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Link between stochastic grid perturbation and location uncertainty framework

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Key Points:

- A rapidly moving grid can be a valid implementation of the Location Uncertainty (LU) framework in the absence of stochastic forcing
- Correlated noise in time and a compensating advection term are introduced to preserve both LU properties and structure of the original grid
- A statistical analysis highlights the importance of the compensation term in the implementation of the method

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Abstract

This paper investigates the relationship between a Stochastic Grid Perturbation (SGP) and Location Uncertainty (LU). The LU formulation, which introduces random velocity fluctuations, has shown efficacy in organizing large-scale flow and replicating long-term statistical characteristics. SGP was created as a simpler approach which perturbs the computational grid for ensemble members, aiming to simulate small uncertainties in high-resolution predictability studies. We aim to clarify the link between SGP and LU. After introducing the LU formalism, we derive the SGP method and discuss its connection to LU. Correlated noise in time is introduced in the SGP method to preserve the structure of the original grid. A compensating advection term is shown to preserve LU properties despite the latter correlated noise. Numerical experiments on a 3-layer Quasi-Geostrophic model compare various SGP implementations with an explicit LU implementation, highlighting the importance of the compensating advection term to achieve strict equivalence.

Plain Language Summary

This paper examines two methods to improve ocean and climate predictions: Stochastic Grid Perturbation (SGP) and Location Uncertainty (LU).

Location Uncertainty (LU): LU adds small, random changes to current speed and direction in models, helping to capture large-scale ocean patterns and maintain important physical properties like energy balance.

Stochastic Grid Perturbation (SGP): SGP slightly shifts the positions of grid points in numerical models to study the impact of small uncertainties in ocean forecasts, originally used for high-resolution studies of specific regions.

We explore the relationship between SGP and LU, finding that SGP can be adjusted to work similarly to LU. Through computer simulations, we validate our findings and examine some consequences of the possible discrepancies between the theoretical LU method and the practical SGP method. Understanding the link between SGP and LU can lead to better description of uncertainties in ocean and climate forecasts, aiding in planning and responding to extreme events and understanding climate change. Our goal is to make advanced techniques like LU more accessible for broader scientific use.

1 Introduction

The Location Uncertainty (LU) formulation introduced by Mémin (2014), which considers small random velocity fluctuations, has proven to be very precise in organizing large-scale flow (Bauer et al., 2020a) and in replicating long-term statistical characteristics (Bauer et al., 2020b; Li et al., 2023a) within the barotropic and baroclinic quasi-geostrophic models. It offers a rigorous alternative to inflation in data assimilation (Dufée et al., 2022) and strikes a favorable balance between representing model errors and ensemble spread (Brecht et al., 2021; Resseguier et al., 2021) across both the rotating shallow water model and the surface quasi-geostrophic model. The conservation properties observed in the deterministic model (e.g. energy or tracer’s moments) can also hold true in its stochastic counterpart (Brecht et al., 2021; Li et al., 2023a; Resseguier et al., 2017a) as well as their main theoretical convergence properties (Debussche et al., 2023; Lang et al., 2023). The theoretical respect for these invariants is essential as they ensure, for instance, a balance between variance production and dissipation. LU, for example, naturally incorporates a direct expression of the fluctuation-dissipation theorem, maintaining a strict equilibrium between the energy introduced by the noise and the energy dissipated by the system. Furthermore, convergence for vanishing noise to the deterministic equation (Chapron et al., 2018; Debussche et al., 2023), which is — like grid con-

vergence — not trivial for any stochastic parameterization, provides this scheme with physical consistency in terms of large-scale representation.

However, even if stochastic equations are more and more recommended for proper parameterizations as well as for ensemble simulation, the perceived difficulty of understanding and implementation is a barrier to widespread adoption.

Using another point of view, Leroux et al. (2022) proposed a method called here “Stochastic Grid Perturbation” (SGP) to control the covariance of their ensemble by rapidly perturbing the computational grid for each ensemble member. The aim was to simulate a small uncertainty in the numerical model in order to study its impact as part of a very high-resolution predictability study of the Western Mediterranean. This method resembles the Location Uncertainty formalism, where the position of the points fluctuate randomly.

In a data assimilation context, Zhen et al. (2023) replaced the inflation step by the application of an uncorrelated in time transport map (i.e. the state variables are modified along a displacement in the underlying coordinates). They formally find links to the LU framework and to the stochastic advection by Lie transport proposed by Holm (2015). Remapping the physical space is analogous to perturbing the grid points ; this indicates a possible connection between “Stochastic Grid Perturbation” (SGP) and the LU approach.

In this paper, we present a first attempt to clarify the link between SGP and Location Uncertainty (LU) and discuss the benefits of such Lagrangian parameterization. The plan is as follows: the LU formalism is first introduced in Section 2. The derivation of the SGP method is then discussed in Section 3 with a link to the LU formalism. Numerical experiments are carried out to compare several SGP implementations with an explicit LU implementation in Section 4. Finally, the link between LU and SGP is summarized in Section 5 together with a discussion on the application scenarios of SGP.

2 Equations of fluids under Location Uncertainty

This section presents the main points of the derivation of the Location Uncertainty framework. A more explicit derivation can be found in the Chapter 2 of Li (2021). The notations and properties are presented in a concise way in §2.1, and §2.2 details the derivation which will be linked to the Stochastic Grid Perturbation method.

2.1 Location Uncertainty formalism

The central hypothesis of the LU framework is the identification of two scales of motion: similarly to a Reynolds averaging, the evolution of the position of a particle \mathbf{X}_t has a large-scale contribution which is smooth and explicitly resolved and a small-scale unresolved component uncorrelated in time and referred to as noise:

$$d\mathbf{X}_t = \underbrace{\mathbf{v}(\mathbf{X}_t, t)dt}_{\text{Large scale motion}} + \underbrace{\sigma(\mathbf{X}_t, t)d\mathbf{B}_t}_{\text{Small scale uncertainty}} \quad (1)$$

The cylindrical Brownian motion $\mathbf{B}_t(\mathbf{x})$ is uncorrelated in time but correlated in space. The absence of time correlation can be seen as the assumption that the characteristic time of turbulence is much smaller than the numerical model’s time step. This implies that turbulent fluctuations decorrelate rapidly within each time step, allowing them to be treated as independent from one step to the next. The spatial correlation of the noise is enforced through the operator $\sigma(\mathbf{X}_t, t)$. The latter is a Hilbert-Schmidt integral operator and can thus be defined through a kernel $\check{\sigma}$:

$$\sigma(\mathbf{X}_t, t)d\mathbf{B}_t \triangleq \int_{\Omega} \check{\sigma}(\mathbf{X}_t, \mathbf{y}, t)d\mathbf{B}_t(\mathbf{y})d\mathbf{y}.$$

At this point, we need to make several comments on our notations:

- bold letters indicate that the values are in \mathbb{R}^2 . \mathbf{B}_t has hence two components and the kernel $\check{\sigma}$ is a 2×2 matrix.
- The computational domain Ω is a bounded domain of \mathbb{R}^2 .
- The differential notation used in (1) actually represents the equality between the integrated terms $\mathbf{X}_t - \mathbf{X}_0 = \int_0^t \mathbf{v} dt + \int_0^t \sigma d\mathbf{B}_t$ where the last integral is a Itô stochastic integral. The Itô integral is a martingale of null ensemble mean, which is why it is preferred to the Stratonovich integral in most settings based on LU. Despite the martingale property, the noise features a non-zero mean component through the introduction of a Girsanov Drift (see Li et al., 2023b): it consists in a change of probability measure and resembles a smooth transport term.

Finally, if q is a quantity such that $dq = 0$ (i.e. $q(\mathbf{X}_{t+\delta t}, t + \delta t) = q(\mathbf{X}_t, t)$) one can use the stochastic calculus tools to obtain the definition of the *stochastic transport operator*:

$$\mathbb{D}_t q \triangleq d_t q + (\mathbf{v}^* dt + \sigma d\mathbf{B}_t) \cdot \nabla q - \frac{1}{2} \nabla \cdot (\mathbf{a} \nabla q) dt = 0. \quad (2)$$

The variance \mathbf{a} of the noise (or one-point-one-time correlation matrix) is defined by $\mathbf{a}(\mathbf{x}, t) \triangleq \int_{\Omega} \check{\sigma}(\mathbf{x}, \mathbf{y}, t) \check{\sigma}^T(\mathbf{x}, \mathbf{y}, t) d\mathbf{y}$. The effective velocity \mathbf{v}^* is defined by $\mathbf{v}^* \triangleq \mathbf{v} - \frac{1}{2} \nabla \cdot \mathbf{a} + \sigma^T (\nabla \cdot \sigma)$.

