Modelling uncertainty using circulation-preserving stochastic transport noise in a 2-layer quasi-geostrophic model

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Abstract

The stochastic variational approach for geophysical fluid dynamics was introduced by Holm (Proc Roy Soc A, 2015) as a framework for deriving stochastic parameterisations for unresolved scales. The key feature of transport noise is that it respects the Kelvin circulation theorem. This paper applies the variational stochastic parameterisation in a two-layer quasi-geostrophic model for a β-plane channel flow configuration. The parameterisation is tested by comparing it with a deterministic high resolution eddy-resolving solution that has reached statistical equilibrium. We describe a stochastic time-stepping scheme for the two-layer model and discuss its consistency in time. Then we describe a procedure for estimating the stochastic forcing to approximate unresolved components using data from the high resolution deterministic simulation. We compare an ensemble of stochastic solutions at lower resolution with the numerical solution of the deterministic model. These computations quantify the uncertainty of the coarse grid computation relative to the fine grid computation. The results show that the proposed parameterisation is efficient and effective for both homogeneous and heterogeneous flows, and they lay a solid foundation for data assimilation.

Keywords: Stochastic parameterisations, Stochastic Lie transport, Geophysical fluid dynamics, Multi-layer quasi-geostrophic model

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1 Introduction

1.1 Motivation

To be useful for input to computational simulations and verification of output from these simulations, the observed data that numerical computations of weather and climate cannot resolve well enough to simulate in real time must be interpolated, extrapolated and spread over scales that allow real-time computational simulations. This is the process of “upscaling”, or “coarse graining” of the fine-scale data for use in computational simulations at coarser scales.

The goal of the present paper is to quantify the uncertainty in the process of upscaling, or coarse graining of fine-scale computationally simulated data for use in computational simulations at coarser scales, in the example of two-level quasigeostrophic channel flow. Accomplishing this goal corresponds to taking the step from (ii) to (iii) in the well-known linked chain of discovery in climate science, which is

(i) driven by large datasets and new methods for its analysis;
(ii) informed by rigorous mathematical derivations and analyses of stochastic geophysical fluid equations;
(iii) quantified using computer simulations, evaluated for uncertainty, variability and model error;
(iv) optimized by cutting edge data assimilation techniques, then
(v) compared with new observation datasets to determine what further analysis and improvements will be needed.

The question for coarse graining that we address in this paper is the following:

How can we use computationally simulated surrogate data at highly resolved scales, in combination with the mathematics of stochastic processes in nonlinear dynamical systems, to estimate and model the effects on the simulated variability at much coarser scales of the computationally unresolvable, small, rapid, scales of motion at the finer scales?

We will address this question in the context of two-level quasigeostrophic channel flow.

Our approach is guided by recent results in [Cotter et al., 2017] which showed that a multi-scale decomposition of the deterministic Lagrange-to-Euler fluid flow map $g_t$ into a slow large-scale mean and a rapidly fluctuating small-scale map leads to Lagrangian fluid paths $x_t = g_t X$ with $g_0 = I_d$ on a manifold $\mathcal{D}$ governed by the stochastic process $g_t \in \text{Diff}(\mathcal{D})$ on the Lie group of diffeomorphic flows, which appears in the same form as had been proposed and studied for fluids in [Holm, 2015]; namely,

$$
\begin{align*}
    dx_t &= dg_t X = u_t(x) dt + \sum_{i=1}^{N} \xi_i(x) \circ dW^i_t = u_t(g_t X) dt + \sum_{i=1}^{N} \xi_i(g_t X) \circ dW^i_t, \quad (1)
\end{align*}
$$

where $x = g_t X$, $d$ represents stochastic differentiation, the vector fields $\xi_i(x)$ for $i = 1, 2, \ldots, N$, are prescribed functions of the Eulerian spatial coordinates, $x$ in the domain of flow $\mathcal{D}$, and $\circ dW^i(t)$ denotes the Stratonovich differential with independent Brownian motions $dW^i(t)$. The stochastic process for the evolution of the Lagrangian process $g_t$ in equation (1) involves the pullback of the Eulerian total velocity vector field, which comprises the sum of a drift displacement vector field $u_t(x) dt$ plus a sum over terms in $\xi_i(x)$ representing the (assumed stationary) spatial correlations of the temporal noise in the Stratonovich representation, each with its own independent Brownian motion in time.

In [Holm, 2015] the velocity decomposition formula (1) was applied in the Hamilton-Clebsch variational principle to derive coadjoint motion equations as stochastic partial differential equations (SPDEs) whose ensemble of realizations can be used to quantify the uncertainty in the slow dynamics of the resolved mean velocity $u_t(x)$. Under the conditions imposed in the derivation of formula (1) in [Cotter et al., 2017] using homogenization theory, the sum of vector fields in (1) that had been treated in [Holm, 2015] from the viewpoint of stochastic coadjoint motion was found to represent a bona fide decomposition of the fluid transport velocity into a mean plus fluctuating flow.
1.2 Data-driven modelling of uncertainty

As opposed to theory-driven models such as Newtonian force laws and thermodynamic processes for the subgrid-scale dynamics, here we will make use of stochastic geometric mechanics as an opportunity to consider a stochastic version of data-driven modelling. In data-driven modelling, one seeks to model properties of a subsystem of a given dynamical system which, for example, may be observable at length or time scales which are below the resolution of available initial and boundary conditions, or scales finer than the resolution of numerical simulations of the dynamical system based on the assumed exact equations.

The most familiar example of data-driven modelling occurs in numerical weather prediction (NWP). In NWP, various numerically unresolvable, but observable, local subgrid-scale processes, such as formation of fronts and generation of tropical cyclones, are expected to have profound effects on the variability of the weather. These subgrid-scale processes must be parameterized at the resolved scales of the numerical simulations. Of course, the accuracy of a given parameterization model often remains uncertain. In fact, even the possibility of modelling subgrid-scale properties in terms of resolved-scale quantities available to simulations may sometimes be questionable. However, if some information about the statistics of the small-scale excitations is known, such as the spatial correlations of its observed transport properties at the resolved scales, one may arguably consider modelling the effects of the small scale dynamics on the resolved scales by a stochastic transport process whose spatial correlations match the observations, at the computationally unresolvable scales. As we will see, the eigenvectors of the correlation matrix of the observations will provide the modes of the subscale motion, to be modelled by applying stochasticity with the statistics of the unresolved scales.

1.3 The main content of the paper

The rest of the paper is structured as follows. Section 2 focuses on the derivation of the stochastic multilayer quasi-geostrophic (QG) equations using the variational approach proposed by Holm [2015]. It starts from the derivation of the deterministic \(N\)-layer QG model in Section 2.1 followed by the Hamiltonian formulation for the stochastic \(N\)-layer QG equations given in Section 2.2, which is then specialised to the case of two layers with a flat bottom for the remainder of this paper.

Section 3 describes our numerical approach to the deterministic and stochastic QG equations. In particular, Section 3.1.1 focuses on the numerical method for the deterministic QG model, and Section 3.1.2 presents numerical results for the case of heterogeneous (Figure 2) and homogeneous (Figure 3) flow, namely

- High-resolution deterministic solution \(q^f\);
- Low-resolution deterministic solution (also referred to as the truth or the true solution), \(q^a\), computed as the solution of the elliptic equation (22) with the stream function \(\psi^a\), where \(\psi^a\) is computed by spatially averaging the high-resolution stream function \(\psi^f\) over the coarse grid cell;
- Low-resolution deterministic solution, \(q^m\), computed by simulating the QG model;
- Decorrelation time for the true solution \(q^a\) (Figure 4).

