A methodology to obtain model-error covariances due to the discretization scheme from the parametric Kalman filter perspective

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Model-error for the advection

As a simple example, consider that the nature is given by the advection

$$\partial_t c + \mathbf{u}\partial_x c = 0, \tag{1}$$

where $\mathbf{u}(t,x) > 0$ is an heterogeneous wind field and $c(t,x)$ a passive scalar field.

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Note that c is conserved along the characteristic curves (see *e.g.* [Boyd, 2001, chap. 14]), that is

$$\frac{dx}{dt} = u, \tag{2a}$$

$$\frac{dc}{dt} = 0. \tag{2b}$$

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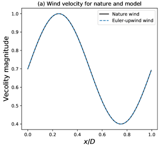
Now suppose the dynamics is numerically solved by the Euler-upwind scheme,

$$\frac{c_i^{q+1} - c_i^q}{\delta t} = -u_i \frac{c_i^q - c_{i-1}^q}{\delta x}, \tag{3}$$

$\mathbf{u}(x) \rightarrow$ 

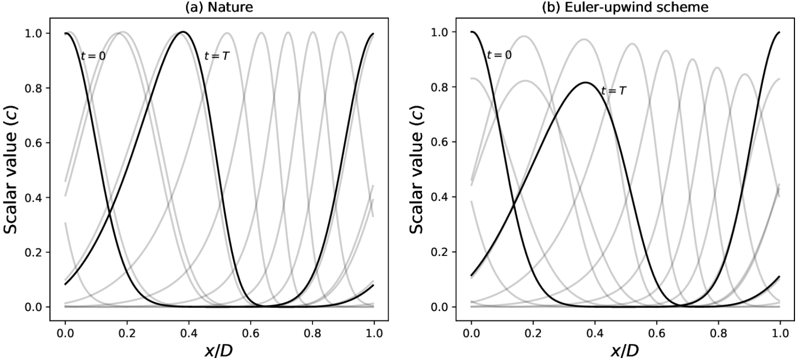


Figure: Nature versus numerical dynamics

Transport with conservation for the nature
but heterogeneous damping for the num. model == model error.

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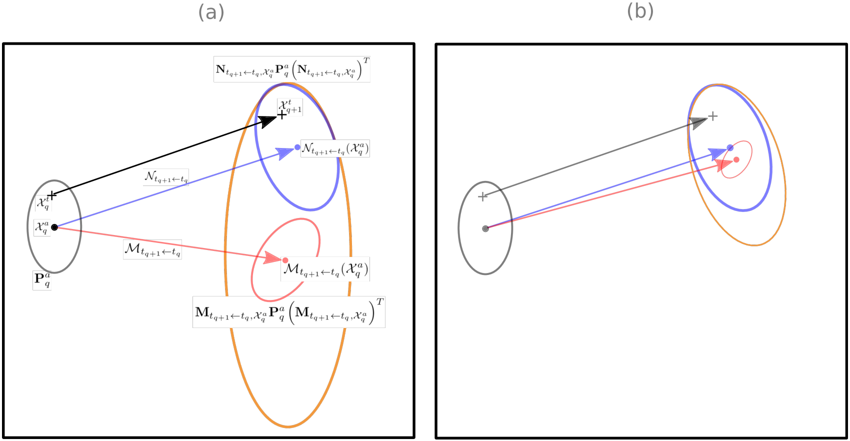
Dynamics of the model-error covariance

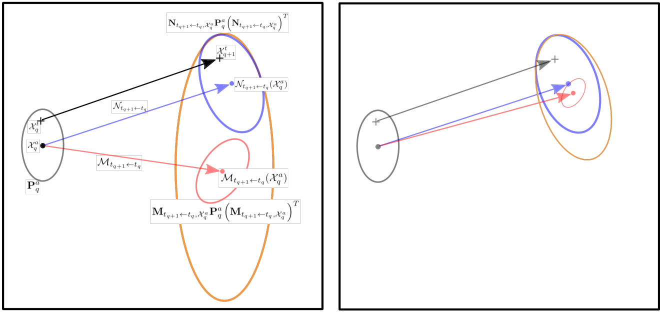
Sketch of the uncertainty evolution in presence of model-error



$\mathcal{N}$ (resp. $\mathcal{M}$) denotes the nature (the numerical model). The orange ellipse represents the forecast-error covariance matrix $\mathbf{P}_{q+1}^f$.