The differences between the total (Lagrangian) derivative $dq \triangleq q(X_{t+\delta t}, t + \delta t) - q(X_t, t)$, the temporal Eulerian increment $d_t q \triangleq q(X_t, t + \delta t) - q(X_t, t)$ and the stochastic transport operator $\mathbb{D}_t q$ are essential. Indeed, as we will see in §3, the Stochastic Grid Perturbation method consists in connecting the first two operators and aims to simulate the last one.

2.2 Detailed derivation

This section contains the technical derivation of the stochastic transport operator \mathbb{D}_t which is crucial for the upcoming proof of the Stochastic Grid Perturbation method. Readers focused on the final results can skip this Section without losing the main thread.

The starting point of the LU derivation is the Ito-Wentzell formula (Kunita, 1990) which is a chain rule for random (semimartingale) functions with random (semimartingale) arguments:

Ito-Wentzell formula. *Let $f(\mathbf{x}, t)$ be a C^2 -process over $\mathbf{x} \in \mathbb{R}^d$ and C^1 -semimartingale over $t \in \mathbb{R}^+$; let \mathbf{X} be a semimartingale over $\Omega \subset \mathbb{R}^d$. $f(\mathbf{X}, t)$ is a semimartingale satisfying*

$$df = d_t f + \sum_{i=1}^d \frac{\partial f}{\partial x_i} d\mathbf{X}^i + \frac{1}{2} \sum_{i,j=1}^d \frac{\partial^2 f}{\partial x_i \partial x_j} d\langle X^i, X^j \rangle_t + \sum_{i=1}^d d\langle \frac{\partial f}{\partial x_i}(X, \bullet), X^i \rangle_t \quad (3)$$

Applying the Ito-Wentzell formula (3) to $dq(\mathbf{X}_t, t)$ decomposes the total derivative dq into a time increment $d_t q$ (which plays the role of a partial derivative), a transport term $(v + \sigma d\mathbf{B}_t) \cdot \nabla q$ and additional quadratic co-variation terms:

$$dq = d_t q + \sum_{i=1}^d \frac{\partial q}{\partial x_i} (\sigma d\mathbf{B}_t)^i + \frac{1}{2} \sum_{i,j=1}^d \frac{\partial^2 q}{\partial x_i \partial x_j} d\langle X^i, X^j \rangle_t + \sum_{i=1}^d d\langle \frac{\partial q}{\partial x_i}(X, \bullet), X^i \rangle_t + v \cdot \nabla q dt \quad (4)$$

Following the derivation of Li et al. (2023a), the quadratic co-variation $d\langle X^i, X^j \rangle_t$ is equal to $a_{ij} dt$. The time increment $d_t q$ is then decomposed into its smooth component and its time uncorrelated component:

$$d_t q = f(\mathbf{X}_t, t) dt + \int_{\Omega} \sum_{k=1}^d g_k(\mathbf{X}_t, y, t) d\mathbf{B}_t^k(y) dy. \quad (5)$$

The quadratic co-variation depends only on the uncorrelated parts. The gradient of the tracer can hence be replaced by its uncorrelated component in the quadratic co-variation with the stochastic flow:

$$\left\langle \frac{\partial q}{\partial x_i}, X^i \right\rangle_t = \int_{\Omega} \sum_{j=1}^d \check{\sigma}_{ij}(\mathbf{X}_t, \mathbf{y}, t) \frac{\partial g_j}{\partial x_i}(\mathbf{X}_t, \mathbf{y}, t) d\mathbf{y}, \quad \forall i = 1, \dots, d \quad (6)$$

This leads to use the canonical decomposition of semi-martingales (i.e. the decomposition (5) is unique) to identify f and g in the equation $dq = 0$:

$$\begin{aligned} f &= -\frac{1}{2} \sum_{i,j=1}^d a_{ij} \frac{\partial^2 q}{\partial x_i \partial x_j} - \int_{\Omega} \sum_{j=1}^d \check{\sigma}_{ij}(\mathbf{X}_t, \mathbf{y}, t) \frac{\partial g_j}{\partial x_i}(\mathbf{X}_t, \mathbf{y}, t) d\mathbf{y} - \mathbf{v} \cdot \nabla q \\ g_j &= -\sum_{k=1}^d \check{\sigma}_{jk} \frac{\partial q}{\partial x_k}. \end{aligned} \quad (7)$$

This identification specifies $d_t q$ for a tracer conserved by the flow. It depends notably on the quadratic co-variation (6) which can be further expanded with the substitution of g_j . After some calculus, one obtains

$$\int_{\Omega} \check{\sigma}_{ij} \frac{\partial g_j}{\partial x_i} = -\underbrace{\frac{1}{2} a_{ik} \frac{\partial^2 q}{\partial x_i \partial x_k}}_{\text{cancelled (in } f)} - \underbrace{\frac{1}{2} \frac{\partial}{\partial x_i} \left(a_{ik} \frac{\partial q}{\partial x_k} \right)}_{\nabla \cdot (a \nabla q)} - \underbrace{\frac{1}{2} \frac{\partial a_{ik}}{\partial x_i} \frac{\partial q}{\partial x_k} + \sigma_{jk} \frac{\sigma_{ij}}{\partial x_i} \frac{\partial q}{\partial x_k}}_{(\mathbf{v}^* - \mathbf{v}) \cdot \nabla q} \quad (8)$$

where the summation are dropped for sake of simplicity. By replacing f and g in (5), one obtains the definition of the stochastic transport operator (2):

$$\mathbb{D}_t q \triangleq d_t q + (\mathbf{v}^* dt + \sigma d\mathbf{B}_t) \cdot \nabla q - \frac{1}{2} \nabla \cdot (\mathbf{a} \nabla q) dt = 0.$$

This derivation was based on the assumption $dq = 0$ but it can be extended to other equations involving dq (e.g. Resseguier et al., 2017b).

3 Stochastic Grid Perturbation

Let us consider a Finite Difference space discretization where the grid points are noted \mathbf{x}_i , i being a space index. The Stochastic Grid Perturbation method consists in moving grid points in a Lagrangian manner following the small scale uncertainty (see Figure 1). The continuous formulation in time reads:

$$\mathbf{x}_i^{\text{Brownian}}(t) - \mathbf{x}_i(0) = \int_0^t (\sigma d\mathbf{B}_t)_i \quad (9)$$

This method is illustrated in §3.1 with the simple example of a transport equation and is compared with the Location Uncertainty (LU) framework. Then §3.2 presents how time correlation in the grid motion (to keep the structure of the grid) can be compensated by an additional advection term. The exact link between the Stochastic Grid Perturbation method and Location Uncertainty is then discussed in §3.3.

3.1 Transport equation on a perturbed grid

We first show the effect of using the Stochastic Grid Perturbation method on the transport equation $\partial_t q dt = -\mathbf{v} \nabla q dt$. The left-hand side loses its time differentiability under the Stochastic Grid Perturbation method and becomes

$$q(\mathbf{x}_i^{\text{Brownian}}(t + \delta t), t + \delta t) - q(\mathbf{x}_i^{\text{Brownian}}(t), t).$$

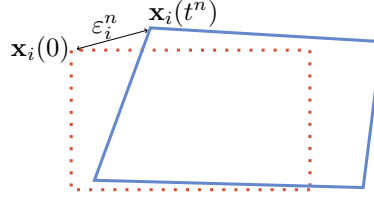


Figure 1. Illustration of the grid perturbation: dotted lines represent the initial grid and solid lines represent the perturbed grid at time t^n . All points are drifted to the right in order to illustrate the fact that the noise is spatially correlated.