The stochastic version of the numerical method is given in Section 3.2.1. We show that the numerical method for the stochastic QG equations is in Stratonovich form and prove its consistency in time (Section 3.2.2). In Section 3.2.3 we present a procedure of computing physically-consistent stochastic initial conditions and numerically test its correctness (Figure 5).

Section 4 describes our algorithm for calibrating the eigenvectors and demonstrates the approach using numerical results. In particular, we use the Lagrangian framework to quantify uncertainty in the homogeneous and inhomogeneous flow regimes and to analyse:

- The relative error between the true deterministic solution and the solution approximated with the leading Empirical Orthogonal Functions (EOFs) and their corresponding principal components, in particular its dependence as a function of EOFs (Figure 6, Section 4.2);
- The spread of stochastic solutions (also referred to as ensemble members), and how it depends on the number of EOFs and the size of the stochastic ensemble (Figures 7 and 8) in instantaneous snapshots (Section 4.3);
• The stochastic spread averaged over the Lagrangian particles in both fast and slow flow regions, and its dependence as a function of the number of EOFs and the size of the ensemble over time (Figures 10 and 11, Section 4.3);

• Along with the uncertainty quantification results for Lagrangian particles, we apply EOFs to the stochastic QG equations in Section 4.4 and study uncertainty quantification with respect to the number of EOFs and the size of the stochastic ensemble for the heterogeneous (Figure 12) and homogeneous (Figure 13) flows;

• In order to compare the modelled deterministic solution $q^m$ and stochastic solution with the true solution $q^a$, we study uncertainty quantification with respect to the number of EOFs and the size of the stochastic ensemble for the heterogeneous (Figure 14) and homogeneous (Figure 15) flows in the deterministic QG model.

In Section 5 we provide conclusions and outlook for future research.

2 Hamiltonian equations of motion for a multi-layer fluid

2.1 A deterministic $N$-layer quasi-geostrophic (NLQG) fluid

Consider a stratified fluid of $N$ superimposed layers of constant densities $\rho_1 < \cdots < \rho_N$; the layers being stacked according to increasing density, such that the density of the upper layer is $\rho_1$. The quasi-geostrophic (QG) approximation assumes that the velocity field is constant in the vertical direction and that in the horizontal direction the motion obeys a system of coupled incompressible shallow water equations. We shall denote by $u_i = (-\partial_y \psi_i, \partial_x \psi_i) = \mathbf{z} \times \nabla \psi_i$ the velocity field of the $i^{th}$ layer, where $\psi_i$ is its stream function, and the layers are numbered from the top to the bottom. We define the generalised total vorticity of the $i^{th}$ layer as

$$\omega_i = q_i + f_i = \Delta \psi_i + \alpha_i \sum_{j=1}^N T_{ij} \psi_j + f_i = \sum_{j=1}^N E_{ij} \psi_j + f_i, \quad i = 1, \ldots, N, \tag{2}$$

where the generalised total vorticity is defined as $\omega_i = q_i + f_i$, the elliptic operator $E_{ij}$ defines the layer vorticity,

$$q_i = \sum_{j=1}^N E_{ij} \psi_j := \Delta \psi_i + \alpha_i \sum_{j=1}^N T_{ij} \psi_j,$$

and the constant parameters $\alpha_i, f_i, f_0, \beta, f_N$ are

$$\alpha_i = \left(\frac{f_0}{g}\right)(\rho_{i+1} - \rho_i)/\rho_0 D_i, \quad i = 1, \ldots, N,$$

$$f_i = f_0 + \beta y, \quad i = 1, \ldots, N - 1,$$

$$f_N = f_0 + \beta y + f_0 d(y)/D_N,$$

$$f_0 = 2\Omega \sin(\phi_0), \quad \beta = 2\Omega \cos(\phi_0)/R,$$

where $g$ is the gravitational acceleration, $\rho_0 = (1/N)(\rho_1 + \cdots + \rho_N)$ is the mean density, $D_i$ is the mean thickness of the $i^{th}$ layer, $R$ is the Earth’s radius, $\Omega$ is the Earth’s angular velocity, $\phi_0$ is the reference latitude, and $d(y)$ is the shape of the bottom. The $N \times N$ symmetric tri-diagonal matrix $T_{ij}$ represents the second-order difference operator,

$$\sum_{j=1}^N T_{ij} \psi_j = (\psi_{i-1} - \psi_i) - (\psi_i - \psi_{i+1}), \tag{4}$$

so that

$$T_{ij} = \begin{bmatrix} -1 & 1 & 0 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & \cdots & 1 & 0 \\ 0 & \cdots & \cdots & 0 & 1 & -2 \\ 0 & \cdots & \cdots & 0 & 0 & 1 \\ 0 & \cdots & \cdots & 0 & 0 & -1 \end{bmatrix}, \quad i, j = 1, \ldots, N. \tag{5}$$

With these standard notations, the motion of the NLQG fluid is given by

$$\partial_t q_i \equiv \left\{ \omega_i, \psi_i \right\}_{xy} \cdot \nabla \psi_i = -\mathbf{z} \times \nabla \psi_i \cdot \nabla \omega_i = -u_i \cdot \nabla \omega_i, \quad i = 1, \ldots, N, \tag{6}$$
where \( \mathbf{z} \) is the vertical unit vector, \( \mathbf{u}_i = \mathbf{z} \times \nabla \psi_i \) is the horizontal flow velocity in the \( i^{th} \) layer, and the brackets in

\[
\{ \omega, \psi \} = J(\omega, \psi) = \omega_x \psi_y - \omega_y \psi_x = \mathbf{z} \cdot \nabla \omega \times \nabla \psi
\]  

(7)
denote the usual \( xy \) canonical Poisson bracket in \( \mathbb{R}^2 \). The boundary conditions in a compact domain \( D \subset \mathbb{R}^2 \) with smooth boundary \( \omega_j \partial D_j = \text{constant} \), whereas in the entire \( \mathbb{R}^2 \) they are \( \lim_{(x,y) \to \infty} \nabla \psi_j = 0 \). The space of variables with canonical Poisson bracket in (7) consists of \( N \)-tuples \( (q_1, \ldots, q_N) \) of real-valued functions on \( D \) (the “generalized vorticities”) with the above boundary conditions and certain smoothness properties that guarantee that solutions are at least of class \( C^1 \). The Hamiltonian for the \( N \)-layer vorticity dynamics in (6) is the total energy

\[
H(q_1, \ldots, q_N) = \frac{1}{2} \int_D \left[ \sum_{i=1}^N \frac{1}{\alpha_i} |\nabla \psi_i|^2 + \sum_{i=1}^{N-1} (\psi_{i+1} - \psi_i)^2 \right] dx \, dy, \quad i = 1, \ldots, N,
\]  

(8)
with stream function \( \psi_i \) determined from vorticity \( \omega_i \) by solving the elliptic equation (2) for \( q_i = \omega_i - f_i \) with

\[
q_i = \sum_{j=1}^N E^{-1}_{ij} \psi_j,
\]  

(9)
for the boundary conditions discussed above. Hence, we find that

\[
H(q_1, \ldots, q_N) = -\frac{1}{2} \int_D \sum_{i,j=1}^N q_i E_{ij} \psi_j dx \, dy = -\frac{1}{2} \int_D \sum_{i,j=1}^N q_i E^{-1}_{ij} * q_j dx \, dy = -\frac{1}{2} \int D \sum_{i=1}^N q_i \psi_i dx \, dy,
\]  

(10)
where \( E^{-1}_{ij} * q_j = \psi_i \) denotes convolution with the Greens function \( E^{-1}_{ij} \) for the symmetric elliptic operator \( E_{ij} \). The relation (10) means that \( \delta H/\delta q_i = \psi_i \) for the variational derivative of the Hamiltonian functional \( H \) with respect to the function \( q_j \).

