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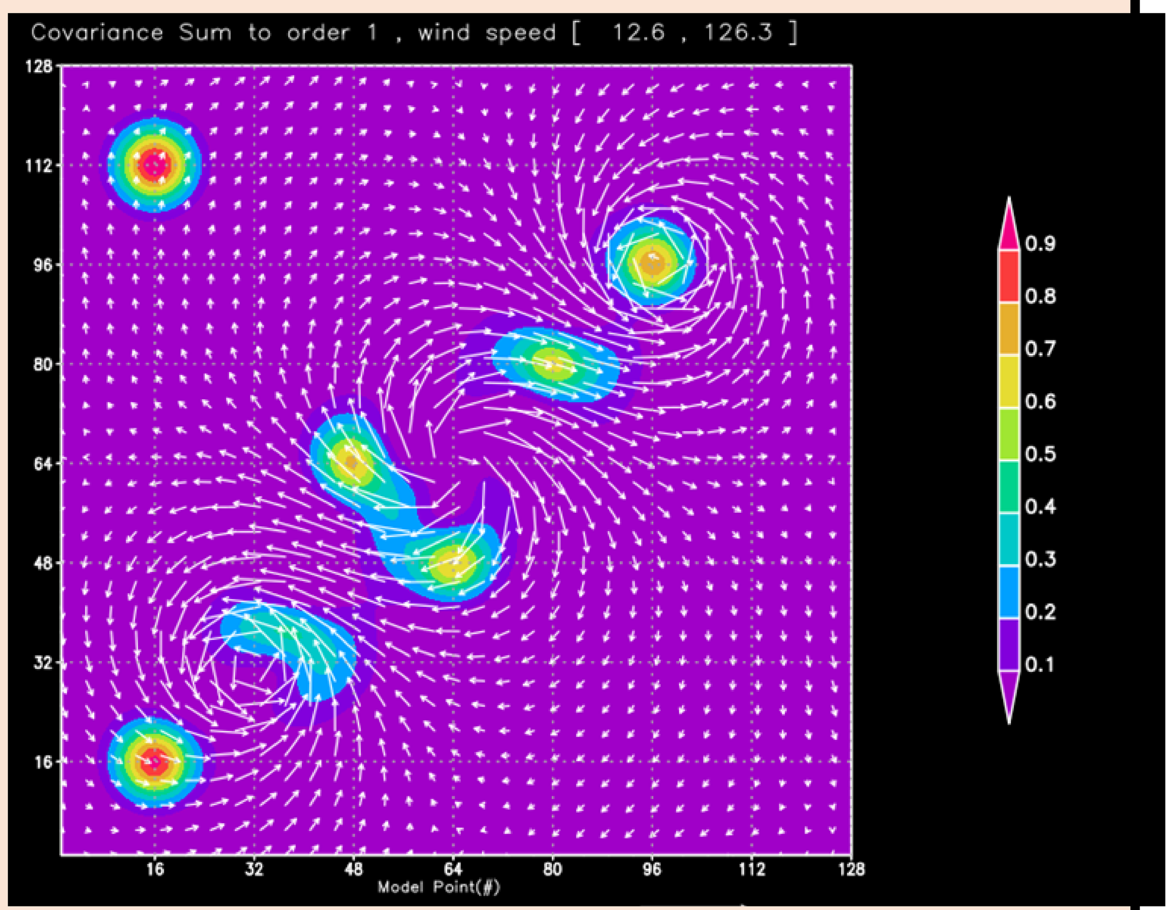
A Gaussian Approach to Flow-dependent Correlations

Green Functions and Correlation Functions

Green functions (GF) for differential equations often exhibit properties that make them suitable models for correlation functions. Loosely speaking, the GF of a differential self-adjoint operator is symmetric in its arguments and in many cases, depending on the specific problem, it is of definite sign. *GFs for generalized diffusion equations have been used to model correlation functions for many years in Ocean Data Assimilation*. The starting point here is the exploration of this analogy between GFs and correlation functions by following methods in other areas of physics where GFs play a prominent role. This is the case of Quantum Field Theory (QFT) where GFs are key ingredients at the time of calculating parameters like scattering cross-sections, transition probabilities, etc… that have to be interpreted in probabilistic terms. In this context one is often interested in corrections to probabilities that characterize a quantum system when this system is embedded in a classical (not random) external field. The solution is found by employing perturbative methods that calculate how this external field alters the propagation of the quantum system (its GF) with respect to the free dynamics described by a baseline GF_o



