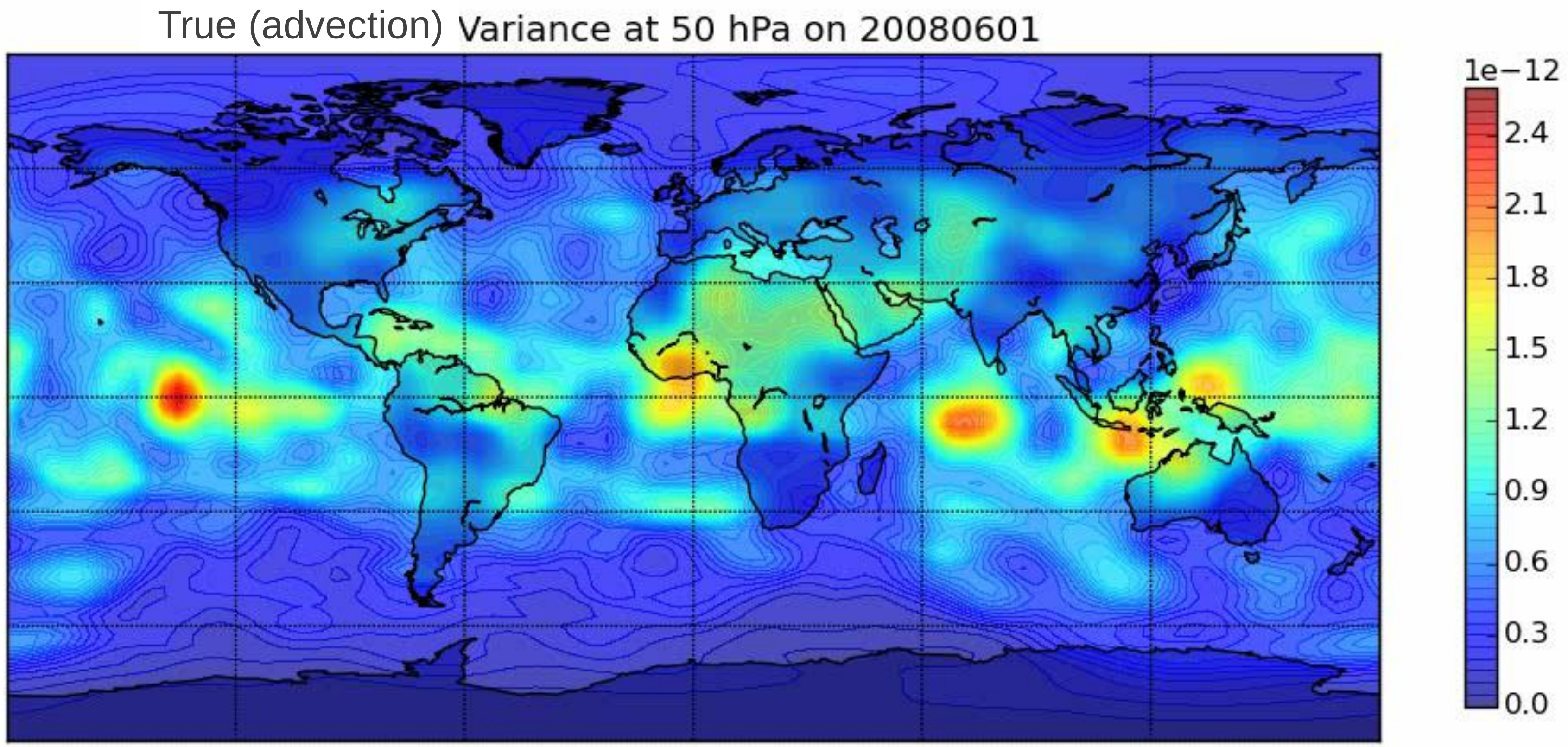
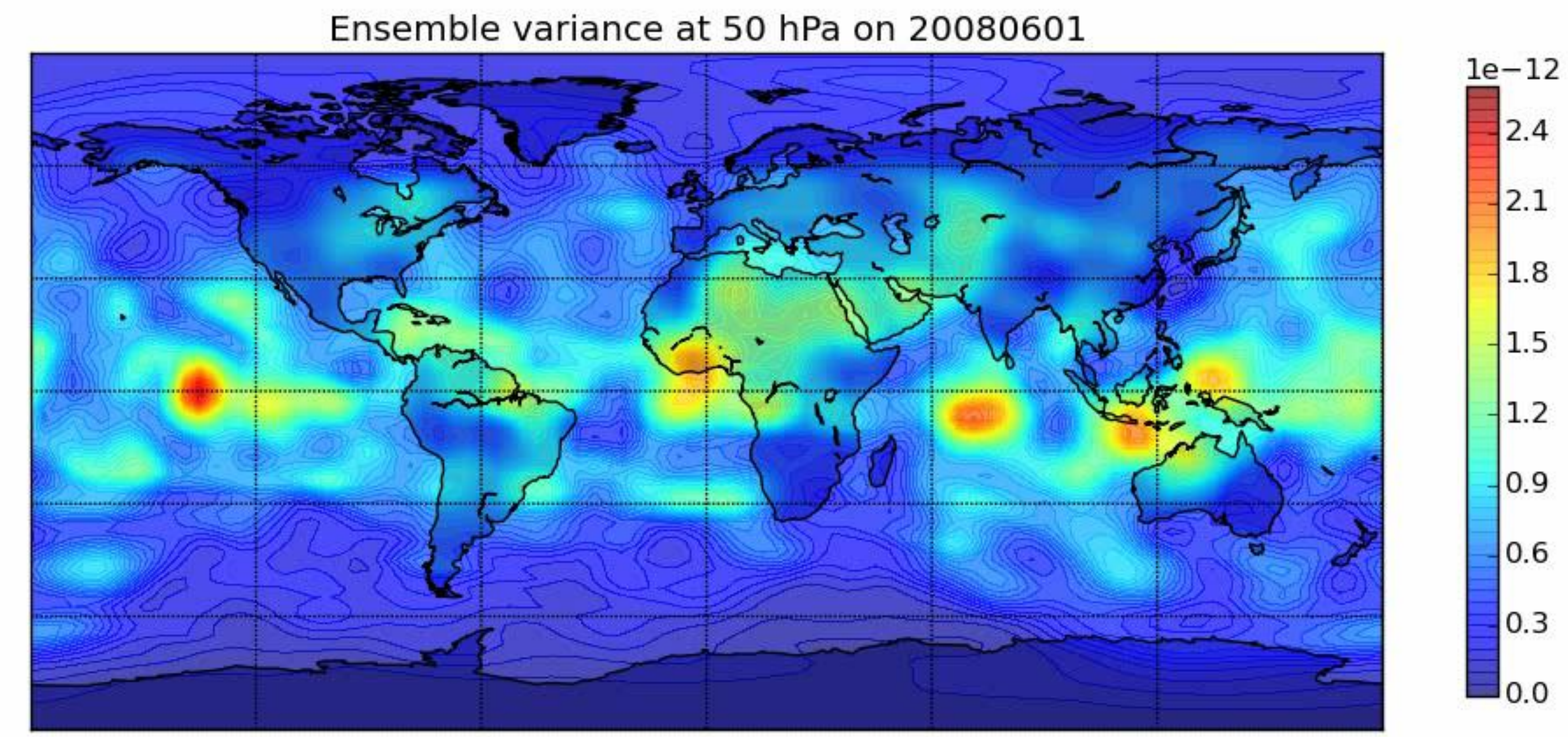