**Lie–Poisson bracket.** Equations (6) are Hamiltonian with respect to the Lie–Poisson bracket on the dual of \( \bigoplus \sum_{i=1}^N \mathcal{F}(D) \) given by

\[
\{ F, H \}(q_1, \ldots, q_N) = \sum_{i=1}^N \int_D (q_i + f_i(x)) \left\{ \frac{\delta F}{\delta q_i}, \frac{\delta H}{\delta q_i} \right\}_{xy} dx \, dy,
\]  

(11)
provided the domain of flow \( D \) is simply connected.\(^1\)

The motion equations (6) for \( q_i \) now follow from the Lie–Poisson bracket (11) after an integration by parts to write it equivalently as

\[
\frac{dF}{dt} = \{ F, H \}(q_1, \ldots, q_N) = -\sum_{i=1}^N \int_D \frac{\delta F}{\delta q_i} \left\{ q_i + f_i(x), \frac{\delta H}{\delta q_i} \right\}_{xy} dx \, dy,
\]  

(12)
and recalling that \( \delta H/\delta q_i = -E^{-1}_{ij} * q_j = -\psi_i, i = 1, 2, \ldots, N \), so that equations (6) follow.

**Constants of motion.** According to equations (6), the material time derivative of \( \omega_i(t, x, y) \) vanishes along the flow lines of the divergence-free horizontal velocity \( \mathbf{u}_i = \mathbf{z} \times \nabla \psi_i \). Consequently, for every differentiable function \( \Phi_i : \mathbb{R} \to \mathbb{R} \) the functional

\[
C_{\Phi_i}(\omega_i) = \int_D \Phi_i(\omega_i) \, dx \, dy
\]  

(13)
is a conserved quantity for the system (6) for \( i = 1, \ldots, N \), provided the integrals exist. By Kelvin’s circulation theorem, the following integrals over an advected domain \( S(t) \) in the plane are also conserved,

\[
I_i(t) = \int_{S(t)} \omega_i \, dx \, dy = \int_{\partial S(t)} \nabla \psi_i \cdot \mathbf{n} \, ds,
\]  

(14)
where \( \mathbf{n} \) is the horizontal outward unit normal and \( ds \) is the arclength parameter of the closed curve \( \partial S(t) \) bounding the domain \( S(t) \) moving with the flow.

\(^1\)If the domain \( D \) is not simply connected, then variational derivatives such as \( \delta H/\delta q_i \) must be interpreted with care, because in that case the boundary conditions on \( \psi_i \) will come into play [McWilliams, 1977].
2.2 Hamiltonian formulation for the stochastic NLQG fluid

Having understood the geometric structure (Lie–Poisson bracket, constants of motion and Kelvin circulation theorem) for the deterministic case, we can introduce the stochastic versions of equations (6) by simply making the Hamiltonian stochastic while preserving the previous geometric structure, as done in the previous section. Namely, we choose

\[ dh = H(\{q\}) dt + \int_D \sum_{i=1}^{N} \sum_{k=1}^{K} q_i(t, x, y) \zeta_k^i(x, y) \circ dW_k(t) \, dx \, dy, \]

where the \( \zeta_k^i(x, y) \), \( k = 1, \ldots, K \) represent the correlations of the Stratonovich noise we have introduced in (15).

For this stochastic Hamiltonian, the Lie–Poisson bracket (11) leads to the following stochastic process for the transport of the \( N \)-layer generalised vortices,

\[ dq_i = \omega_i dt + J(\psi_i, dq_i) = \nabla(d\psi_i) \times \hat{z} \cdot \nabla \omega_i = -d\mathbf{u}_i \cdot \nabla \omega_i, \quad i = 1, \ldots, N, \]

in terms of its stochastic stream function

\[ d\psi_i := \psi_i dt + \sum_{k=1}^{K} \zeta_k^i(x, y) \circ dW_k(t) = \frac{\delta(h)}{\delta q_i}, \quad i = 1, \ldots, N, \]

determined from the variational derivative of the stochastic Hamiltonian in (15) with respect to the generalised vorticity \( q_i \) in the \( i^{th} \) layer.

**Constants of motion.** The constants of motion \( C_\Phi \) in (13) and the Kelvin circulation theorem for the integrals \( I_i \) in (14) persist for the stochastic generalised vorticity equations in (16). This is because both of these properties follow from the Lie-Poisson bracket in (11). However, the stochastic Hamiltonian in (15) is not conserved, since it depends explicitly on time, \( t \), through its Stratonovich noise term.

**The case of two layers.** In the case of two layers with a flat bottom which we study in the remainder of this paper, the 2-layer generalised vorticity equations in (16) become

\[ dq_1 + J(\psi_1, dq_1) = (\nu \Delta^2 \psi_1) \, dt, \]

\[ dq_2 + J(\psi_2, dq_2) = (\nu \Delta^2 \psi_2 - \mu \Delta \psi_2) \, dt, \]

in which viscosity and drag terms with constant parameters \( \nu \) and \( \mu \), respectively, have also been introduced.

3 The two-dimensional multilayer quasi-geostrophic model

3.1 Deterministic case

To recap the previous section, the two-layer deterministic QG equations for the potential vorticity (PV) \( q \) in a domain \( \Omega \) are given by the PV material conservation law augmented with forcing and dissipation [Pedlosky, 1987; Vallis, 2006]:

\[ \partial_t q_1 + J(q_1, q_1 + \beta y) = \nu \Delta^2 \psi_1, \]

\[ \partial_t q_2 + J(q_2, q_2 + \beta y) = \nu \Delta^2 \psi_2 - \mu \Delta \psi_2, \]
where $\psi$ is the stream function, $J(f, g) = f_x g_y - f_y g_x$ is the Jacobian, the planetary vorticity gradient is given by parameter $\beta$, $\mu$ is the bottom friction parameter, and $\nu$ is the lateral eddy viscosity. The computational domain $\Omega = [0, L_x] \times [0, L_y] \times [0, H]$ is a horizontally periodic flat-bottom channel of depth $H = H_1 + H_2$ given by two stacked isopycnal fluid layers of depth $H_1$ and $H_2$, respectively (Figure 1). A mollified version of the existence and uniqueness theorem for the QG model can be found in [Farhat et al., 2012].

![Diagram of the computational domain](image)

Figure 1: The present investigation involves a two-layer horizontally periodic channel $\Omega$ of horizontal length $L_x$, vertical length $L_y$ and depth $H = H_1 + H_2$, given by two stacked isopycnal fluid layers of depth $H_1$ and $H_2$, respectively. We set periodic boundary conditions for the stream function $\psi$ on the lateral boundaries $\Gamma_2$ and $\Gamma_4$, namely $\psi|_{\Gamma_2} = \psi|_{\Gamma_4} = 0, i = 1, 2$; and no-slip boundary condition on the top, $\Gamma_3$, and bottom, $\Gamma_1$, boundary: $\partial_n \psi|_{\Gamma_1} = \partial_n \psi|_{\Gamma_3} = 0, i = 1, 2$. For all numerical simulations presented in this paper we take $L_x = 3840$ km, $L_y = 1920$ km, and total depth $H = H_1 + H_2$, with $H_1 = 1.0$ km, $H_2 = 3.0$ km.