Modelling Flow-Dependent Covariances with Gaussian Integrals

Let then Δ be the random NWP model error field on an *N x N regular grid without boundaries*. The order-zero assumption for the statistics of this field is to consider it Gaussian and invariant by translations over the grid. According to the proposed analogy we think the B^{-1} term as the "kinetic term" of a Lagrangian, it represents the "free propagation" from node to node without external forces. For the interaction with an ambient field **V** there are different options at modeller's disposal, but there are also restrictions in order to guarantee the correctness of the model. For example, we can take the sum over the grid nodes of squares of error advection by **V**. The corrected covariances would then be given by

$$< \Delta_i \Delta_j > [\vec{V}] = \frac{1}{N(\vec{V})} \int \prod_h d\Delta_h \, \Delta_i \Delta_j \, e^{-\frac{1}{2}\left(\Delta^T B^{-1} \Delta + \mu \, tr\, [\vec{V} \vec{\nabla} \Delta] \, [\vec{V} \vec{\nabla} \Delta]^T\right)} \quad \textbf{(1)}$$

The notation emphasizes that the covariances are now functions of **V**, and therefore not anymore translational invariant, and that the normalization will depend also on this **V** field. The parameter μ is necessary to make the quantity in the exponent dimensionally homogeneous, and is a free parameter in the scheme. The expression **(1)** makes it apparent that the covariances computed by this method are symmetric and it also makes sense because that Gaussian integral exists, it gives a finite calculation because the exponent is a quadratic positive definite form

Formulation of the Algorithm. Choosing a Model

Consider a Gaussian random error field with covariance $B_o^{-1} = \frac{1}{\sigma} C_o^{-1} \frac{1}{\sigma}$ with C_o a baseline homogeneous and isotropic correlation matrix and then diagonal in k-space and dependent on the modulus of k only. The proposed model is this

$$B^{-1} = \frac{1}{\sigma} \, C^{-1} \frac{1}{\sigma} = \frac{1}{\sigma} \left[C_o^{-T/2} + \mu \, M^+ \right] \left[C_o^{-1/2} + \mu \, M \right] \frac{1}{\sigma} \quad \textbf{(2)}$$

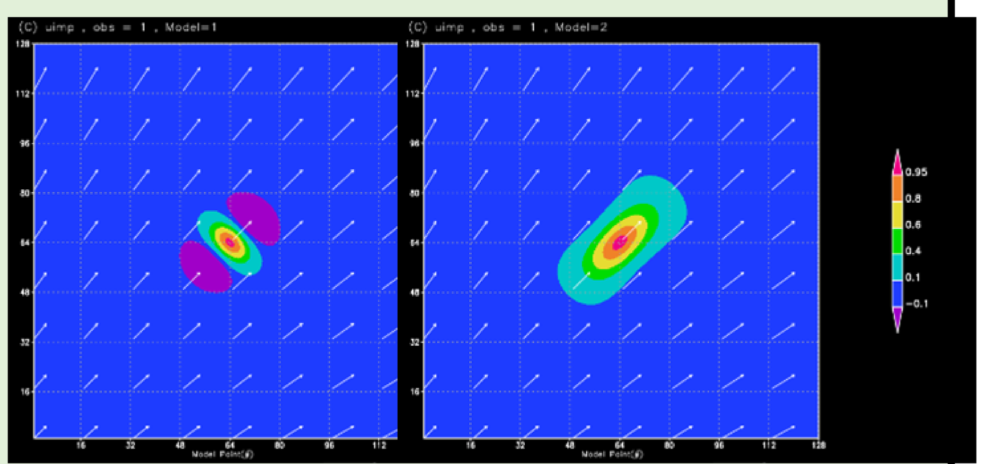
where M is the operator that implements our model and M^+ its adjoint. The real and positive parameter μ is necessary for dimensional reasons and will be important when calibrating the scheme. This B is obviously self-adjoint and positive and therefore a valid k-space representation of a covariance. For the actual computation of C a perturbative method in μ is proposed.