B - EnKF variance for linear transport



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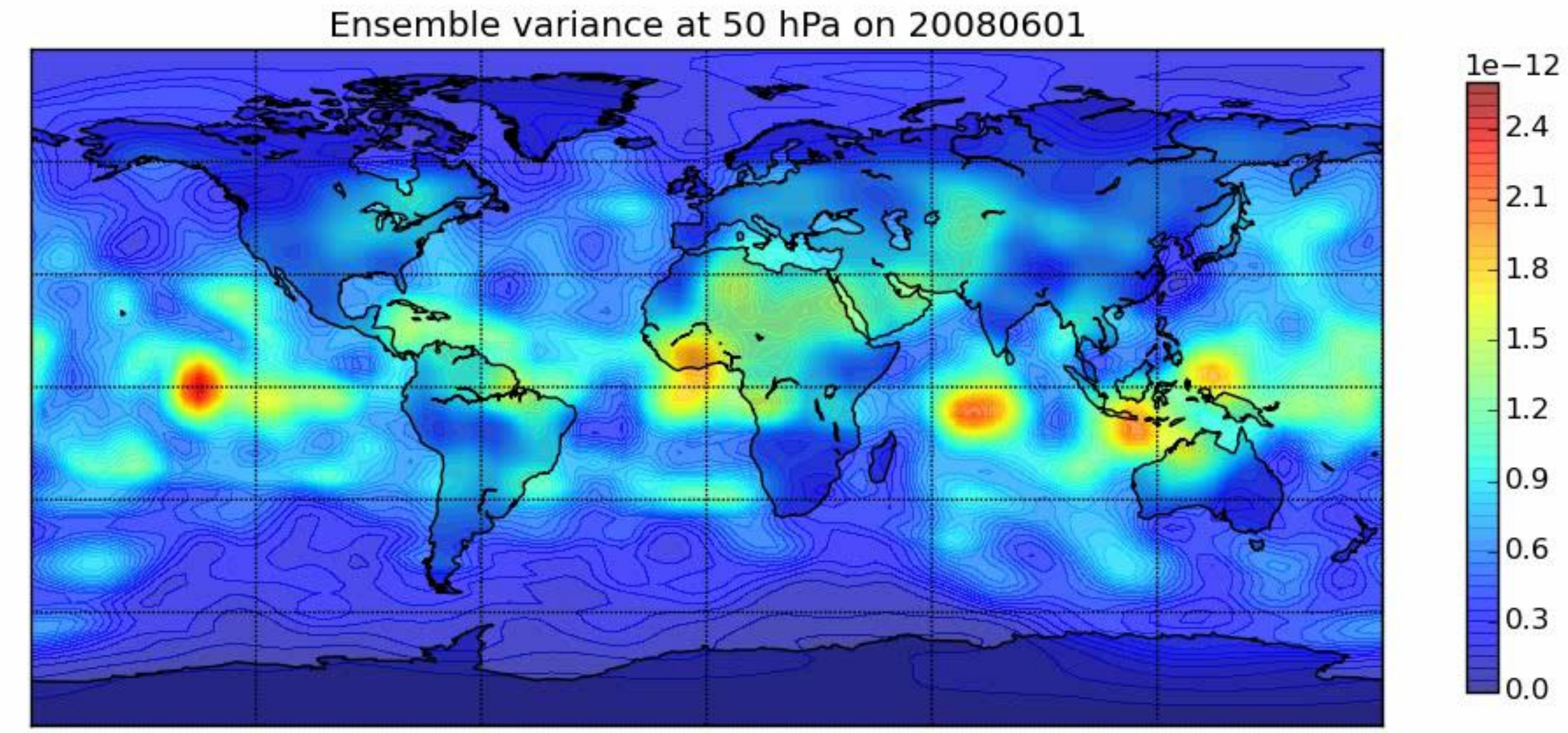
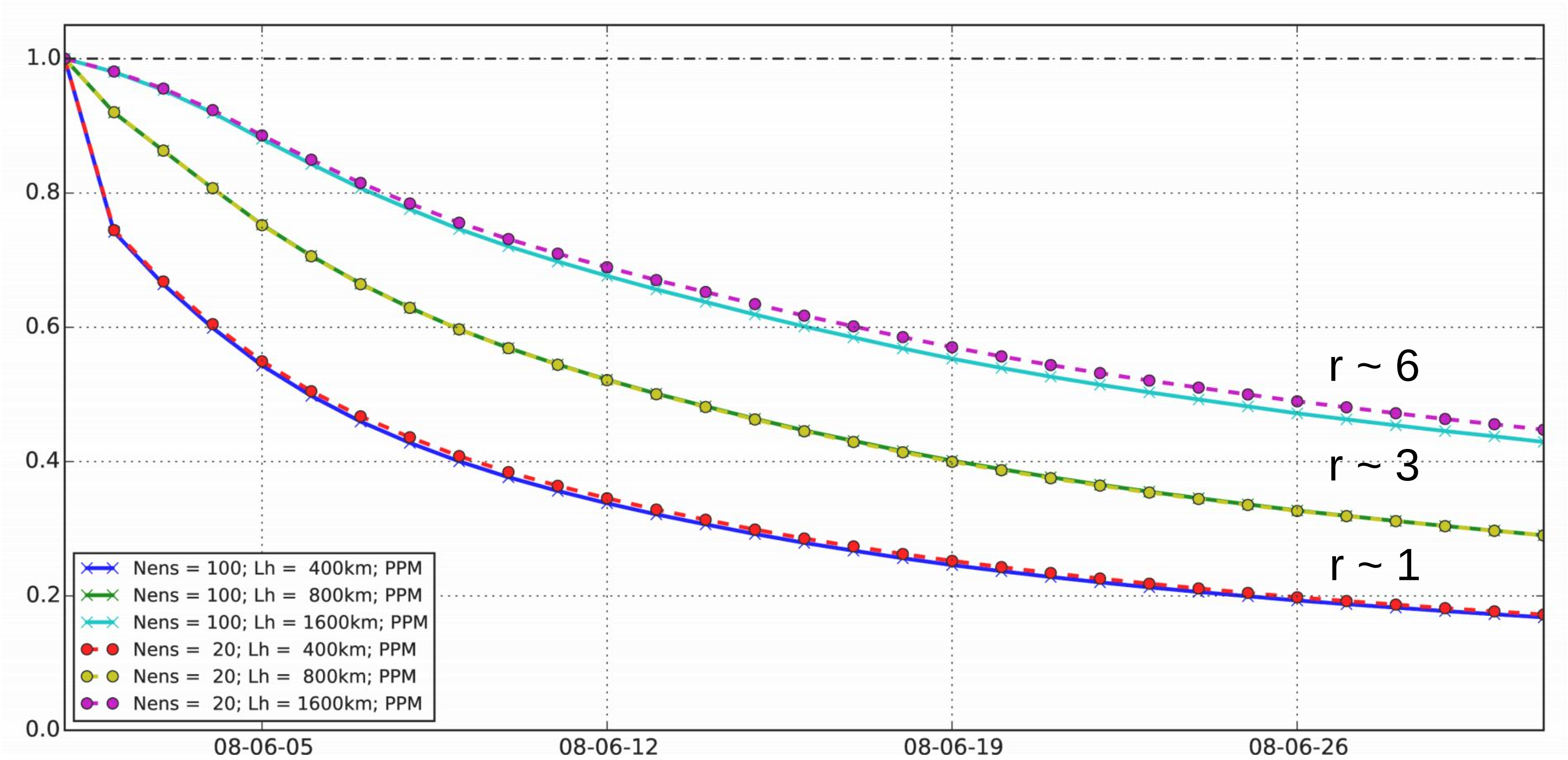