- In the particular case where $\mathbf{v} = 0$, one can recognize a Lagrangian discretization of a cancelling total derivative $dq = 0$. The total derivative and the presence of noise is at the heart of the LU framework. Following the derivation of the stochastic transport operator in §2.2 with $\mathbf{v} = 0$, one then obtains

$$\begin{cases} d\mathbf{x}_i^{\text{Brownian}} &= (\sigma d\mathbf{B}_t)_i \\ dq(\mathbf{x}_i, t) &= 0 \end{cases} \implies \mathbb{D}_t q = 0, \quad (\mathbf{v} = 0) \quad (10)$$

- In the general case with any \mathbf{v} , the left-hand side can be noted $d_t(q \circ \mathbf{x}_i^{\text{Brownian}})$ (where \circ is the composition) and represents a material derivative taking only the uncorrelated part of the velocity into account (see §3.3). The derivation of §2.2 can still be followed by applying the Ito-Wentzell formula (3) on $d_t(q \circ \mathbf{x}_i^{\text{Brownian}}, t) + v \cdot \nabla q dt$ which gives the right-hand side of (4). The canonical decomposition of semimartingales is then used on the equation $d_t(q \circ \mathbf{x}_i^{\text{Brownian}}, t) = -v \cdot \nabla q dt$, which yields the system (7). Assuming a perfect discretization of ∇q , one finally obtains

$$\begin{cases} d\mathbf{x}_i^{\text{Brownian}} &= (\sigma d\mathbf{B}_t)_i \\ d_t(q \circ \mathbf{x}_i^{\text{Brownian}}) &= -\mathbf{v}(\mathbf{x}_i, t) \cdot \nabla q dt \end{cases} \implies \mathbb{D}_t q = 0 \quad (11)$$

For the transport equation, the perturbed grid ($\mathbf{x}_i^{\text{Brownian}}$) hence implements the stochastic transport operator \mathbb{D}_t defined in (2).

However, $\int_0^t \sigma d\mathbf{B}_t$ is not bounded and the distance between a grid point $\mathbf{x}_i^{\text{Brownian}}(t)$ and its original location $\mathbf{x}_i^{\text{Brownian}}(0)$ possibly increases infinitely. As consequences, the grid loses its structure with time and the evaluation of ∇q potentially reduces its accuracy. Two solutions can be applied to keep the grid close to its original disposition:

- Restore the grid to its original state by interpolating all the variables. However, this global interpolation has a significant cost. It is interesting to note that in the particular case of some semi-Lagrangian models, an interpolation is already implemented to realign the grid points to their original positions.
- Introduce a time-correlated noise which keeps $\mathbf{x}_i(t) - \mathbf{x}_i(0)$ close to zero. This is the subject of §3.2.

3.2 Ornstein-Uhlenbeck processes in Stochastic Grid Perturbation

In their grid perturbation, Leroux et al. (2022) did not use a Brownian motion but an auto-regressive process. The crucial property of auto-regressive processes is their possible bounded variance which removes the problem of grid divergence mentioned earlier. Let us note the current perturbation of a grid point $\varepsilon_i^n = \mathbf{x}_i(t^n) - \mathbf{x}_i(0)$ as in Figure 1. The first order Auto-Regressive process AR(1) is

$$\varepsilon_i^n = e^{-\alpha \delta t} \varepsilon_i^{n-1} + \sigma(B(t_n) - B(t_{n-1})) \quad (12)$$

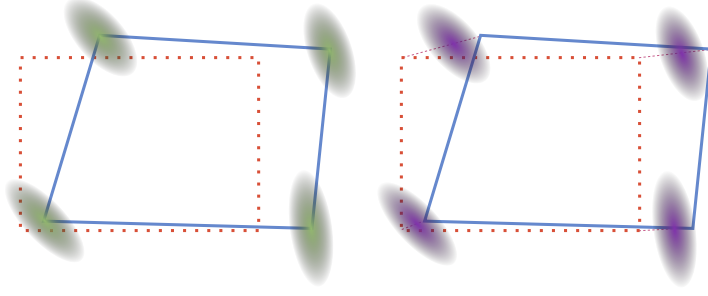


Figure 2. Representation of Brownian (left) and Auto-Regressive (right) noises for the grid perturbation. Dotted lines are the initial grid, solid lines are the current perturbed grid, and the ellipses represent the positions of the future grid points. Auto-Regressive processes perform a translation of the probability density function from the current grid towards the initial grid.

where $e^{-\alpha\delta t}$ is slightly smaller than 1 to ensure that the variance of AR(1) is bounded for $n \rightarrow \infty$. The continuous counterparts of AR(1) are Ornstein-Uhlenbeck processes R_t , which satisfy the stochastic differential equation

$$dR_t = -\alpha R_t dt + \sigma d\mathbf{B}_t, \quad R_0 = 0. \quad (13)$$

Injecting equation (13) in (11) yields

$$\begin{cases} d\mathbf{x}_i^{\text{Brownian}} &= \alpha R_t dt + dR_t \\ d_t(q \circ \mathbf{x}_i^{\text{Brownian}}) &= -\mathbf{v}(\mathbf{x}_i, t) \cdot \nabla q dt \end{cases} \implies \mathbb{D}_t q = 0 \quad (14)$$

Similarly to §3.1, the nudging term $\alpha R_t dt$ can be “transferred” from the first line to the second line of the system. The effect is to change the noise of the perturbation and to compensate this change by an additional advection term which depends on the current displacement of the grid:

$$\begin{cases} d\mathbf{x}_i^{\text{O-U}} &= dR_t \\ d_t(q \circ \mathbf{x}_i^{\text{O-U}}) &= (-\mathbf{v}(\mathbf{x}_i, t) + \alpha R_t) \cdot \nabla q dt \end{cases} \implies \mathbb{D}_t q = 0 \quad (15)$$

Figure 2 represents the difference between Brownian and Auto-Regressive processes in the Stochastic Grid Perturbation method. It should be noted that the probability density function is simply translated towards the initial grid in the second case.

Remark. *In a discrete in time setting, the AR(1) process can replace Ornstein-Uhlenbeck process in the previous operations and the compensation can be derived at the discrete level. One then obtains*

$$\underbrace{\sigma(\mathbf{B}(t_n) - \mathbf{B}(t_{n-1}))}_{\text{“}\sigma d\mathbf{B}_t\text{”}} = \underbrace{(\varepsilon_i^n - \varepsilon_i^{n-1})}_{\text{“}dR_t\text{”}} + \underbrace{(1 - e^{-\alpha\delta t})\varepsilon_i^{n-1}}_{\text{“}\alpha R_t dt\text{”}}$$

Following the continuous case, the compensation term $\alpha R_t \cdot \nabla q dt$ can be discretized by $((1 - e^{-\alpha\delta t})\varepsilon_i^{n-1}) \cdot \nabla q$. It is interesting to note that the compensation uses the grid displacement at the former time step and not at the current one. The grid at the former time step must hence be stored to implement this discrete compensation term.

3.3 General link between SGP and LU

Let us define the operator ∂_t^{SGP} which represents (at the continuous level in time) a partial derivative in time under the Stochastic Grid Perturbation method: for a quantity θ , its definition is $\partial_t^{\text{SGP}} \theta \triangleq d_t(\theta \circ \mathbf{x}_i^{\text{Brownian}})$. If a Ornstein-Uhlenbeck is used to

keep the grid close to its original state (as it was proposed in §3.2), then one can use an alternative (but equivalent) definition: $\partial_t^{\text{SGP}}\theta \triangleq d_t(\theta \circ \mathbf{x}_i^{\text{O-U}}) - \alpha R_t \cdot \nabla\theta dt$. This Section clarifies the links and differences between $\partial_t^{\text{SGP}}\theta$, the total variation $d\theta$ and the stochastic transport operator $\mathbb{D}_t\theta$.

Applying the Ito-Wentzell formula (3) to $\partial_t^{\text{SGP}}\theta$, one obtains:

$$\partial_t^{\text{SGP}}\theta = d_t\theta + \sum_{i=1}^d \frac{\partial\theta}{\partial x_i} (\sigma d\mathbf{B}_t)^i + \frac{1}{2} \sum_{i,j=1}^d \frac{\partial^2\theta}{\partial x_i \partial x_j} d\langle X^i, X^j \rangle_t + \sum_{i=1}^d d\left\langle \frac{\partial\theta}{\partial x_i} (X, \bullet), X^i \right\rangle_t. \quad (16)$$

This operator ∂_t^{SGP} takes into account only the uncorrelated component of the velocity. The variations $d\theta$ and $\partial_t^{\text{SGP}}\theta$ (given by equations (4) and (16), respectively) differ only from the presence of a transport by the smooth component of the velocity:

$$\partial_t^{\text{SGP}}\theta = d\theta - \mathbf{v} \cdot \nabla\theta dt. \quad (17)$$

The SGP operator is hence equivalent to the total derivative without the smooth velocity.