Forcing in system (20) is introduced through a vertically sheared, baroclinically unstable background flow (e.g., [Berloff and Kamenkovich, 2013])

$$\psi_i \rightarrow -U_i y + \psi_i, \quad i = 1, 2,$$

(21)

where the parameters $U_i$ are background-flow zonal velocities.

The PV and stream function are related through two elliptic equations:

$$q_1 = \Delta \psi_1 + s_1 \psi_{[21]},$$

$$q_2 = \Delta \psi_2 + s_2 \psi_{[12]},$$

(22a)

(22b)

with stratification parameters $s_1$, $s_2$; $\psi_{[ij]} := \psi_i - \psi_j$.

System (20)-(22) is augmented by the integral mass conservation constraint [McWilliams, 1977]

$$\partial_t \int_{\Omega} \psi_{[12]} \, dydx = 0,$$

(23)

as well as by the periodic horizontal boundary conditions,

$$\psi|_{\Gamma_2} = \psi|_{\Gamma_4} = 0, \quad \psi = (\psi_1, \psi_2),$$

(24)

and no-slip boundary conditions at the top and bottom of the channel,

$$\partial_n \psi|_{\Gamma_1} = \partial_n \psi|_{\Gamma_3} = 0,$$

(25)

where $n$ is the outward normal unit vector.

### 3.1.1 Numerical method

The QG model (20)-(25) is solved using the high-resolution CABARET method, which is based on a second-order, non-dissipative and low-dispersive, conservative advection scheme [Karabasov et al., 2009]. The distinctive feature of this scheme is its ability to simulate large-Reynolds-number flow regimes at much lower computational costs compared to conventional methods (see, e.g., [Arakawa, 1966; Woodward and Colella, 1984; Shu and Osher, 1988; Hundsdorfer et al., 1995]). The CABARET method is a predictor-corrector scheme in which the components of the
conservative variables are updated at half time steps. Algorithm 1 illustrates the principal steps of the CABARET method adopted from [Karabasov et al., 2009]. To make the notation more concise, we introduce the forward difference operators in space

\[
\Delta_x[f] = \frac{f_{i+1,j} - f_{ij}}{\Delta x}, \quad \Delta_y[f] = \frac{f_{i,j+1} - f_{ij}}{\Delta y},
\]

and omit spatial and layer indices wherever possible, unless stated otherwise.

**Algorithm 1** CABARET scheme for the deterministic QG system (20)-(25)

**Predictor**

\[
q_{i+1/2,j+1/2}^{n+1} = q_{i+1/2,j+1/2}^n + \frac{\Delta t}{2} F\left(q^n, u(q^n), v(q^n)\right) + \Delta t F_\beta\left(v^n, v^{n-1}\right) + \Delta t F_{\text{visc}}\left(\psi^n_{i+1/2,j+1/2}\right),
\]

\[
F\left(q^n, u(q^n), v(q^n)\right) = - \left(\Delta_x \left[u(q^n)_{i,j+1/2}\right] + \Delta_y \left[v(q^n)_{i+1/2,j}\right]\right),
\]

\[
F_\beta\left(v^n, v^{n-1}\right) = \frac{3}{2} R^n - \frac{1}{2} R^{n-1}, \quad R^n = \frac{\beta}{2} \left(v^n_{i+1/2,j+1} + v^n_{i+1/2,j}\right).
\]

The forcing term

\[
F_{\text{visc}}\left(\psi^n_{i+1/2,j+1/2}\right) = \nu \left(\Delta^2 \psi_i\right)_{i+1/2,j+1/2} - \frac{\nu}{\Delta x} \Delta_x \left[\Delta y \left(\psi_q\right)_{i+1/2,j+1/2}\right],
\]

is added in the prediction step after the elliptic problem is solved.

**Solve the elliptic system of equations with respect to** \((\psi_1)_{i+1/2,j+1/2}^{n+1}\) and \((\psi_2)_{i+1/2,j+1/2}^{n+1}\)

\[
(q_1)_{i+1/2,j+1/2}^{n+1/2} = \left(\Delta \psi_1\right)_{i+1/2,j+1/2}^{n+1} + s_1 (\psi_{21})_{i+1/2,j+1/2}^{n+1} \quad \text{and} \quad (q_2)_{i+1/2,j+1/2}^{n+1/2} = \left(\Delta \psi_2\right)_{i+1/2,j+1/2}^{n+1} + s_2 (\psi_{12})_{i+1/2,j+1/2}^{n+1}.
\]

**Calculate**

\[
\psi_{1,i,j+1/2}^{n+1/2} = \left(\psi_{1,i,j+1/2}^{n+1} + \psi_{1,i,j-1/2}^{n+1} + \psi_{1,i+1/2,j}^{n+1} + \psi_{1,i-1/2,j}^{n+1}\right)/4.
\]

**Update velocity components at the cell faces**

\[
u_{i+1/2,j}^{n+1/2} = \Delta_x \left[\psi_{1,i,j+1/2}^{n+1/2}\right], \quad (v_1)_{i+1/2,j}^{n+1/2} = -\Delta_x \left[\psi_{1,i,j-1/2}^{n+1/2}\right].
\]

**Extrapolator**

\[
u_{i+1/2,j+1/2}^{n+1} = \frac{3}{2} \nu_{i,j+1/2}^{n+1/2} - \frac{1}{2} \nu_{i+1,j+1/2}^{n+1/2}, \quad \nu_{i+1/2,j}^{n+1} = \frac{3}{2} \nu_{i,j+1/2}^{n+1/2} - \frac{1}{2} \nu_{i+1/2,j-1/2}^{n+1/2}.
\]

\[
q_{i+1,j+1/2}^{n+1} = 2\nu_{i+1/2,j+1/2}^{n+1} - q_{i,j+1/2}^{n+1} \quad \text{if} \quad \nu_{i+1,j+1/2}^{n+1} > 0; \quad q_{i+1,j+1/2}^{n+1} = 2\nu_{i+1/2,j+1/2}^{n+1} - q_{i+1,j+1/2}^{n+1} \quad \text{if} \quad \nu_{i+1,j+1/2}^{n+1} < 0.
\]

\[
q_{i+1/2,j+1}^{n+1} = 2\nu_{i+1/2,j+1}^{n+1} - q_{i+1/2,j}^{n+1} \quad \text{if} \quad \nu_{i+1/2,j}^{n+1} > 0; \quad q_{i+1/2,j+1}^{n+1} = 2\nu_{i+1/2,j+1}^{n+1} - q_{i+1/2,j}^{n+1} \quad \text{if} \quad \nu_{i+1/2,j}^{n+1} < 0.
\]