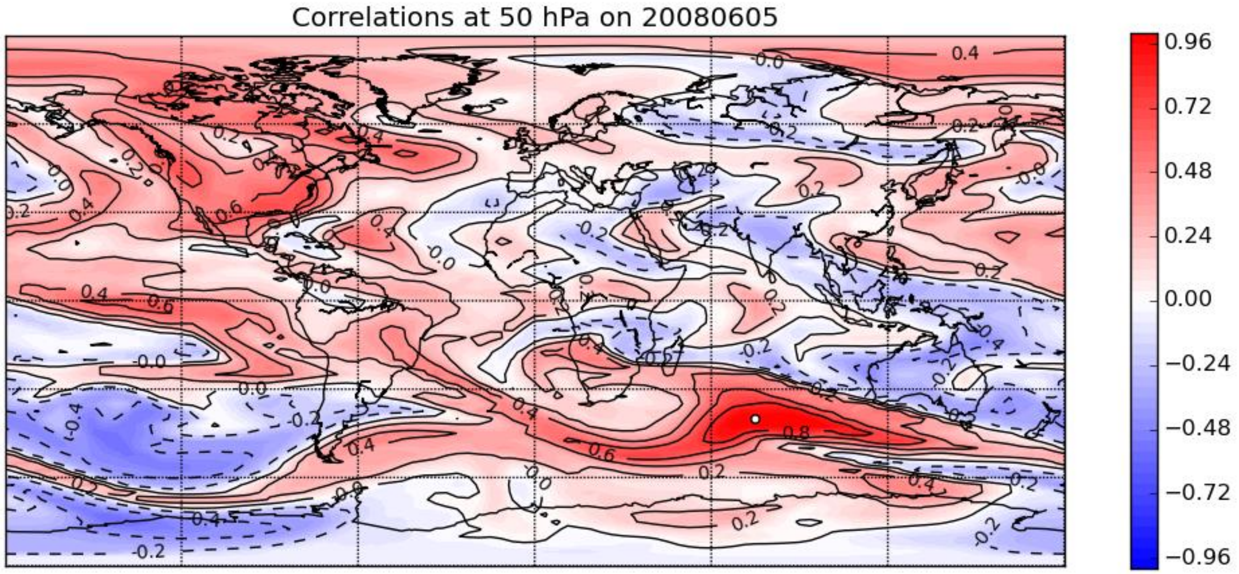
B/A : Ratio of the EnKF error variance with the advection of error variance



- The variance loss depends on the ratio of **r = correlation length / model resolution**
- Differences with small sample size (Nens = 20) is due to sampling errors