Modelling of the model-error covariance

(a) (b)



In the diffusive case (b) the forecast-error covariance matrix writes [Pannekoucke et al., 2021]

$$\mathbf{P}^f{}_{q+1} \approx \mathbf{P}^p_{q+1} + \Pi^m_{q+1} + \mathbf{Q}_{q+1}, \tag{4}$$

with $\mathbf{P}^p_{q+1} = \mathbf{M}\mathbf{P}^a{}_q\mathbf{M}^T$ the predictability-error covariance matrix and

$$\Pi^m_{q+1} = \mathbf{N}\mathbf{P}^a{}_q\mathbf{N}^T - \mathbf{M}\mathbf{P}^a{}_q\mathbf{M}^T. \tag{5}$$

Dynamics of the model-error covariance

With $\mathbf{P}^f{}_{q+1} \approx \mathbf{P}^p_{q+1} + \mathbf{P}^m_{q+1}$, it results that the model-error covariance matrix

$$\mathbf{P}^m_{q+1} = \Pi^m_{q+1} + \mathbf{Q}_{q+1}, \tag{6}$$

expands as a

- flow-dependent part $\Pi^m_{q+1} = \mathbf{N}\mathbf{P}^a{}_q\mathbf{N}^T - \mathbf{M}\mathbf{P}^a{}_q\mathbf{M}^T$,
- climatological part $\mathbf{Q}_{q+1}$.

So to focuse on the flow-dependent part, we need to compute the predictability-error covariance matrices $\mathbf{N}\mathbf{P}^a{}_q\mathbf{N}^T$ and $\mathbf{M}\mathbf{P}^a{}_q\mathbf{M}^T$.

From $\mathbf{M}$ we can compute $\mathbf{M}\mathbf{P}^a{}_q\mathbf{M}^T$ from an ensemble. But in practice since we don't have $\mathbf{N}$, so we cannot compute $\mathbf{N}\mathbf{P}^a{}_q\mathbf{N}^T$.

We propose to performed the computation by using the parametric approach.

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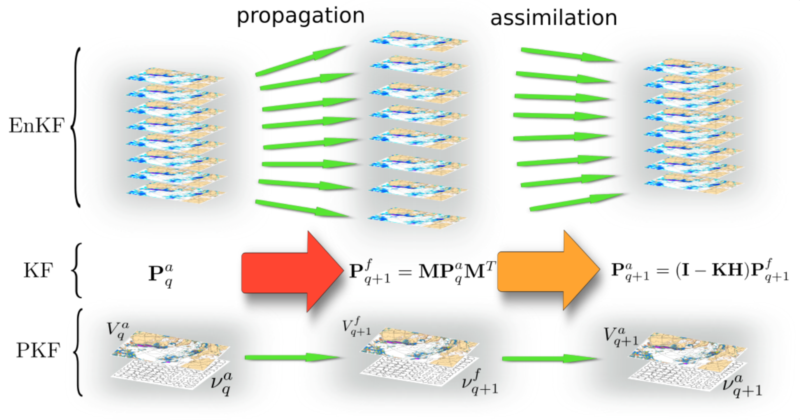
Parametric Kalman Filter



What are the PKF equations for the forecast steps ?

VLAT covariance matrices

In this talk we consider covariance models parameterized by the variance and the local anistropy tensor fields – the VLATcov model [Pannekoucke, 2021]. For an error field $\varepsilon(t,x)$,

- the variance is defined as $V(t,x) = \mathbb{E}\left[\varepsilon^2\right]$

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- the variance is defined as $V(t,x) = \mathbb{E}\left[\varepsilon^2\right]$
- the local anisotropy tensor is given either by the metric tensor, $\boldsymbol{g}(t,x)$, which measures the anisotropy of the correlation function

$$\rho(t,x,x+\delta x) = \frac{\mathbb{E}\left[\varepsilon(t,x)\varepsilon(t,x+\delta x)\right]}{\sqrt{V_x V_{x+\delta x}}} \underset{\delta x \to 0}{=} 1 - \frac{1}{2}||\delta x||^2_{\boldsymbol{g}_x} + \mathcal{O}(\delta x^2),$$

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or the the aspect tensor, $\boldsymbol{s}(t,x)$, which is the matrix inverse of the metric tensor