Note that in (16) that the last term $d\langle \frac{\partial\theta}{\partial x_i} (X, \bullet), X^i \rangle_t$ depends on the equation under consideration: for instance for $\partial_t^{\text{SGP}}\theta + \mathbf{v} \cdot \nabla\theta dt = 0$, this term leads (as explained in §2.2) to $\partial_t^{\text{SGP}}\theta + \mathbf{v} \cdot \nabla\theta = \mathbb{D}_t\theta$. Conversely, the presence of a non-zero right-hand side can instigate a modification in $\partial_t^{\text{SGP}}\theta$, causing it to diverge from \mathbb{D}_t (which is defined independently of the equation). The rest of this Section focuses on explaining this difference between the Stochastic Grid Perturbation and Eulerian implementations of the Location Uncertainty parameterization.

The appendix B of Resseguier et al. (2017a) derives the difference between the material derivative and the stochastic transport operator. This difference is non-zero only in the presence of a stochastic forcing. They decompose $\mathbb{D}_t\theta$ into a smooth part $f dt$ and an uncorrelated component $\mathbf{h}^T d\mathbf{B}_t$:

$$\mathbb{D}_t\theta = f dt + \mathbf{h}^T d\mathbf{B}_t. \quad (18)$$

This decomposition leads them to $d\theta = \mathbb{D}_t\theta + tr(\sigma^T \nabla \mathbf{h}^T) dt$, which gives us a relation between the stochastic transport operator and the partial derivative in time under Stochastic Grid Perturbation:

$$\partial_t^{\text{SGP}}\theta + \mathbf{v} \cdot \nabla\theta dt = d\theta = \mathbb{D}_t\theta + tr(\sigma^T \nabla \mathbf{h}^T) dt. \quad (19)$$

To illustrate the importance of the term $tr(\sigma^T \nabla \mathbf{h}^T)$, let us consider the example of the Quasi-Geostrophic (QG) equations. In the numerical experiments of Section 4, the QG equations will be based on the transport of potential vorticity and feature no stochastic forcing (see §4.1). This formulation ensures that $tr(\sigma^T \nabla \mathbf{h}^T) = 0$. Conversely, in Li et al. (2023a) one can see that when considering Quasi-Geostrophic equations based on the momentum $\mathbf{u} = (u, v)$ one has $\mathbf{h}^T d\mathbf{B}_t = \beta y \mathbf{k} \times \sigma_h d\mathbf{B}_t$. More precisely,

$$\begin{pmatrix} \mathbf{h}_u^T d\mathbf{B}_t \\ \mathbf{h}_v^T d\mathbf{B}_t \end{pmatrix} = \beta y \mathbf{k} \times \sigma_h d\mathbf{B}_t = \beta y \begin{pmatrix} -(\sigma_h d\mathbf{B}_t)_y \\ (\sigma_h d\mathbf{B}_t)_x \end{pmatrix} = \beta y \begin{pmatrix} -\sigma_{21} & -\sigma_{22} \\ \sigma_{11} & \sigma_{12} \end{pmatrix} d\mathbf{B}_t.$$

This noise is additive and a simplified form of $tr(\sigma^T \nabla \mathbf{h}_u^T)$, $tr(\sigma^T \nabla \mathbf{h}_v^T)$ can be derived. The difference between $(\partial_t^{\text{SGP}}\mathbf{u} + \mathbf{v} \cdot \nabla\mathbf{u} dt)$ and $\mathbb{D}_t\mathbf{u}$ is finally

$$\begin{pmatrix} tr(\sigma^T \nabla \mathbf{h}_u^T) \\ tr(\sigma^T \nabla \mathbf{h}_v^T) \end{pmatrix} dt = \beta y \begin{pmatrix} -\sum_i \sigma_{i\bullet} \partial_i \cdot \sigma_{2\bullet} \\ \sum_i \sigma_{i\bullet} \partial_i \cdot \sigma_{1\bullet} \end{pmatrix} dt + \beta \begin{pmatrix} \sigma_{21}^2 + \sigma_{22}^2 \\ \sigma_{1\bullet} \cdot \sigma_{2\bullet} \end{pmatrix} dt \quad (20)$$

Injecting the values of β, y, σ used in the numerical experiments of Section 4, we numerically obtain that $\frac{\|tr(\sigma^T \nabla \mathbf{h}^T) dt\|_\infty}{\|d\mathbf{u}\|_\infty} < 10^{-4}$ and $\frac{\|tr(\sigma^T \nabla \mathbf{h}^T) dt\|_2}{\|d\mathbf{u}\|_2} < 10^{-3}$. This suggests that the difference between SGP and LU is minimal in practice.

In the opposite case of systems which do not contain any stochastic forcing the SGP is strictly equivalent to the stochastic transport operator:

$$\partial_t^{\text{SGP}} q + \mathbf{v} \cdot \nabla q dt = \mathbb{D}_t q \quad (21)$$

This strict equivalence notably occurs in the equations numerically studied in the following Section.

4 Numerical Experiments

In this section we examine the Stochastic Grid Perturbation method applied on a 3-layer Quasi-Geostrophic (QG) model described in §4.1. Several simulations using different approaches are described in §4.2. Those simulations are compared qualitatively in §4.3 then quantitatively in §4.4.

4.1 Numerical Model description

The numerical model we used was created by Thiry et al. (2023) and slightly modified to make the Stochastic Grid Perturbation possible. This model is described here again for completeness. In all the numerical experiments the prognostic variables are the potential vorticity $\mathbf{q} = \begin{bmatrix} q_1 \\ q_2 \\ q_3 \end{bmatrix}$ (in s^{-1}) and the dynamic pressure $\mathbf{p} = \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}$ (in $\text{m}^2 \cdot \text{s}^{-2}$), stacked in three isopycnal layers. The 3-layer QG equations read:

$$\partial_t \mathbf{q} = \frac{1}{f_0} J(\mathbf{q}, \mathbf{p}) + f_0 B \mathbf{e} - \frac{a_4}{f_0} \Delta^2 (\Delta \mathbf{p}), \quad (22)$$

$$(\Delta - f_0^2 A) \mathbf{p} = f_0 \mathbf{q} - f_0 \beta (y - y_0), \quad (23)$$

where Δ is the horizontal Laplacian, Δ^2 the biharmonic operator, $J(a, b) = \partial_x a \partial_y b - \partial_x b \partial_y a$ stands for the Jacobi operator, $f_0 + \beta(y - y_0)$ is the Coriolis parameter under beta-plane approximation with the meridional axis centered on y_0 , and a_4 is the biharmonic viscosity coefficient.

The three-layer QG equations are integrated in a mid-latitude-centered rectangular ocean box model configuration, similar to the implementation used by Hogg et al. (2005). The ocean circulation is driven by a stationary, symmetrical wind stress at the surface and a linear Ekman stress at the bottom, generating an eastward turbulent jet featuring an idealized Gulf Stream in which spontaneous eddy production takes place. Despite its simplicity, such an idealized model is capable of producing meaningful mesoscale dynamics provided horizontal resolution is sufficiently high and viscosity is relatively low. In this paper, simulations were carried out with a horizontal resolution of 40, 10 and 5 km. The numerical model setup was further modified by Thiry et al. (2023) to make the Stochastic Grid Perturbation method possible.