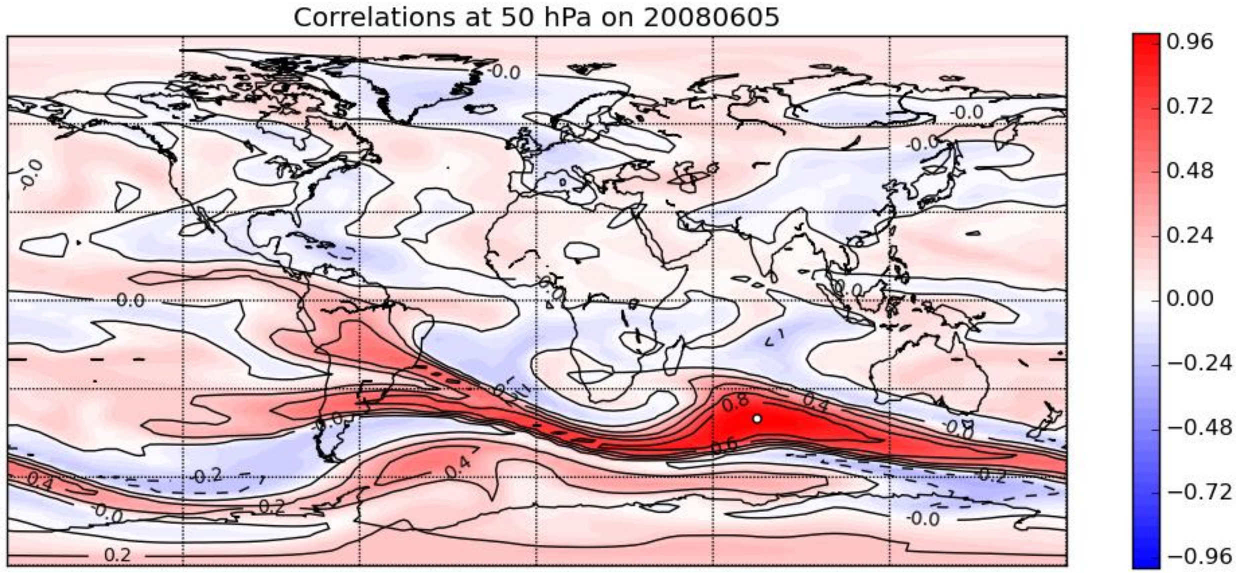
- As *N* increase the correlation becomes less noisy

***N* = 20**



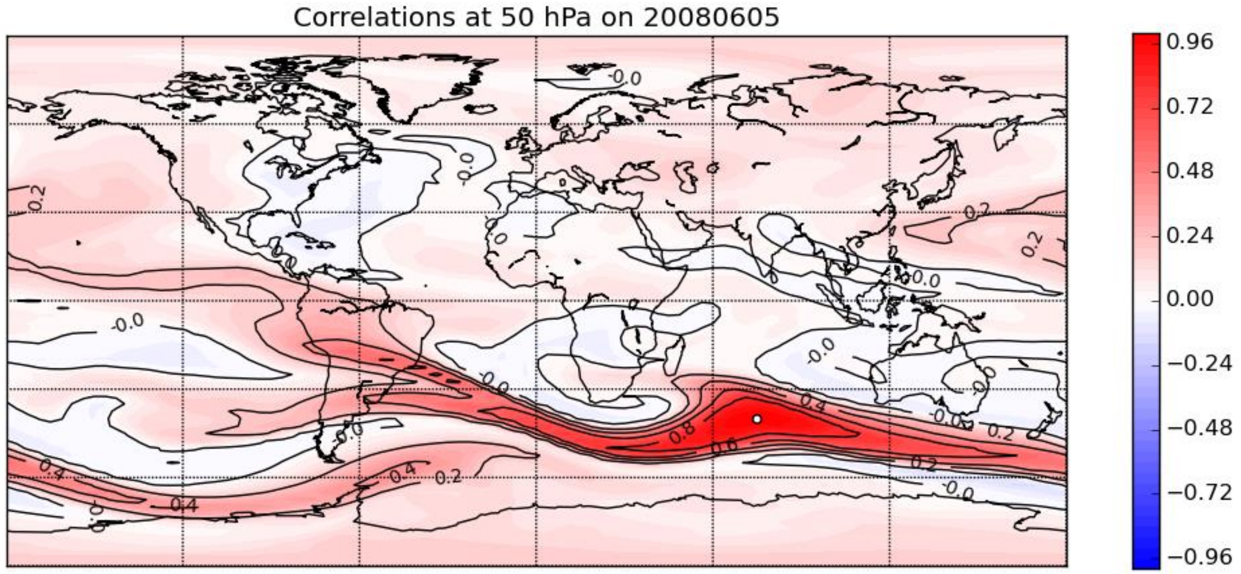
- As *N* increase the correlation becomes less noisy