$$< (\Delta/\sigma)_k (\Delta/\sigma)_l > = L_k^m (L^+)_m^{-l} \approx C_o(k) \, \delta_k^{-l} - \mu \left(C_o^{1/2}(k) \, M_k^{-l} C_o(-l) + C_o(k) (M^+)_k^{-l} \, C_o^{1/2}(-l) \right) + \mu^2 \left(C_o^{1/2}(k) \sum_p M_k^p C_o(p) \, (M^+)_p^{-l} \, C_o^{1/2}(-l) \right) \quad \textbf{(3)}$$

For the specification of M we consider as basic building bloc the advection operator $Ad_x \equiv (\vec{V} \vec{\nabla} \Delta)_x$. In k-space we have the pair : $Ad_G^l = \frac{i}{N} \vec{V}_{G-l} \vec{S}_l$; $(Ad^+)_l^G = (Ad_G^l)^* = \frac{-i}{N} \vec{V}^*_{G-l} \vec{S}_l$

The first choice for M_k^l is just Ad_k^l. With this choice, the correlation model **(2)** reads in x-space

$$\Delta^T C^{-1} \Delta = \Delta^T C_o^{-1} \Delta + tr \left[\mu^2 (\vec{V} \vec{\nabla} \Delta) \, (\vec{V} \vec{\nabla} \Delta)^T \right] + \mu \left(\Delta^T C_o^{-\frac{T}{2}} (\vec{V} \vec{\nabla} \Delta) + (\vec{V} \vec{\nabla} \Delta)^T C_o^{-\frac{1}{2}} \Delta \right) \quad \textbf{(4)}$$



The last terms connect, through the baseline model error correlation (square-root) matrix, error in one location with error advection rate in another location. This is meaningful from the modeller's perspective but at difference with the other two terms, these terms have no definite sign. **(4)** is the exponent of the Gaussian pdf. Random configurations of Δ that give the smallest possible value to **(4)** are favoured. The first two terms cannot decrease more than zero, but the last terms (with μ positive) can become negative for advection down the gradient. This effect squeezes the Δ correlation isolines along the **V** direction (left panel of the figure). This deformation pattern may look unnatural.

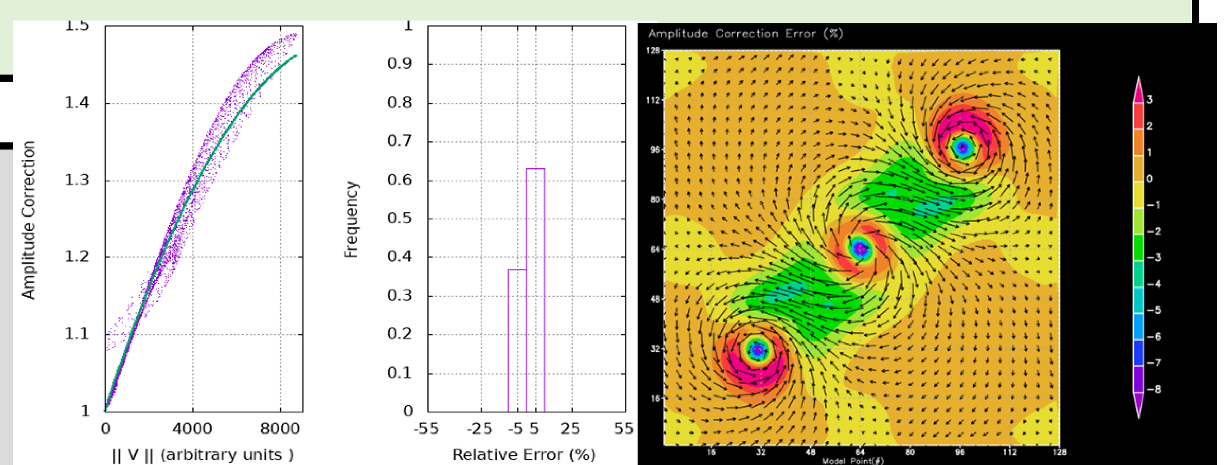
Other possibility is $M_k^l = (Ad^+)_k^s Ad_s^l$. It corresponds in x-space to the second term in **(4)** and we readily see that it favours an orthogonal relation between **V** and grad (Δ), with the result that correlation isolines are stretched along the **V** direction (right panel). In x-space, acting on the left, this operator is the familiar inhomogeneous diffusion operator