Table 1 gives the values of the parameters shared by all simulations. The values of B , \mathbf{e} , A , given by Thiry et al. (2023), are:

$$B = \begin{bmatrix} \frac{1}{H_1} & \frac{-1}{H_1} & 0 & 0 \\ 0 & \frac{1}{H_2} & \frac{-1}{H_2} & 0 \\ 0 & 0 & \frac{1}{H_3} & \frac{-1}{H_3} \end{bmatrix}, \quad \mathbf{e} = \begin{bmatrix} \partial_x \tau^y - \partial_y \tau^x \\ 0 \\ 0 \\ \frac{\delta_{ek}}{2|f_0|} \Delta p_3 \end{bmatrix}, \quad \vec{\tau} = \tau_0 \begin{bmatrix} -\cos(2\pi y/L_y) \\ 0 \end{bmatrix}, \quad (24)$$

where τ_0 represents the surface wind magnitude, H_k is the background thickness of the k -th layer and δ_{ek} is the thickness of the lower Ekman layer. The vertical stratification

L_x, L_y	Double-gyre 3-layer QG (3840 × 4800)km
H_k	(350, 750, 2900)m
$g'_{k+0.5}$	(0.025, 0.0125) ms ⁻²
δ_{ek}	2m
τ_0	2×10^{-5} m ² s ⁻²
Simulation time	1 year
Time step	2 hours
Temporal scheme	SSRK3
a_4	5×10^{11} m ⁴ s ⁻¹
f_0	9.37×10^{-5} s ⁻¹
β	1.75×10^{-11} m ⁻¹ s ⁻¹
α	5×10^{-5} s ⁻¹

Table 1. Model parameters shared by all simulations.

of this model is described by the term $-f_0^2 A \mathbf{p}$ where

$$A = \begin{bmatrix} \frac{1}{H_1 g'_{1.5}} & \frac{-1}{H_1 g'_{1.5}} & 0 \\ \frac{-1}{H_2 g'_{1.5}} & \frac{1}{H_2} \left(\frac{1}{g'_{1.5}} + \frac{1}{g'_{2.5}} \right) & \frac{-1}{H_2 g'_{2.5}} \\ 0 & \frac{-1}{H_3 g'_{2.5}} & \frac{1}{H_3 g'_{2.5}} \end{bmatrix}, \quad (25)$$

with $g'_{k+0.5}$ the reduced gravity defined between layers k and $k + 1$.

The noise $\sigma d\mathbf{B}_t$ is computed through offline analysis of high-resolution simulations based on Empirical Orthogonal Functions (see Li et al., 2023b). Specifically, high-pass filtering is applied to high-resolution simulation data to extract streamfunction fluctuations, from which velocity fluctuations are derived and aggregated into $N = 50$ orthogonal modes via the EOF procedure. The semi-martingale associated with the noise is then represented as a linear combination of these modes, weighted by standard Brownian motions:

$$\sigma(\mathbf{x})d\mathbf{B}_t = \sum_{i < N} \sqrt{\lambda_i} \Phi_i(\mathbf{x}) d\xi_t^i + \mathbf{\Gamma}(\mathbf{x}) dt$$

where λ_i is the eigenvalue associated with the spatial mode Φ_i and $(d\xi_t^i)_{i < N}$ denote independent and identically distributed standard Brownian motions. The drift term $\mathbf{\Gamma}$ is introduced through Girsanov transformation (change of probability measure), with the aim of replicating the mid-latitude jet observed in the high-resolution experiment.

This choice of σ is tailored for the LU model to resemble a high-resolution simulation. Consequently, if a method differs from the LU model, using the same noise parameterization is likely to result in a solution that does not resemble the high-resolution simulation. This discrepancy indicates a divergence from the LU model rather than an absolute measure of the method’s performance. In fact, it would be possible to parameterize σ specifically for this method to achieve better results.

4.2 Stochastic Grid Perturbation and Metric Perturbation

The perturbation described in Leroux et al. (2022) does not consist in perturbing the grid points but instead the grid metric. The associated experiment is hence called “Perturbed Steps” and will be compared to the Stochastic Grid Perturbation presented in this paper, named “Perturbed Points”. Figure 3 illustrates the difference between the two approaches. In a rectangular grid, the perturbation of the space steps amounts to modify $\sigma d\mathbf{B}_t$ with a cumulative sum from the lower space indices to the greater ones. This is illustrated on the bottom of Figure 3 where the grid points with a cumulative

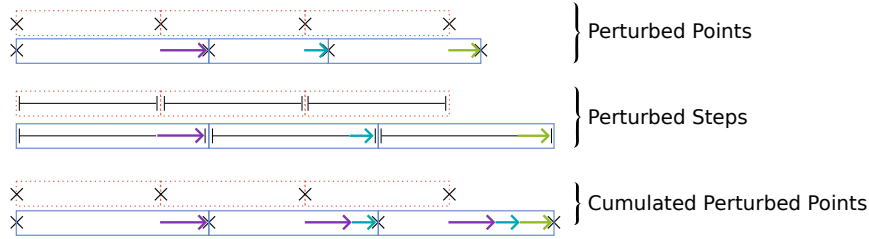


Figure 3. Illustration of the grid perturbation methods “Perturbed Points” (top) where the noise is applied to the grid points and “Perturbed Steps” (center) where the noise is applied to the space steps. The dotted orange rectangles represent the initial grid and blue rectangles represent the perturbed grid. On the bottom is an illustration of the equivalence between “Perturbed Points” with a cumulative sum of the noise and “Perturbed Steps”.

noise are aligned with the grid points of the “Perturbed steps” method. Inversely, moving the grid points would amount to modify the “Perturbed steps” noise by taking its difference between consecutive steps. There is hence no fundamental difference behind the distinction between “Perturbed Steps” and “Perturbed Points”. Nevertheless, we will see that the choice between the two methods significantly changes the behavior of the model if σ is kept the same.

In both cases, an Auto-Regressive process is used to preserve the structure of the grid. As it is explained in §3.2, a compensation (i.e. the additional advective term) is introduced in the “Perturbed points” method to recover the effects of an uncorrelated noise in time.

Remark. *The choice of the nudging intensity parameter α depends on the structure and intensity of the noise. In our numerical simulations, $\alpha = 5 \times 10^{-5} \text{ s}^{-1}$ which gives $e^{-\alpha \delta t} \approx 0.7$ for our choice of δt . The goal was to minimise α while keeping the perturbation small compared to the space step: $\epsilon_i \ll \delta x$. The value of α was chosen by hand through numerical experiments to prevent negative space steps and avoid reliance on numerical thresholds.*

To focus on the effect of the grid perturbation, the same advective term is applied to the “Perturbed steps” method. As it is illustrated on the bottom of Figure 3, the displacement of the grid points can be large in the latter method, especially with space-correlated noise. The control of the parameters of such a noise is also a difficult task because of a possible strong accumulation effect. Using this displacement to compute the compensation term leads to high advection speed which would require to drastically decrease the time step. Consequently, at the price of a possible theoretical inconsistency, the displacement of the “Perturbed points” method was used to compute the compensation, even in the “Perturbed steps” method. We consider 6 ensemble simulations (30 members each):

- Deterministic : High¹ (10km) and low (40km) resolution
- Explicit LU
- Perturbed Steps
- Perturbed Points

¹In the high resolution simulation the hyper-viscosity parameter was reduced to $a_4 = 10^{10} \text{ m}^4 \cdot \text{s}^{-1}$. Keeping this parameter constant does not significantly change the simulation compared to the low resolution simulation, but would require a time step 10 times smaller.

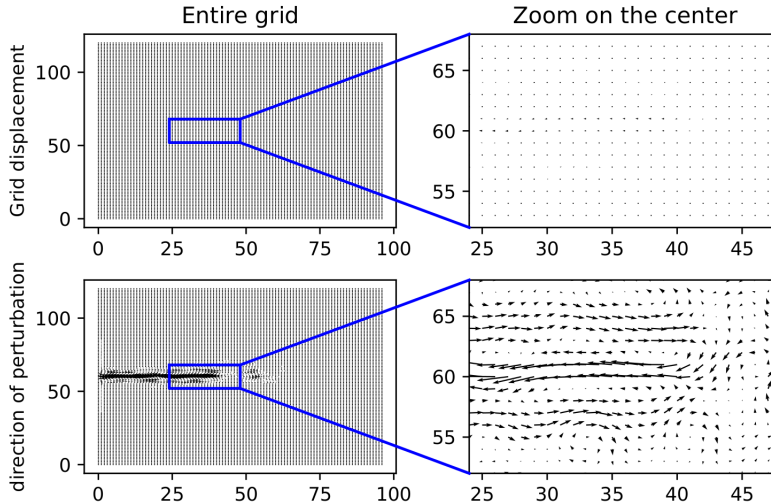


Figure 4. Visualization of the perturbation of the grid generated by the SGP method for one of the ensemble members at the end of a one-year simulation. Arrows linking the initial grid to the perturbed grid are plotted: the length of the arrows was multiplied tenfold in the bottom part to better visualise the direction of the perturbation. On the left, the whole grid is represented and the right panel is a zoom on a smaller portion.