***N* = 100**



- As *N* increase the correlation becomes less noisy

***N* = 500**

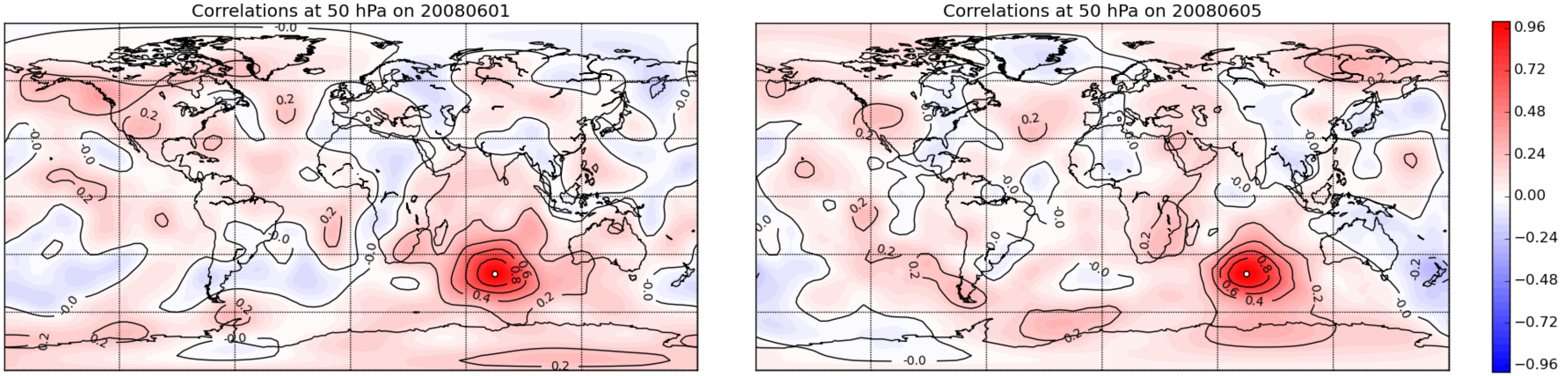


Variance loss occurs because we apply an advection scheme on filamentary covariance structures, created by wind shear

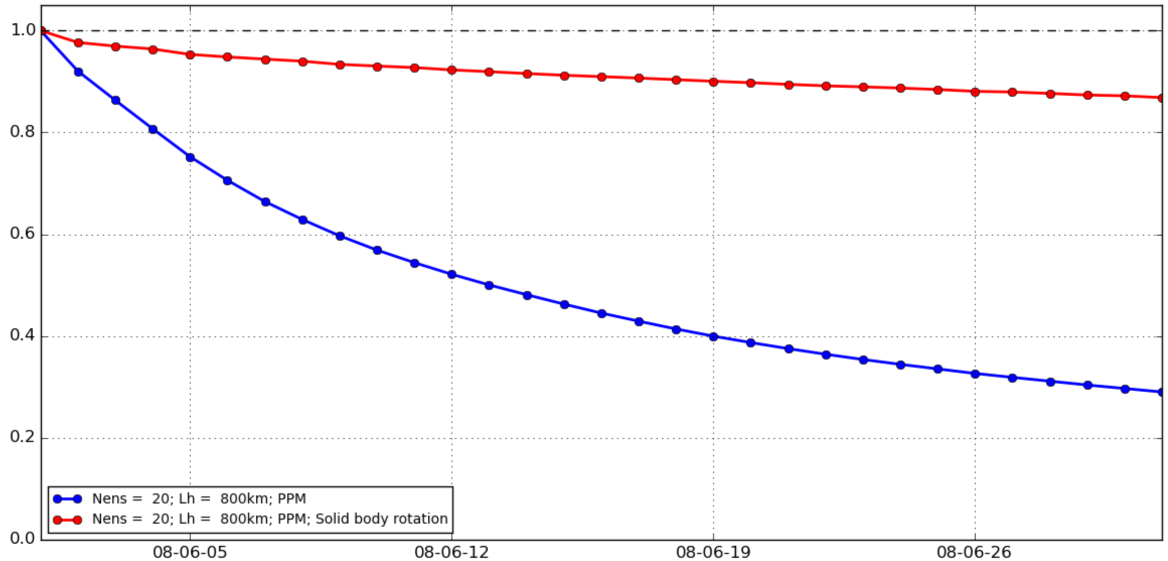
Solid body rotation winds

Initial error correlation

Error correlation after 4 days



Variance loss: **solid body rotation winds**, **ERA interim winds**



Consider 1D advection uniform wind. J grid points.
simple upstream differencing

$$\tilde{q}_j(t+\Delta t) = (1-c)\,\tilde{q}_j(t) + c\,\tilde{q}_{j-1}(t)$$

where c is the Courant number.

The forecast error variance at grid point j is given by

$$\left\langle \tilde{q}_j(t+\Delta t)\,\tilde{q}_j(t+\Delta t) \right\rangle = (1-c)^2 \left\langle \tilde{q}_j(t)\,\tilde{q}_j(t) \right\rangle + 2c(1-c)\left\langle \tilde{q}_{j-1}(t)\,\tilde{q}_j(t) \right\rangle + c^2 \left\langle \tilde{q}_{j-1}(t)\,\tilde{q}_{j-1}(t) \right\rangle$$

whereas the advection of error variance should be

$$\left\langle \tilde{q}_j(t+\Delta t)\,\tilde{q}_j(t+\Delta t) \right\rangle = (1-c)\left\langle \tilde{q}_j(t)\,\tilde{q}_j(t) \right\rangle + c\left\langle \tilde{q}_{j-1}(t)\,\tilde{q}_{j-1}(t) \right\rangle$$

the difference between the two expression is

$$c(c-1)\left\{ \left\langle \tilde{q}_j(t)\,\tilde{q}_j(t) \right\rangle - \left\langle \tilde{q}_j(t)\,\tilde{q}_{j-1}(t) \right\rangle - \left\langle \tilde{q}_{j-1}(t)\,\tilde{q}_j(t) \right\rangle + \left\langle \tilde{q}_{j-1}(t)\,\tilde{q}_{j-1}(t) \right\rangle \right\}$$

is actually a spitting error term

How could we fix this ?
(although this is not the object of this study)