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Note that $(\boldsymbol{g}_x)_{ij} = \mathbb{E}\left[\partial_i\left(\frac{\varepsilon}{\sqrt{V}}\right)\partial_j\left(\frac{\varepsilon}{\sqrt{V}}\right)\right].$

PKF for VLATcov models

The parametric Kalman filter dynamics for the variance and the local anisotropy writes as

$$\partial_t V = 2\mathbb{E}\left[\varepsilon \partial_t \varepsilon\right], \tag{7}$$

$$\partial_t \boldsymbol{g} = \partial_t \mathbb{E}\left[\partial_i \left(\frac{\varepsilon}{\sqrt{V}}\right) \partial_j \left(\frac{\varepsilon}{\sqrt{V}}\right)\right], \tag{8}$$

which can be computed by using a computer algebra system.

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SymPKF performs the symbolic computation of the PKF for VLATcov model and can also automatically generate a finite difference implementation for the numerical exploration [Pannekoucke and Arbogast, 2021].

see https://github.com/opannekoucke/sympkf

Predictability-error covariance dynamics: the nature

The PKF dynamics for the transport equation, over a 1D domain, computed with SymPKF leads to the predictabilty error dynamics for the nature:

$$\partial_t \tilde{c} = -u\partial_x \tilde{c}, \tag{9}$$

$$\partial_t \tilde{V}^p = -u\partial_x \tilde{V}^p, \tag{10}$$

$$\partial_t \tilde{s}^p = -u\partial_x \tilde{s}^p + 2\tilde{s}^p \partial_x u, \tag{11}$$

stands for $\mathbf{N}\mathbf{P}^a{}_q\mathbf{N}^T$, where $\tilde{\cdot}$ denotes the statistics for the nature.

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stands for $\mathbf{NP}^a{}_q\mathbf{N}^T$, where $\tilde{\cdot}$ denotes the statistics for the nature.

The variance is conserved, while the anisotropy is stretched by the shear (the term $2s\partial_x u$).

Predictability-error covariance dynamics: the model

The modified equation associated with the Euler-upwind scheme

$$\frac{c_i^{q+1}-c_i^q}{\delta t} = -u_i\frac{c_i^q - c_{i-1}^q}{\delta x}, \tag{12}$$

reads as

$$\partial_t C + U\partial_x C = \kappa\partial_x^2 C, \tag{13}$$

where

$$\begin{cases} U(t,x) = u - \frac{\delta t}{2}\partial_t u + \frac{\delta t}{2}u\partial_x u, \\ \kappa(t,x) = \frac{u}{2}\left(\delta x - u\delta t\right). \end{cases} \tag{14}$$

which shows that the num. model is suffering from dispersion and dissipation.

Note that similar expressions are obtained for semi-Lagrangian discretization as used in NWP and air quality.

Predictability-error covariance dynamics: the model

The PKF dynamics for the num. model, computed with SymPKF, reads as

$$
\begin{aligned}
\partial_t c &= -U\partial_x c + \kappa\partial_x^2 c,\\
\partial_t V^p &= U\partial_x V^p - \frac{2V^p\kappa}{s^p} + \kappa\partial_x^2 V^p - \frac{\kappa\left(\partial_x V^p\right)^2}{2V^p}\\
\partial_t s^p &= -U\partial_x s^p + 2\kappa {s^p}^2\mathbb{E}\left(\tilde{\varepsilon^p}\partial_x^4\tilde{\varepsilon^p}\right) - 3\kappa\partial_x^2 s^p - 2\kappa + \frac{6\kappa\left(\partial_x s^p\right)^2}{s^p}\\
&\quad - \frac{2\kappa s^p\partial_x^2 V^p}{V^p} + \frac{\kappa\partial_x V^p\partial_x s^p}{V^p} +\\
&\quad \frac{2\kappa s^p\left(\partial_x V^p\right)^2}{{V^p}^2} + 2s^p\partial_x U + \partial_x\kappa\partial_x s^p - \frac{2s^p\partial_x\kappa\partial_x V^p}{V^p},
\end{aligned}
$$

where $\tilde{\varepsilon^p} = \varepsilon^p/\sqrt{V^p}$ is the normalized error. This stands for $\mathbf{M}{\mathbf{P}^a}_q\mathbf{M}^T$ and appears as a coupled system due to the numerical diffusion which needs a closure