- Perturbed Points without the compensation term

Figure 4 shows the perturbation applied in the “Perturbed Points” case, and serves also as a representation of the noise. The noise features a so-called Girsanov drift to obtain a jet that is similar to the one in the deterministic High Resolution (HR) simulation (Li et al., 2023a).

Creation of the initial ensemble A very high resolution (5km, with the hyper-viscosity coefficient reduced to $a_4 = 2.10^9 \text{ m}^4\text{s}^{-1}$) deterministic simulation at statistical equilibrium is used to create the initial ensemble. Assuming that the turbulence is sufficiently decorrelated in time, a snapshot of the very high resolution simulation is taken every 6 months in a 15-year simulation. To adjust the level of energy to the low resolution experiments, the (low resolution) explicit LU code then integrates in time all those snapshots for one year. For the 10km-resolution deterministic experiments, the snapshots of the 5km-resolution are used directly.

4.3 Qualitative study

In this section we focus on the solution profile at the end of the one-year simulation. Figures 5 and 6 respectively present the averaged pressure and potential vorticity. The average is computed both over the ensemble and over the last week of a one-year simulation. Firstly, it can be observed that the LU formalism allows for the generation of a jet that is much more pronounced than without noise injection. The solutions of the “Perturbed Points” and “Perturbed Steps” methods do exhibit such an energetic jet: the behaviour of SGP is hence similar to LU in this regard. However, in the absence of the compensation term (experiment “Without compensation”), the jet is slightly less pronounced.

Figure 7 provides the standard deviation of the surface pressure of the ensemble simulations. The standard deviation is also computed both over the ensemble and over

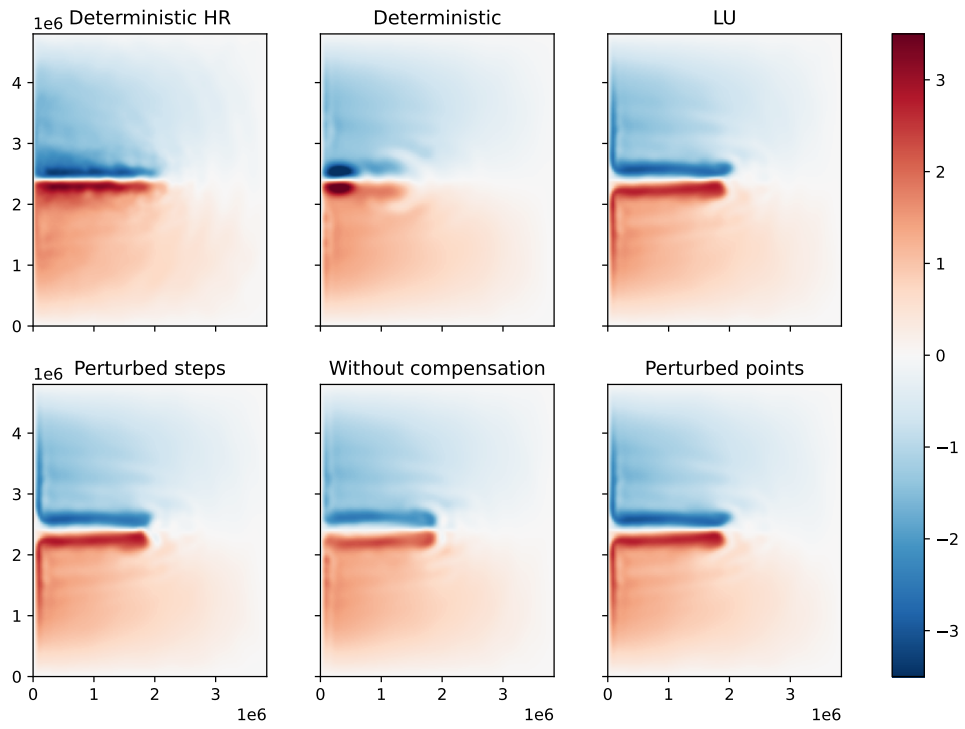


Figure 5. Surface pressure (in $\text{m}^2 \cdot \text{s}^{-2}$) averaged over the last week of a one-year simulation.

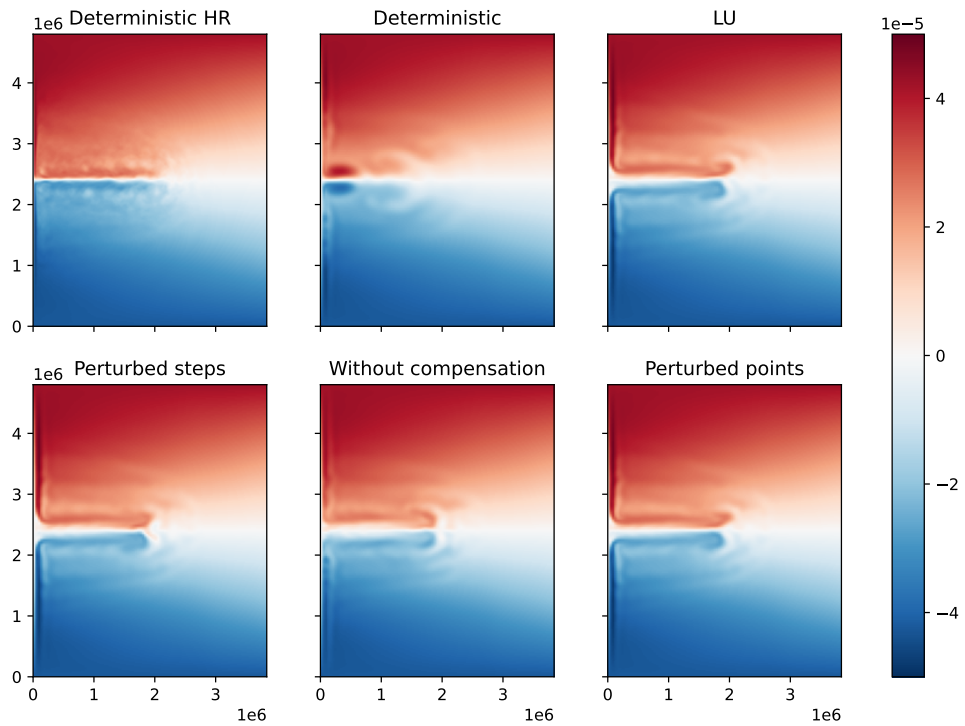


Figure 6. Surface potential vorticity (in s^{-1}) averaged over the last week of a one-year simulation.

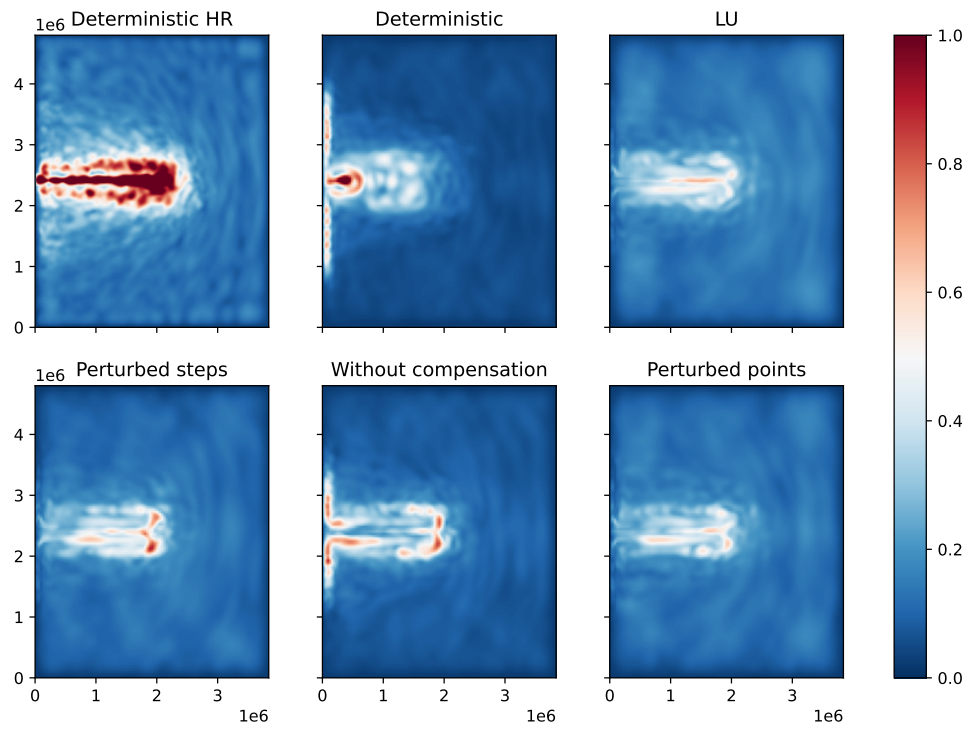


Figure 7. Point-wise standard deviation of surface pressure computed over the ensemble and over the last week of a one-year simulation.