- By applying inflation (to augment the variance). If multiplicative inflation a Schur product is also needed to reduce the correlation length-scale

- For transport problems;
  - A - replace the EnKF variance by the advection of variance solution. Need a Schur product compensation to reduce the resulting correlation lengths
  - B – To use a Lagrangian advection of error covariances (i.e. Lagrangian KF (Lyster et al 2004)). Because of trajectory collapse remapping of the error covariance is needed and this created variance loss.
  - C – Use the Parametrized Kalman filter where variances and length-scales are evolved and updated by analysis (see Pannoucke poster)

- Second order splitting (Strang Splitting) but this only affects the time time discretization issue, whereas the spatial discretization is the important aspect to consider

- Is the use non-diffusive transport schemes like the Prather scheme

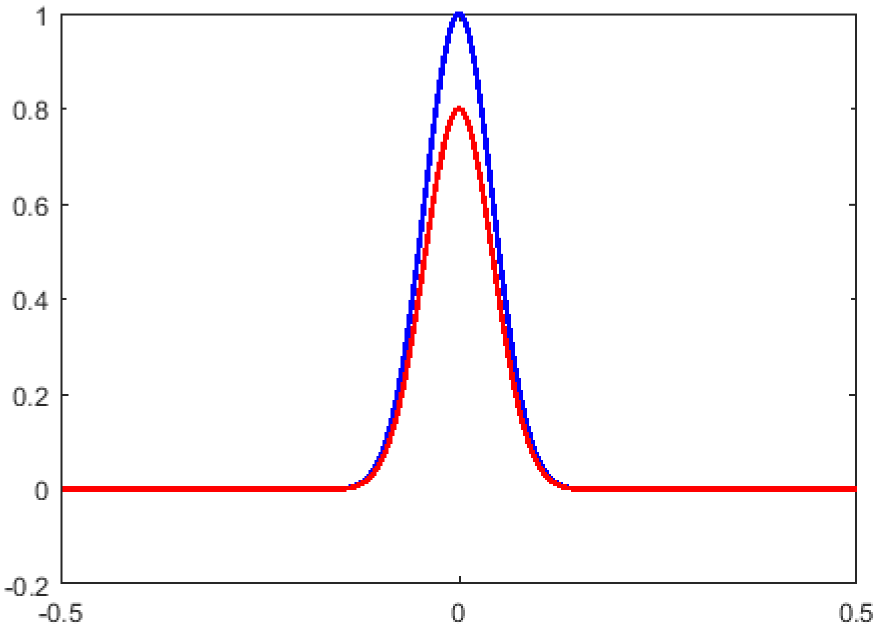
- To propagate error covariance is an alternative covariance space
  Instead of $(\mathbf{x}_1, \mathbf{x}_2)$ consider $(\mathbf{x}, \boldsymbol{\xi})$ where $\mathbf{x} = \frac{1}{2}(\mathbf{x}_1 + \mathbf{x}_2)$; $\boldsymbol{\xi} = \frac{1}{2}(\mathbf{x}_1 - \mathbf{x}_2)$
  This requires however a rewrite of existing transport models

- Evaluate the splitting error term. But this depends on the specifics of the numerical scheme

Splitting error – illustration in a 1D case simple upstream scheme

EnKF numerical solution = Advection of variance + error term

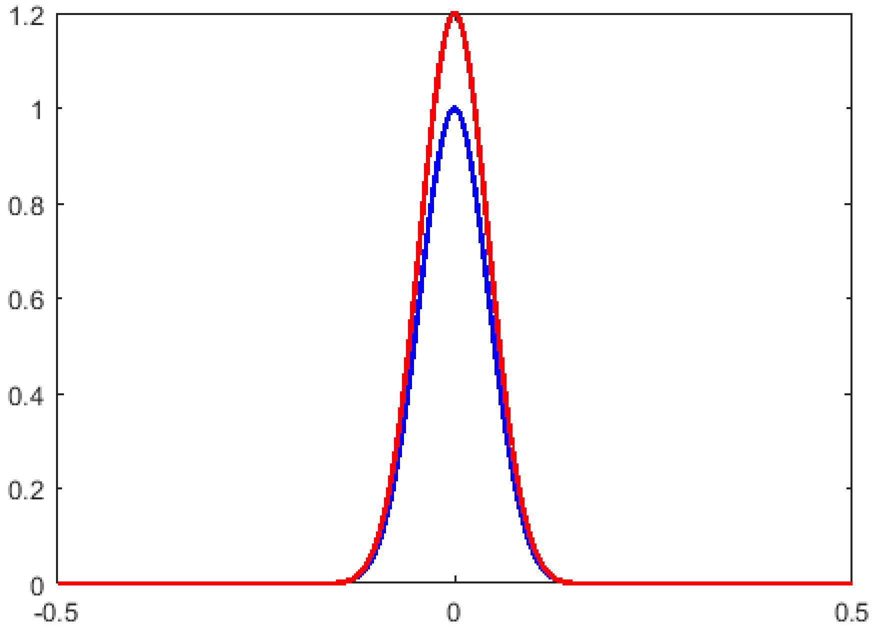
with a simple upstream scheme the error term = $u(x_1)u(x_2)\Delta t^2 \nabla_{x2}\nabla_{x1}P$