Predictability-error covariance dynamics: the model

With the local Gaussian closure [Pannekoucke et al., 2018] $\mathbb{E}\left(\tilde{\varepsilon^p}\partial_x^4\tilde{\varepsilon^p}\right) = \frac{2\partial_x^2 s^p}{s^{p2}} + \frac{3}{s^{p2}} - \frac{4(\partial_x s^p)^2}{s^{p3}}$, the predictability-error covariance dynamics reads as

$$\partial_t c = -U\partial_x c + \kappa\partial_x^2 c,$$

$$\partial_t V^p = U\partial_x V^p - \frac{2V^p\kappa}{s^p} + \kappa\partial_x^2 V^p - \frac{\kappa\left(\partial_x V^p\right)^2}{2V^p}$$

$$\partial_t s^p = -U\partial_x s^p + (2\partial_x U)s^p +$$

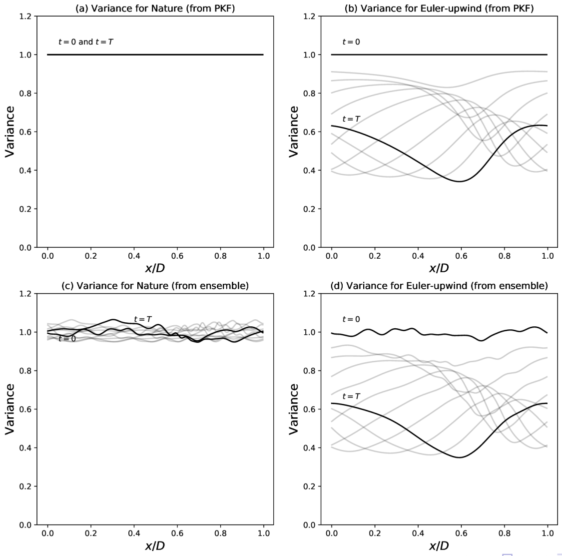
$$\kappa\partial_x^2 s^p + 4\kappa - \frac{2\left(\partial_x s^p\right)^2}{s^p}\kappa + \partial_x\kappa\partial_x s^p - \frac{2\partial_x^2 V^p}{V^p}\kappa s^p +$$

$$\frac{\partial_x V^p}{V}\kappa\partial_x s^p - \frac{2\partial_x V^p}{V^p}s^p\partial_x\kappa + \frac{2\left(\partial_x V^p\right)^2}{V^{p2}}\kappa s^p,$$

Note that closures can be found from data-driven physics considering an hybridization of physics and AI *e.g.* PDE-NetGen [Pannekoucke and Fablet, 2020] see https://github.com/opannekoucke/pdenetgen

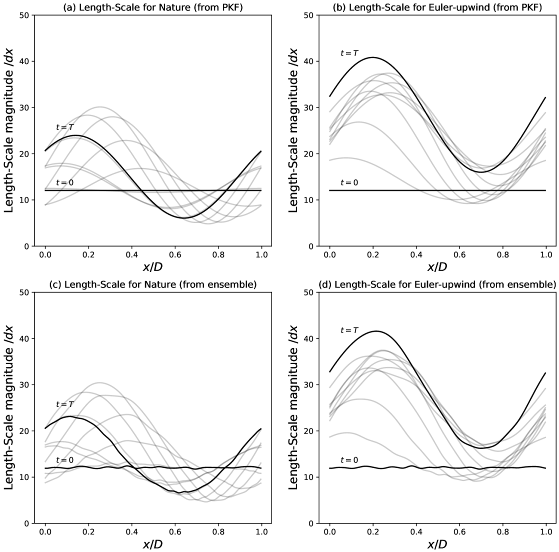
Predictability-error covariance dynamics PKF

(validated by an ensemble estimation with 6400 members, [Evensen, 2009])



Predictability-error covariance dynamics PKF

(with the correlation length-scale defined as $\sqrt{s}$)



Predictability-error covariance dynamics: the model

Note that, using the spatial averaged over the domain, $\langle\cdot\rangle = \frac{1}{D}(\int)\cdot dx$, the predictability-error dynamics for $\mathcal{M}$ approximately reads as