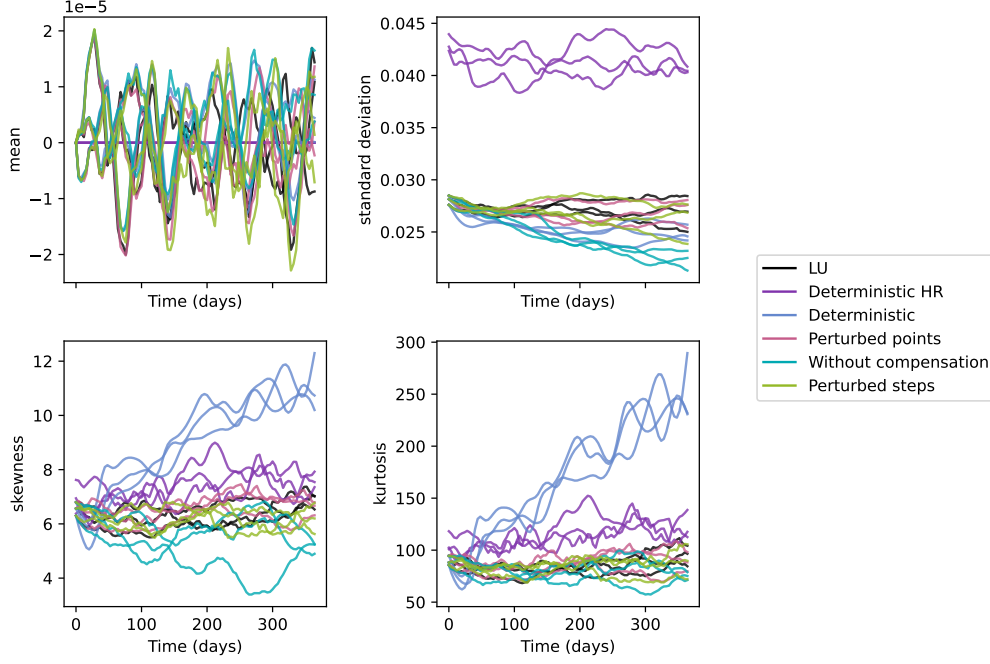


Figure 8. First four standardized moments of the variable u (reconstructed from p). Only 3 ensemble members out of 30 are displayed for each ensemble to facilitate better visualization.

the last week of the one-year simulation. It shows that, without the compensation term (“Without compensation”), the standard deviation is more concentrated at the center of the domain: it is stronger at the jet level and globally weaker in the rest of the basin. The compensation term seems hence to play a crucial role in transferring ensemble variability from grid points to the state variables. Interestingly, the “Perturbed steps” simulation also seems to exhibit a higher ensemble variance at the jet level compared to the LU approach.

4.4 Quantitative study

Figures 8 and 9 display the first four spatially computed standardized moments of u and q , respectively. We note $m_i(u, t) = \frac{1}{V} \iiint (u(\mathbf{x}, t) - \bar{u}(\mathbf{x}, t))^i d\mathbf{x}$ the i -th order central moment ($i \geq 2$), where V is the basin volume and $\bar{u}(\mathbf{x}, t)$ is the ensemble average of u . The standard deviation, skewness and kurtosis are respectively defined by $\sqrt{m_2}$, $\frac{m_3}{(m_2)^{1.5}}$ and $\frac{m_4}{(m_2)^2}$. One can see on those figures that the statistics of the “Perturbed points” ensemble are close to those of the “LU” ensemble. The two other presented methods approximate certain statistics at the expense of others:

- The mean vorticity with the “Perturbed steps” method significantly differs from other methods. Cumulative noise from low to high indices results in stronger noise in one gyre, creating average vorticity. In a separate experiment (not depicted), cumulative sum in each gyre leads indeed to a fourfold smaller vorticity creation. It was also tested to remove the compensation term in this “Perturbed steps” experiment: doing so also reduce by half the vorticity creation. The displacement of the “Perturbed points” method used to compute the compensation (see §4.1) may be a cause of vorticity creation. However there is still an unidentified vor-

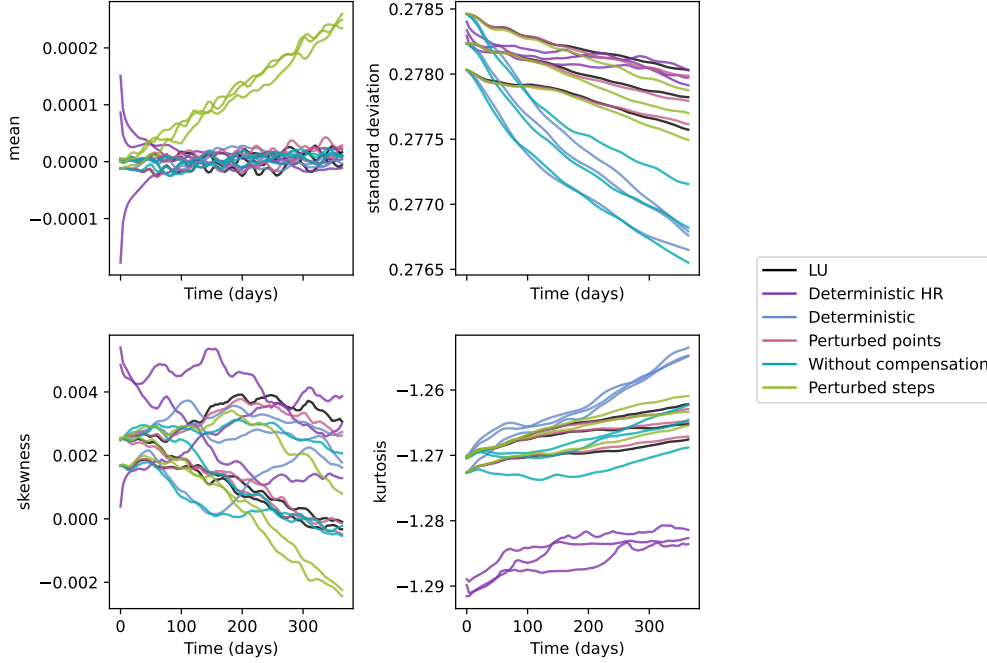


Figure 9. First four standardized moments of the variable q . As in Figure 8, only 3 ensemble members out of 30 are displayed for each ensemble simulation.

ticity source, as removing the compensation term while using the cumulative sum in each gyre does not completely cancel the vorticity creation.

- The standard deviation for both variables is underestimated with the method “Without compensation”. The compensation term of the “Perturbed points” method is indeed one of the keys of the transfer of the variability from the grid points to the variables u and q .

Figure 8 also features interesting characteristics of skewness and kurtosis. First, the positive skewness of the variable u suggests that extreme values are predominantly positive. The latter observation is expected, as this double-gyre configuration is characterized by the east-directed flow concentrating the extreme values. Second, the kurtosis of u in the deterministic case is much larger than in the stochastic cases, indicating more extreme values. It can be noted that the deterministic simulation appears to have a slightly higher variance than the noise without compensation. This suggests that the high skewness and kurtosis of the low resolution deterministic simulation does not come from small values of the variance. Figure 6 hints that in the absence of a clear jet, the deterministic (LR) experiment may create extreme values located on the west side between the two gyres. Note that the spatial statistics of the high-resolution deterministic experiments are displayed for completeness but are difficult to compare to the low-resolution experiments.