**Correction of the computed cell-face PV values**

\[
\begin{align*}
\text{If} \quad q_{i,j+1/2}^{n+1} > M_{i,j+1/2}^{n+1} & \Rightarrow q_{i,j+1/2}^{n+1} = M_{i,j+1/2}^{n+1}, \\
\text{If} \quad q_{i,j+1/2}^{n+1} < M_{i,j+1/2}^{n+1} & \Rightarrow q_{i,j+1/2}^{n+1} = M_{i,j+1/2}^{n+1}, \\
\text{If} \quad q_{i+1/2,j}^{n+1} > M_{i+1/2,j}^{n+1} & \Rightarrow q_{i+1/2,j}^{n+1} = M_{i+1/2,j}^{n+1}, \\
\text{If} \quad q_{i+1/2,j}^{n+1} < M_{i+1/2,j}^{n+1} & \Rightarrow q_{i+1/2,j}^{n+1} = M_{i+1/2,j}^{n+1}, \\
\text{If} \quad q_{i+1,1/2,j}^{n+1} > 0 & \Rightarrow q_{i+1,1/2,j}^{n+1} = \max\left(q_{i+1,1/2,j}^{n+1-1}, q_{i+1,1/2,j}^{n+1}, q_{i+1,1/2,j}^{n+1+1}\right) + \frac{2}{\Delta t} F\left(q_{i+1/2,j}^{n+1-1}, q_{i+1/2,j}^{n+1}, q_{i+1/2,j}^{n+1+1}\right), \\
\text{If} \quad q_{i+1,1/2,j}^{n+1} < 0 & \Rightarrow q_{i+1,1/2,j}^{n+1} = \min\left(q_{i+1,1/2,j}^{n+1-1}, q_{i+1,1/2,j}^{n+1}, q_{i+1,1/2,j}^{n+1+1}\right) + \frac{2}{\Delta t} F\left(q_{i+1/2,j}^{n+1-1}, q_{i+1/2,j}^{n+1}, q_{i+1/2,j}^{n+1+1}\right), \\
\end{align*}
\]

**Corrector**

\[
q_{i+1/2,j+1/2}^{n+1} = q_{i+1/2,j+1/2}^{n+1} + \frac{\Delta t}{2} F\left(q^n, u(q^n), v(q^n)\right), \quad \text{where} \quad q^n, u(q^n), v(q^n) \text{ are computed in the extrapolation step.}
\]

An efficient parallelization of the QG model has allowed us to carry out high-performance computations in eddy-resolving regimes. In particular, for the purpose of this paper we computed three solutions for the case of homogeneous and heterogeneous flow (Figures 2 and 3):

- High-resolution deterministic \(q^f\) computed on the fine grid \(G^f = \{N_x \times N_y\}, \quad N_x = 2049, \quad N_y = 1025\) (\(dx = dy = 1.9\) km);
Low-resolution deterministic solution \( q^a \) computed on the coarse grid \( G^c = 129 \times 65 \) \((dx = dy = 299 \text{ km})\) as the solution of the elliptic equation (22) with the stream function \( \psi^a \), where \( \psi^a \) is computed by spatially averaging the high-resolution stream function \( \psi^f \) over the coarse grid cell \( G^c \). We refer to \( q^a \) as the truth or the true solution, and use it for comparison with the parameterised solution;

Low-resolution solution \( q^m \) (also referred to as the coarse-grain modelled solution) computed on the coarse grid \( G^c \) by simulating the QG model. This solution is used for parameterisation.

### 3.1.2 Numerical results

We define the computational domain \( \Omega = [0, L_x] \times [0, L_y] \times [0, H] \) as a horizontally periodic flat-bottom channel with \( L_x = 3840 \text{ km}, \ L_y = L_x/2 \text{ km}, \) and total depth \( H = H_1 + H_2, \) with \( H_1 = 1.0 \text{ km}, \ H_2 = 3.0 \text{ km} \) (Figure 1). We choose governing parameters of the QG model that are typical to a mid-latitude setting. These comprise the planetary vorticity gradient \( \beta = 2 \times 10^{-11} \text{ m}^{-1} \text{ s}^{-1} \), lateral eddy viscosity \( \nu = 3.125 \text{ m}^2 \text{ s}^{-1} \), and the bottom friction parameters \( \mu = \{4 \times 10^{-8}, 4 \times 10^{-7}\} \text{ s}^{-1} \). We will explain this choice below, as well as the reason for studying two different flow regimes. The background-flow zonal velocities in (21) are given by \( U = [6.0, 0, 0] \text{ m s}^{-1} \), while the stratification parameters in system (22) are \( s_1 = 4.22 \times 10^{-3} \text{ km}^{-2}, \ s_2 = 1.41 \times 10^{-3} \text{ km}^{-2}; \) chosen so that the first Rossby deformation radius is \( Rd_1 = 25 \text{ km} \). In order to ensure that the numerical solutions are statistically equilibrated, the model is initially spun up from the state of rest to \( t = 0 \) over the time interval \( T_{spin} = [-100, 0] \) years.

For smaller bottom friction, we find that jet-like structures (also referred to as striations) emerge in the simulations, resulting from interplay of forcing, damping and baroclinic instability. In contrast, for larger bottom friction, the flow pattern is essentially homogeneous and no coherent structures are seen in the simulations. This nonlinear emergent asymptotic behaviour runs counter to what one might have expected from linear analysis; in which the onset of baroclinic instability in a two-layer channel flow occurs when the PV changes sign in the two layers and its onset occurs at lower drag, for a given forcing.

In this paper we consider both heterogeneous (Figure 2) and homogeneous (Figure 3) flow regime (which correspond to flows with low (\( \mu = 4 \times 10^{-8} \)) and high (\( \mu = 4 \times 10^{-7} \)) drag, respectively) and study how the parameterisation performs in each case.
Figure 2: The series of snapshots shows the high-resolution solution \( q_f \) computed on the fine grid \( G_f = 2049 \times 1025 \) \((dx = dy = 1.9 \text{ km})\), the true solution \( q_a \) computed on the coarse grid \( G_c = 129 \times 65 \) \((dx = dy = 299 \text{ km})\), and the low-resolution solution \( q_m \) (also referred to as the coarse-grain modelled solution) computed on the coarse grid \( G_c \) by simulating the QG model for the low drag \( \mu = 4 \times 10^{-8} \text{ s}^{-1} \). All the fields are given in units of \([s^{-1} f_0^{-1}]\), where \( f_0 = 0.83 \times 10^{-4} \text{ s}^{-1} \) is the Coriolis parameter. As seen in the figure, the flow is more energetic and small-scale features are prevalent in the first layer. The true solution \( q_a \) captures the small-scales features of the high-resolution solution \( q_f \) in the first and second layer, and also has the same energy. On the contrary, the coarse-grain modelled solution \( q_m \) (which must be parameterised and will be used in uncertainty quantification tests presented in Section 4.4) is much less energetic than the true solution, and does not capture the correct structure (the number of striations and their positions) of the true flow \( q_a \). The lower resolution of the modelled solution \( q_m \) arrests the small-scale eddies which take part in the jet-maintaining mechanism [Kamenkovich et al., 2009]. Note that in order to visualize all the solutions on the same color scale we have multiplied the modelled solution by a factor of 5.
Figure 3: The series of snapshots in the figure shows the high-resolution solution $q^f$ computed on the fine grid $G^f = 2049 \times 1025$ ($dx = dy = 1.9$ km), the true solution $q^a$ computed on the coarse grid $G^c = 129 \times 65$ ($dx = dy = 299$ km), and the low-resolution solution $q^m$ (also referred to as the coarse-grain modelled solution) computed on the coarse grid $G^c$ by simulating the QG model for the high drag $\mu = 4 \times 10^{-7}$ s$^{-1}$. All the fields are given in units of [s$^{-1}$f$^{-1}$ 0], where $f_0 = 0.83 \times 10^{-4}$ s$^{-1}$ is the Coriolis parameter. As in the case of the heterogeneous flow (Figure 2), the homogeneous flow is more energetic in the first layer. However, this difference is less pronounced than that in the heterogeneous case. Moreover, the homogeneous flow teems with small-scale eddies not only in the first but also in the second layer, while the whole flow dynamics is more damped by higher drag and therefore less energetic in contrast to the heterogeneous flow. This, in turn, suppresses the zonally uniform eigenmodes which are responsible for maintaining the jet-like structure of the flow [Berloff et al., 2011]. The true solution $q^a$ captures the small-scales features of the high-resolution solution $q^f$ in both layers and has the same energy. As opposed to the heterogeneous flow, the coarse-grain modelled solution $q^m$ (which must be parameterised and then used in uncertainty quantification tests presented in Section 4.4) is also homogeneous and has the same energy as the true solution $q^a$. The figure shows that the coarse-grain model can adequately represent the large-scale flow dynamics.
For the low drag, which corresponds to the bottom friction coefficient $\mu = 4 \times 10^{-8}$, flow dynamics is highly-heterogeneous (Figure 2). The high-resolution flow $q^f$ (computed on the fine grid $G^f = 2049 \times 1025$ with the resolution $dx = dy = 1.9\text{ km}$) in the first layer consists of two flow regions: the fast flow within the striations and the slow flow between striations. The flow dynamics in the first layer teems with small-scale eddies which, in turn, maintain the striated structure of the flow (see, e.g. [Kamenkovich et al., 2009]). On the contrary, the dynamics of the second layer is much less energetic than that of the first one, and exhibits neither small-scale features nor striations. The striated flow structure as well as flow energetics are captured by the true solution $q^a$ computed on the coarse grid $G^c = 129 \times 65 \ (dx = dy = 299\text{ km})$. However, the low-resolution solution $q^m$ (the solution which has to be parameterised and then used in uncertainty quantification tests presented in Section 4.4) computed on the coarse grid $G^c$ by simulating the QG model is much less energetic in both the first and second layer than the true solution $q^a$, and cannot capture the correct structure (the number of striations and their positions) of the true flow dynamics. Thus, the coarse-grain QG equations fail to model the proper jet-like structure of the flow. Apparently, the coarse resolution suppresses the small-scale eddies, which are thought to be one of the mechanisms responsible for maintaining these structures (see, e.g. [Kamenkovich et al., 2009]).