$$\vec{\nabla} \bullet \left(\vec{V} \, (\vec{V} \bullet \vec{\nabla} \Delta) \right) = \vec{\nabla} \bullet \left((\vec{V} \otimes \vec{V}) \vec{\nabla} \Delta \right)$$

The diffusion tensor here is singular, with (in 2D) one eigenvalue 0 and the other $v_1^2 + v_2^2$, with eigenvectors $(-v_2, v_1)$ and (v_1, v_2) respectively, there is no diffusion in the direction orthogonal to **V**. This is not a fundamental restriction of the method. We can consider two ambient fields **V, W**, and get a symmetric full-rank diffusion tensor. the M operator becomes

$$\left(Ad^+[\vec{V}]\right)_k^s \left(Ad[\vec{W}]\right)_s^l + \left(Ad^+[\vec{W}]\right)_k^s \left(Ad[\vec{V}]\right)_s^l \quad \leftrightarrow \quad \vec{\nabla} \bullet \left((\vec{V} \otimes \vec{W} + \vec{W} \otimes \vec{V}) \vec{\nabla} \Delta \right)$$

One advantage of this method is that we are not constrained to specific correlation models (Gaussian, Matérn, etc …). Any translation invariant baseline C_o function can be used in this scheme. We also notice that a linear combination of several choices is a valid option for M in **(2),** and also are operators with higher number of factors $(Ad^+)_k^l$ and/or $(Ad)_k^l$ .However, the computational burden increases when we introduce more complexity in M and gains in utility of the algorithm are arguable.



Calibration, Normalization and Implementation in an Operational Variational DA System

- The value for μ is determined by taking that value that makes the O (μ) term in **(3)** not bigger than a given fraction of the first term in **(3)** at any given location. This is a crude but practical way of introducing in the scheme the need for "convergence" of the perturbative computational method where **(3)** comes from

- The flow-dependent correlations so obtained do not satisfy the condition $C(\vec{x}\,\vec{x}) = 1 \; \forall \, \vec{x}$, which is necessary in order to conserve the amount of variance in the model error field. Inspired by methods used in the diffusion equations approach (which faces the same difficulty), we consider statistical regressions between the values of $tr[\vec{V}\vec{V}^T](\vec{x})$ and the amplitude corrections $ac(\vec{x})$ obtained by running equation **(3)** on unit-impulses at selected points in the domain. The amplitude correction parameter regresses well (left panel) with the trace of the deformation tensor built with **V,** although it can less accurate in areas of strong shear (right panel). The maximum relative error is below 10% , which is acceptable considering that model error variances are usually known with limited precision .

- The path to implement this scheme in the formulation of the background error covariance matrix B described in Derber and Bouttier (1999) is clear. This DB1999 formulation of B is integrated in many 3D-Var and 4D-Var DA systems exploited currently every day in many weather centres. In their notation, the covariance error matrix for the univariate controls is $B_u = B_u^{1/2} B_u^{T/2}$, which in turn decomposes as $B_u = V^{1/2} EDE^T V^{1/2}$ with V a diagonal matrix of variances on the model grid and EDE^T the covariance matrix for the vertical modes, one for each wavenumber. With this structure, a first implementation is to consider 2D **V** fields (one at each level) and reduces to the following substitution

$$V^{1/2} \;\Rightarrow\; \sigma \left(C_o^{1/2} - \mu \, C_o^{1/2} \, M C_o^{1/2} \right)$$