An additional moment analysis (not shown) centered on the jet area yields the same conclusions, except that the variance, kurtosis and skewness of the low-resolution deterministic simulation are a lot smaller, indicating the absence of a clear jet. The vorticity creation of the “Perturbed steps” method is also largely reduced, indicating that it does not come from the jet.

Finally, these figures (for the sake of readability) only display 3 out of the 30 ensemble members. Comparing the statistics of two ensembles can be done using the Wasser-

	Deterministic	Perturbed points	Without compensation	Perturbed steps
MEAN	1.502	0.048	1.730	0.074
STD	2.272	0.155	4.436	0.416
SKEWNESS	33.139	0.471	5.772	0.738
KURTOSIS	92.389	0.420	1.435	0.567

Table 2. Relative distance to LU for the velocity u .

	Deterministic	Perturbed points	Without compensation	Perturbed steps
MEAN	0.168	1.466	0.293	643.695
STD	7.442	0.005	7.423	0.056
SKEWNESS	0.746	0.040	0.172	0.907
KURTOSIS	1.581	0.012	0.771	0.098

Table 3. Relative distance to LU for the vorticity q .

stein distance. This involves finding the permutation $\pi : \llbracket 1, 30 \rrbracket \rightarrow \llbracket 1, 30 \rrbracket$ that minimizes the term-wise distance: $\inf_{\pi} \left(\frac{1}{30} \sum_{i=1}^{30} \|X_i - Y_{\pi(i)}\|^2 \right)^{\frac{1}{2}}$. This allows for the comparison of ensemble simulations for a given statistic. Tables 2 and 3 (summarized in Figure 10, (a)) provide the *relative distance to LU*. A reference is calculated by taking the Wasserstein distance between the first 15 and the last 15 members of the same ensemble from the 'LU' experiment (for a given turbulent statistic). The *relative distance to LU* is the Wasserstein distance between two ensembles divided by the latter reference. It can be understood as the member-to-member distance divided by the distance between members of the LU ensemble.

Figure 10 presents on radar charts the relative distance to LU for each standardized moments of u and q . The left panel (a) is a summary of Tables 2 and 3 where the moments take into account the whole computational domain. Conversely, the moments are computed only on an area around the jet to create the right panel (b). Those radar charts are in line with the previous conclusions: the statistics of the ‘‘Perturbed points’’ ensemble are indeed close to those of the ‘‘LU’’ ensemble. All the methods introducing a stochastic noise are closer to LU than the deterministic simulation, with the exception of the systematic creation of vorticity of the ‘‘Perturbed steps’’ method. The latter remark does not apply as strongly when the moments are computed in the vicinity of the jet only. Finally, it is also seen that the relative difference to LU is often smaller than 1. This means that the variability of the LU ensemble for those moments is larger than the difference between the studied approaches.

5 Conclusion

5.1 Summary

This paper has presented a Stochastic Grid Perturbation method based on autoregressive processes that is equivalent to an explicit implementation of the LU method. To achieve strict equivalence, a compensation term has been added in the form of advection. The importance of this compensation has been numerically studied, and the validity of the grid perturbation method has been confirmed. Perturbing grid steps differs from perturbing grid points: transitioning between the two is akin to modifying the operator σ fundamentally, altering the statistical characteristics of the solutions.

In the model employed here, the stochastic transport operator applied to q was a significant choice. As it was mentioned in Section 3.3 considering velocity u as a prognostic variable under LU assumptions results in a system with distinct properties. It has

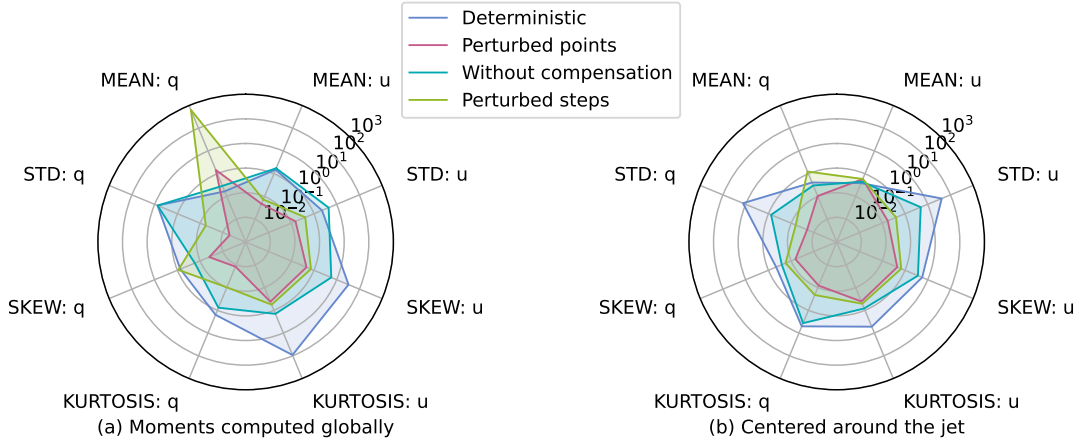


Figure 10. Log scaled radar chart showing the relative distance to LU for the first four standardized moments of the variables u and q . Left panel (a): summary of Tables 2 and 3: the standardized moments are computed on the whole computational domain. Right panel (b): additional analysis where the standardized moments are computed on a smaller portion of the domain, including the jet area.

been shown that with the presence of a stochastic right-hand side, the effect of grid perturbation can differ from the stochastic transport operator although a numerical estimation hints that this difference may be small for the Quasi-Geostrophic equations.

This paper addresses the link between LU and SGP by modifying the SGP method to make it similar to LU. This approach is quite natural because LU offers more theoretical guarantees such as energy conservation along trajectories. However, one could alternatively design a noise term $\sigma d\mathbf{B}_t$ to express the SGP method as an instance of LU and study its properties. This noise would feature a Girsanov drift based on its past trajectory. Investigating such a noise within the LU framework would be interesting but challenging.

5.2 Application scenarios and limitations of SGP

The starting point of this study is the implementation of SGP in NEMO (Leroux et al., 2022). This implementation was motivated by the apparent simplicity of perturbing the grid to control the spread of an ensemble. However, their goal was not to implement exactly a LU method and the noise introduced was homogeneous. Indeed, the main difficulty of most LU implementation is the parameterization of the operator σ . This can be achieved for instance through offline analysis of high-resolution simulations based on Empirical Orthogonal Functions (Tucciarone et al., 2023) or more elaborate approach (Tucciarone et al., 2024).

When the SGP described in this paper is integrated into an Eulerian code with the compensation term, it combines the stochastic Eulerian transport of the compensation term with grid perturbation. In contrast, explicitly implementing LU would solely necessitate a stochastic Eulerian transport.

Within a code built upon an Arbitrary Lagrangian Eulerian framework, grid points can undergo direct perturbation using $\sigma d\mathbf{B}_t$ without the need for Ornstein-Uhlenbeck processes and a compensation term.

Applying the SGP method amounts to treat the smooth component of the motion in an Eulerian manner while using a Lagrangian method for the uncorrelated motion. This is somewhat similar to the so-called fractional-step methods (e.g. Huerta & Casadei, 1994), widely used in Arbitrary Eulerian Lagrangian frameworks. Therefore, this study presents the option of a semi-Lagrangian implementation of the LU equations, which holds more significance for semi-Lagrangian frameworks. Future work could focus on adapting this semi-Lagrangian setting to other discretization methods, such as Finite Volume methods.

Open Research Section

The numerical model, the code for statistical analyses and the code generating the Figures and Tables can be found in the repository “Stochastic Grid Perturbation” (Clement & Li, 2024) at address https://gricad-gitlab.univ-grenoble-alpes.fr/clemensi/qgm_sgp. The latter Python3.10 code is under MIT license. Moreover, the datasets containing the outputs of the simulations used in the Figures are available in Zenodo (Clement, 2024) at <https://doi.org/10.5281/zenodo.11650897>.

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