For the high drag flows, with bottom friction coefficient $\mu = 4 \times 10^{-7}$, flow dynamics becomes more homogeneous (Figure 3). As in the heterogeneous case, the high-resolution flow $q^f$ is more energetic in the first layer than in the second one, although this difference is less pronounced. In the homogeneous flow, small-scale eddies are ubiquitous in both the first and second layer. Comparing the high-resolution solution $q^f$ with its coarse-grained analogue $q^h$ we conclude that the latter captures the small-scales features as well as the energetics of $q^f$ in both layers. Unlike the heterogeneous flow, the coarse-grain modelled solution $q^m$ (the solution we parameterise and use in uncertainty quantification tests given in Section 4.4) is also homogeneous in structure and adequately restores the energetics of the true solution $q^a$. In other words, the coarse-grain QG model properly represents the large-scale flow dynamics for flows with higher drag, which are more damped and therefore less energetic. In the case of high-drag flows, the zonally uniform eigenmodes responsible for maintaining the jet-like structure of the flow (see, e.g. [Berloff et al., 2011]) become more damped thus making jets much more latent compared with highly-energetic low-drag flows.

Another important characteristic of the flow which can influence the accuracy of the parameterisation is decorrelation time (Figure 4). Only after the decorrelation time we can assume that $\xi(z)$ does not depend on time.

![Figure 4: Evolution of the correlation coefficient $r_{q(0),q(t)} = \frac{\text{cov}(q(0),q(t))}{\sigma_q(0)\sigma_q(t)}$ is shown for the heterogeneous (left) and homogeneous (right) flow. As seen in the figure, the larger the bottom friction coefficient is, the more homogeneous the flow becomes and the faster the correlation coefficient decays. The decorrelation time for the heterogeneous flow is much longer than that of the homogeneous one, as expected. For both homogeneous and heterogeneous flow, the decorrelation time in the first layer (solid black line) is shorter, compared with the second layer (dashed black line). This difference in decorrelation time is also expected, since the flow in the first layer is more energetic. The correlation coefficient of the true solution $r_{q^a(0),q^a(t)}$ (black line) for the heterogeneous flow significantly differs from the correlation coefficient of the modelled solution $r_{q^m(0),q^m(t)}$ (red line), while in the case of the homogeneous flow these coefficients have a similar behavior. Thus, we can conclude that in order for the parameterisation to restore the structure of the flow, it should take into account both spatial and temporal correlations.](image)

(a): Heterogeneous flow ($\mu = 4 \times 10^{-8}\text{s}^{-1}$)  
(b): Homogeneous flow ($\mu = 4 \times 10^{-7}\text{s}^{-1}$)
As seen in Figure 4, the larger the bottom friction coefficient is, the more homogeneous flow becomes and the faster the correlation coefficient decays as expected. The decorrelation time for the heterogeneous flow (Figure 4(a)) is much longer than that of the homogeneous one (Figure 4(b)). For both types of flow, the decorrelation time in the first layer is much shorter than in the second layer, because the flow in the first layer is faster and more energetic, and therefore it faster “forgets” its initial state. Note that for the heterogeneous flow the correlation time of the true solution \( q^* \) differs considerably from the correlation time of the modelled solution \( q^m \). In the case of the homogeneous flow, the decorrelation time of \( q^a \) and \( q^m \) have a similar behavior. Thus, we can conclude from Figure 4 that in order for the parameterisation to restore the structure of the flow it should take into account both spatial and temporal correlations. The simulation results presented in this section show that more interesting and energetic flow dynamics is confined in the first layer. Therefore, from now on we will focus our attention on the first layer unless stated otherwise.

### 3.2 Stochastic case

The stochastic version of the two-layer QG equations is given by system (19). The terms in \( \zeta^k_1 \) and \( \zeta^k_2 \) the only differences from the deterministic QG model, all other equations remain the same as in the deterministic case. However, the CABARET scheme in the stochastic case differs from the deterministic version and therefore its use can only be justified if it is consistent with the stochastic QG model. In other words, the CABARET scheme should be in Stratonovich form.

#### 3.2.1 Numerical method

The CABARET scheme for the stochastic QG system (19) is given by Algorithm 2 (with the stochastic terms highlighted in red).

In order to show that the CABARET scheme is consistent with the stochastic QG model, we rewrite the scheme as the improved Euler method (also known as Heun’s method) [Kloeden and Platen, 1999]

\[
x^* = x^n + \Delta t f(x^n) + \Delta Wg(x^n),
\]

\[
x^{n+1} = x^n + \frac{\Delta t}{2} (f(x^n) + f(x^*)) + \frac{\Delta W}{2} (g(x^n) + g(x^*)),
\]

which solves stochastic differential equations (SDEs) in the form of Stratonovich.