so to compensate for the error term we could use an inflation of the form $-\gamma \nabla_{x2}\nabla_{x1}P$

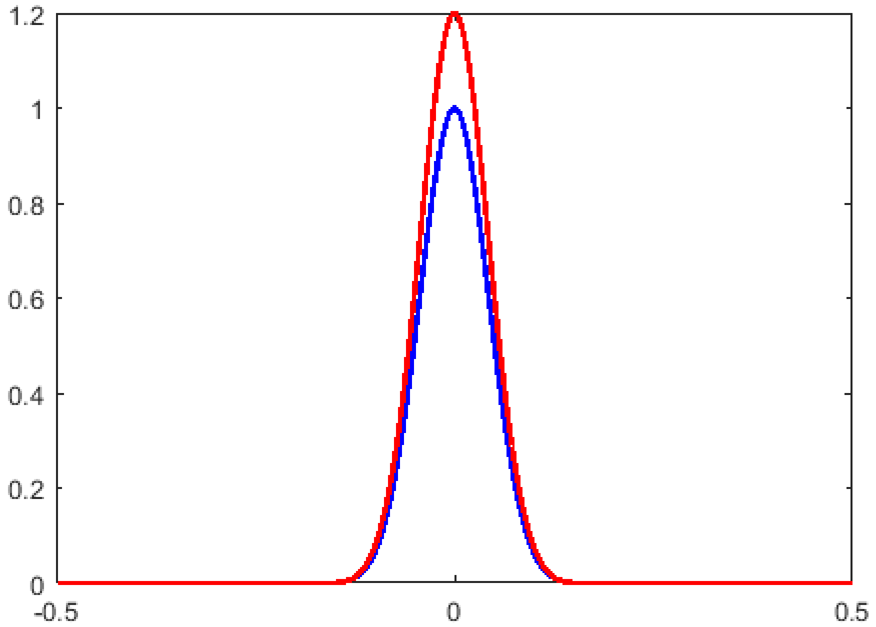
EnKF numerical solution + inflation term

inflation term = $-\gamma \nabla_{x2} \nabla_{x1} P$



EnKF numerical solution + inflation term

inflation term = $-\gamma \nabla_{x2} \nabla_{x1} P$



$\Rightarrow$ compensating for the error term is similar to inflation
but we have here a specific form for it (i.e. the double gradient)

Relevance of this study

- Chemical data assimilation, ex: stratospheric ozone
- CO_2 inverse modeling using EnKF
- Tracer assimilation in oceans
- Assimilation of water vapor
- Could also be relevant in some meteorological applications where cascade to smaller scales is important

Thanks for your attention

extra slide

First-order operator splitting

$$\frac{\partial P}{\partial t} + L(\mathbf{x}_1)P + L(\mathbf{x}_2)P = 0 \quad \text{................(1)}$$

takes the form of a two-step solution:

- First solve $$\frac{\partial P}{\partial t} + L(\mathbf{x}_1)P = 0 \quad \text{....................................(2)}$$
- then with the solution P^* of (2) use it to solve

$$\frac{\partial P}{\partial t} + L(\mathbf{x}_2)P = 0 \quad \text{....................................(3)}$$

Important result: When the operators commute $L(\mathbf{x}_1)L(\mathbf{x}_2) = L(\mathbf{x}_2)L(\mathbf{x}_1)$

the solution of (1) is identical to the solution (2)-(3) by operator splitting

- The spatially continuous advection operators

$$L(\mathbf{x}_1) = \mathbf{V}(\mathbf{x}_1, t)\cdot\nabla_{\mathbf{x}_1} P^e \quad \text{and} \quad L(\mathbf{x}_2) = \mathbf{V}(\mathbf{x}_2, t)\cdot\nabla_{\mathbf{x}_2} P^e$$

do commute, but this is not generally true for their discrete formulations