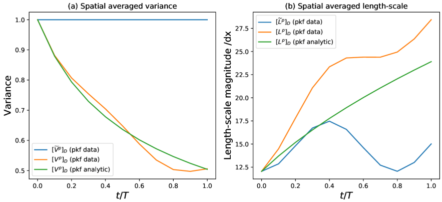
$$\partial_t \langle V^p \rangle = -\frac{\langle 2\kappa \rangle}{\langle s^p \rangle}\langle V^p \rangle, \tag{15}$$

$$\partial_t \langle s^p \rangle = 4\langle \kappa \rangle, \tag{16}$$

of solution

$$\langle V^p \rangle(t) = \langle V^p \rangle(0)\left(\frac{\langle s^p \rangle(0)}{\langle s^p \rangle(0) + 4\langle \kappa \rangle t}\right)^{1/2}, \tag{17}$$

$$\langle s^p \rangle(t) = \langle s^p \rangle(0) + 4\langle \kappa \rangle t. \tag{18}$$



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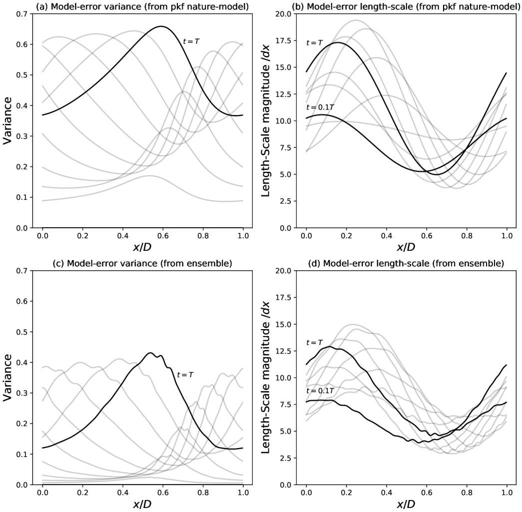
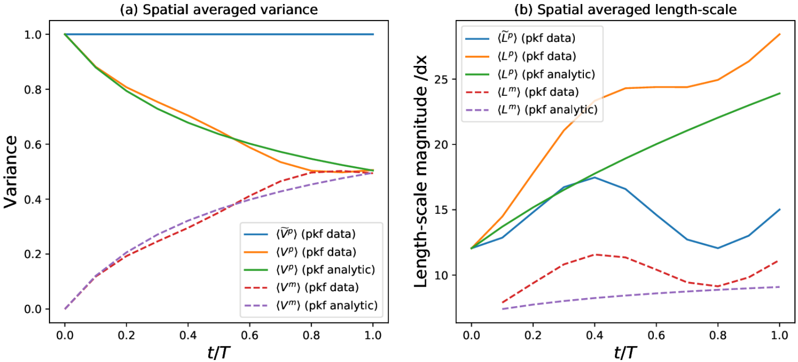
Time evolution of the low-dependent part of $\mathbf{P}^m$



Evolution of the flow-dependent part of the model-error covariance
$\Pi^m_{q+1} = \mathbf{N}\mathbf{P}^a{}_q\mathbf{N}^T - \mathbf{M}\mathbf{P}^a{}_q\mathbf{M}^T$

Spatial averaged of the model-error variance



For the first moments of the experiment, $\langle V^m \rangle(t) \sim t \frac{\langle \kappa \rangle}{\langle \nu^p \rangle(0)} \langle V^p \rangle(0)$,

then $\langle V^m \rangle(t) \sim 1 - \left(\frac{l_h^2}{l_h^2 + 4\langle \kappa \rangle t} \right)^{1/2}$, where $\langle s^p \rangle(0) = l_h^2$.

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Conclusion

For the parametric Kalman filte (PKF):

- In the PKF error-covariance matrix are approximated by some covariance model
- The dynamics of the parameters is an approximation of the dynamics of the real error-covariance matrix, it often needs a closures but gives access to the physics of uncertainty.
- Some applications are under investigation – see the next presentation of Martin Sabathier with the assimilation of the Earth radiation belts

Concerning its application for the model-error covariance properties:

- We can compute the predicatability-error dynamics from the PKF
- This gives a proxy of the flow-dependent part of the model-error covariance that could be interesting in the diffusive case
- We illustrate this on a simple transport over a 1D domain
- Give some clues for inflation in 2D/3D domain applications – see the next presentation of Richard Ménard

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