In doing so, we omit the space indices for the potential vorticity \( q \) to emphasize the functional dependence on \( q \), and introduce an extra variable

\[
q^* = 2q^{n+\frac{1}{2}} - q^n,
\]

which allows to recast (26) and (27) in the form

\[
q^* = q^n + \Delta t F(q^n, u(q^n), v(q^n)) + 2\Delta t F_\beta (v^n, v^{n-1}) + 2\Delta t F_{\text{visc}} \left( \psi \left( q^{n+\frac{1}{2}} \right) \right) + \sum_{k=1}^{m} (G_k(q^n) + G_{k,\beta}) \Delta W_k,
\]

(28a)

\[
q^{n+1} = \frac{q^* + q^n}{2} + \frac{\Delta t}{2} F(q^*, u(q^*), v(q^*)) + \sum_{k=1}^{m} (G_k(q^*) + G_{k,\beta}) \frac{\Delta W_k}{2}.
\]

(28b)

Substitution of (28a) into (28b) and (26) into the forcing term \( F_{\text{visc}} \left( \psi \left( q^{n+\frac{1}{2}} \right) \right) \) leads to

\[
q^{n+1} = q^n + \frac{\Delta t}{2} \left[ F(q^n, u(q^n), v(q^n)) + F(q^n + O_1(\Delta W_k), u(q^n + O_1(\Delta W_k)), v(q^n + O_1(\Delta W_k))) \right]
\]

\[
+ \Delta t \left[ F_\beta (v^n, v^{n-1}) + F_{\text{visc}} \left( \psi \left( q^n + O_2(\Delta W_k) \right) \right) \right] + \sum_{k=1}^{m} (G_k(q^n) + G_{k,\beta}) \frac{\Delta W_k}{2} + \sum_{k=1}^{m} (G_k(q^n + O_1(\Delta W_k)) + G_{k,\beta}) \frac{\Delta W_k}{2},
\]

(29)

where

\[
O_1(\Delta W_k) := \Delta t F(q^n, u(q^n), v(q^n)) + 2\Delta t F_\beta (v^n, v^{n-1})
\]

\[
+ 2\Delta t F_{\text{visc}} \left( \psi \left( q^n + O_2(\Delta W_k) \right) \right) + \sum_{k=1}^{m} (G_k(q^n) + G_{k,\beta}) \Delta W_k,
\]

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Algorithm 2 The CABARET scheme for the stochastic QG system

**Predictor**

\[ q_{n+1/2} = q_{n+1/2} + \frac{\Delta t}{2} F(q^n, u(q^n), v(q^n)) + \Delta t F_{\beta}(v^n, v^{n-1}) + \Delta t F_{\text{visc}}(\psi(q^{n+1/2})) \]

\[ + \sum_{k=1}^{m} (G_k(q^n) + G_{k,\beta}) \frac{\Delta W_k}{2}, \]  

(26)

\[ G_k(q^n) = -\left( \Delta_y \left( \langle \xi_k^u q^n \rangle_{i,j+1/2} \right) + \Delta_y \left( \langle \xi_k^v q^n \rangle_{i+1/2,j} \right) \right), \quad G_{k,\beta} = 3R^n - R^{n-1}, \quad R^n = -\frac{\beta}{2} \left( \langle \xi_k^u \rangle_{i+1/2,j+1} + \langle \xi_k^v \rangle_{i+1/2,j} \right). \]

The forcing term

\[ F_{\text{visc}}(\psi(q^{n+1/2})) = \nu \left( \Delta^2 \psi \right)_{i+1/2,j+1/2} - \delta_{l2} \mu (\Delta \psi)_i^{n+1/2} \]  

is added in the prediction step after the elliptic problem is solved.

Solve the elliptic system of equations with respect to \((\psi_{1,n+1/2})_{i+1/2,j+1/2}\) and \((\psi_{2,n+1/2})_{i+1/2,j+1/2}\)

\[ (q_{1,i+1/2,j+1/2})_{n+1/2} = \left( \Delta \psi_1 \right)_{i+1/2,j+1/2} + \xi_{i+1/2,j+1/2} + \xi_{i+1/2,j+1/2} \]

Calculate

\[ \psi_{ij}^{n+1/2} = \frac{1}{4} \left( \psi_{i+1/2,j+1/2}^{n+1/2} + \psi_{i-1/2,j+1/2}^{n+1/2} + \psi_{i+1/2,j-1/2}^{n+1/2} + \psi_{i-1/2,j-1/2}^{n+1/2} \right). \]

Update velocity components at the cell faces

\[ u_{i+1/2,j}^{n+1/2} = \Delta x \left[ \psi_{ij}^{n+1/2} \right], \quad (v_{i,j+1/2})_{n+1/2} = -\Delta y \left[ \psi_{ij}^{n+1/2} \right]. \]

**Extrapolator**

\[ u_{i+1/2,j+1/2}^{n+1} = \frac{3}{2} u_{i+1/2,j+1/2}^{n+1} - \frac{1}{2} u_{i+1/2,j+1/2}^{n+1}, \quad v_{i+1/2,j+1/2}^{n+1} = \frac{3}{2} v_{i+1/2,j+1/2}^{n+1} - \frac{1}{2} v_{i+1/2,j+1/2}^{n+1}. \]

\[ q_{i+1/2,j+1/2}^{n+1} = \frac{3}{2} q_{i+1/2,j+1/2}^{n+1} - \frac{1}{2} q_{i+1/2,j+1/2}^{n+1} \]

\[ q_{i+1/2,j+1/2}^{n+1} = \frac{3}{2} q_{i+1/2,j+1/2}^{n+1} - \frac{1}{2} q_{i+1/2,j+1/2}^{n+1} \]

\[ q_{i+1/2,j+1/2}^{n+1} = \frac{3}{2} q_{i+1/2,j+1/2}^{n+1} - \frac{1}{2} q_{i+1/2,j+1/2}^{n+1} \]

\[ q_{i+1/2,j+1/2}^{n+1} = \frac{3}{2} q_{i+1/2,j+1/2}^{n+1} - \frac{1}{2} q_{i+1/2,j+1/2}^{n+1} \]

\[ q_{i+1/2,j+1/2}^{n+1} = \frac{3}{2} q_{i+1/2,j+1/2}^{n+1} - \frac{1}{2} q_{i+1/2,j+1/2}^{n+1} \]

\[ q_{i+1/2,j+1/2}^{n+1} = \frac{3}{2} q_{i+1/2,j+1/2}^{n+1} - \frac{1}{2} q_{i+1/2,j+1/2}^{n+1} \]

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\[ q_{i+1/2,j+1/2}^{n+1} = \frac{3}{2} q_{i+1/2,j+1/2}^{n+1} - \frac{1}{2} q_{i+1/2,j+1/2}^{n+1} \]

\[ q_{i+1/2,j+1/2}^{n+1} = \frac{3}{2} q_{i+1/2,j+1/2}^{n+1} - \frac{1}{2} q_{i+1/2,j+1/2}^{n+1} \]

\[ q_{i+1/2,j+1/2}^{n+1} = \frac{3}{2} q_{i+1/2,j+1/2}^{n+1} - \frac{1}{2} q_{i+1/2,j+1/2}^{n+1} \]

\[ q_{i+1/2,j+1/2}^{n+1} = \frac{3}{2} q_{i+1/2,j+1/2}^{n+1} - \frac{1}{2} q_{i+1/2,j+1/2}^{n+1} \]

\[ q_{i+1/2,j+1/2}^{n+1} = \frac{3}{2} q_{i+1/2,j+1/2}^{n+1} - \frac{1}{2} q_{i+1/2,j+1/2}^{n+1} \]

\[ q_{i+1/2,j+1/2}^{n+1} = \frac{3}{2} q_{i+1/2,j+1/2}^{n+1} - \frac{1}{2} q_{i+1/2,j+1/2}^{n+1} \]

\[ q_{i+1/2,j+1/2}^{n+1} = \frac{3}{2} q_{i+1/2,j+1/2}^{n+1} - \frac{1}{2} q_{i+1/2,j+1/2}^{n+1} \]

\[ q_{i+1/2,j+1/2}^{n+1} = \frac{3}{2} q_{i+1/2,j+1/2}^{n+1} - \frac{1}{2} q_{i+1/2,j+1/2}^{n+1} \]

\[ q_{i+1/2,j+1/2}^{n+1} = \frac{3}{2} q_{i+1/2,j+1/2}^{n+1} - \frac{1}{2} q_{i+1/2,j+1/2}^{n+1} \]

\[ q_{i+1/2,j+1/2}^{n+1} = \frac{3}{2} q_{i+1/2,j+1/2}^{n+1} - \frac{1}{2} q_{i+1/2,j+1/2}^{n+1} \]

\[ q_{i+1/2,j+1/2}^{n+1} = \frac{3}{2} q_{i+1/2,j+1/2}^{n+1} - \frac{1}{2} q_{i+1/2,j+1/2}^{n+1} \]

\[ q_{i+1/2,j+1/2}^{n+1} = \frac{3}{2} q_{i+1/2,j+1/2}^{n+1} - \frac{1}{2} q_{i+1/2,j+1/2}^{n+1} \]

\[ q_{i+1/2,j+1/2}^{n+1} = \frac{3}{2} q_{i+1/2,j+1/2}^{n+1} - \frac{1}{2} q_{i+1/2,j+1/2}^{n+1} \]

Correccor

\[ q^n_{i+1/2,j+1/2} = q^n_{i+1/2,j+1/2} + \frac{\Delta t}{2} F(q^n_{i+1/2,j+1/2}, v^n_{i+1/2,j+1/2}) + \sum_{k=1}^{m} (G_k(q^n_{i+1/2,j+1/2}) + G_{k,\beta}) \frac{\Delta W_k}{2}, \]  

(27)

where \(q^{n+1}, u(q^{n+1}), v(q^{n+1})\) are computed in the extrapolation step.
and
\[ O_2(\Delta W_k) := \frac{\Delta t}{2} F(q^n, u(q^n), v(q^n)) + \Delta t F_\beta \left( v^n, v^{n-1} \right) + \sum_{k=1}^{m} (G_k(q^n) + G_{k,\beta}) \frac{\Delta W_k}{2}. \]

Retaining the terms up to order \( \Delta t \) in (29) we get
\[ q^{n+1} = q^n + \Delta t \left[ F(q^n, u(q^n), v(q^n)) + F_\beta \left( v^n, v^{n-1} \right) + F_{\text{visc}}(\psi(q^n)) \right] + \sum_{k=1}^{m} (G_k(q^n) + G_{k,\beta}) \Delta W_k + \sum_{k=1}^{m} \sum_{k_2=1}^{m} G_{k_1} \left( G_{k_2}(q^n) + G_{k_2,\beta} \right) \frac{\Delta W_{k_1} \Delta W_{k_2}}{2} + H.O.T., \quad (30) \]
where \( G_\beta \) does not depend on \( q^n \), and \( H.O.T. \) denotes higher order terms. Thus we have shown that the CABARET scheme is in Stratonovich form up to order \( (\Delta t)^{3/2} \).

### 3.2.2 Consistency

In this section we prove that the stochastic CABARET scheme (30) is consistent with the stochastic QG equation (19) in the mean square sense in time, since its consistency in space is guaranteed by its second order approximation [Karabasov et al., 2009]. We consider a Stratonovich process \( q = q(t, x) \) satisfying the SPDE
\[ d q = a_t \, d t + \sum_{i=1}^{m} b_{i,t} \circ d W_{i,t}, \quad a_t := F(q^n, u(q^n), v(q^n)) + F_\beta + F_{\text{visc}}(\psi(q^n)), \quad b_{i,t} := G_i(q^n) + G_{i,\beta}, \]
and rewrite it in the Itô form
\[ d q = a_t \, d t + \sum_{i=1}^{m} b_{i,t} \, d W_{i,t} + \frac{1}{2} \sum_{i=1}^{m} b_{i,t}(b_{i,t}) \, d t, \]
or alternatively
\[ d q = q_d \, d t + \sum_{i=1}^{m} q^i_{s,t} \, d W_{i,t} \quad (31) \]
with the stochastic and deterministic parts defined as \( q_d := a_t + \frac{1}{2} \sum_{i=1}^{m} b_{i,t}(b_{i,t}) \) and \( q^i_{s,t} := b_{i,t} \), respectively.

We define consistency for SPDE (31) as follows

**Definition 1.** We say that a discrete time-space approximation \( q^n = q^n_d + q^n_s \) of \( q = q_d + q_s \) with the time step \( \Delta t \) and space steps \( \Delta x = (\Delta x_1, \Delta x_2, \ldots, \Delta x_d) \) is consistent in mean square of order \( \alpha > 1 \) and \( \beta > 1 \) in time and space with respect to (31) if there exists a nonnegative function \( c = c((\Delta t)^\alpha, (\Delta x)^\beta) \) with \( \lim_{\Delta t \to 0} c((\Delta t)^\alpha, (\Delta x)^\beta) = 0 \) such that
\[ \mathbb{E}\left[ \| q_s - q^n_s \|_{L^2(\Omega)}^2 \right] \leq c((\Delta t)^\alpha, (\Delta x)^\beta), \quad \mathbb{E}\left[ \| q_d - q^n_d \|_{L^2(\Omega)}^2 \right] \leq c((\Delta t)^\alpha, (\Delta x)^\beta) \]
for all fixed values \( q^n \), time \( n = 0, 1, 2, \ldots \) and space indices.

Since our focus in this section is on consistency in time, we have to prove that the following estimation holds:
\[ \mathbb{E}\left[ \| q_s - q^n_s \|_{L^2(\Omega)}^2 \right] \leq c((\Delta t)^\alpha). \quad (32) \]

**Theorem 2.** Assuming that there exists a constant \( \tilde{C} > 0 \) such that the following assumptions hold

**A1.** \( \mathbb{E}\left[ \| a_r - a_s \|_{L^2(\Omega)} \right] \leq \tilde{C} \sqrt{r - s}, \)

**A2.** \( \mathbb{E}\left[ \| \sum_{i=1}^{m} (b_{i,r} - b_{i,s}) \|_{L^2(\Omega)} \right] \leq \tilde{C} \sqrt{r - s}, \)

**A3.** \( \mathbb{E}\left[ \left\| \sum_{i=1}^{m} \sum_{j=1}^{m} b_{i,j}(s) \right\|_{L^2(\Omega)} \right] \leq \tilde{C}, \) for \( i, j = 1, 2, \ldots, m, \).
A4. \[ E\left[ \left\| \sum_{i=1}^{m} (b_{i,r}(b_{i,r}) - b_{i,s}(b_{i,s})) \right\|_{L^2(\Omega)} \right] \leq \bar{C}\sqrt{r-s}, \]

A5. \[ E[|H.O.T.|] \leq \bar{C}(r-s)^{3/2}, \]

with \(|r-s| \leq \Delta t\), the stochastic CABARET scheme (30) is consistent in mean square with \(c(\Delta t) = (\Delta t)^2\).

**Proof.** Integration of (31) with respect to time over the interval \([s,t]\) gives

\[ q_t = q_s + \int_s^t a_r \, dr + \int_s^t \sum_{i=1}^{m} b_{i,r} \, dW_{i,r} + \frac{1}{2} \int_s^t \sum_{i=1}^{m} b_{i,r}(b_{i,r}) \, dr. \]  \hspace{1cm} (33)

Substitution of (30) and (33) into (32) leads to

\[ E\left[ \left\| \int_s^t a_r \, dr + \int_s^t \sum_{i=1}^{m} b_{i,r} \, dW_{i,r} + \frac{1}{2} \int_s^t \sum_{i=1}^{m} b_{i,r}(b_{i,r}) \, dr \right\|^2_{L^2(\Omega)} \right] \leq c(\Delta t). \]  \hspace{1cm} (34)

By combining the terms in (34), we get

\[ E\left[ \left\| A + B + C \right\|^2_{L^2(\Omega)} \right] \leq c(\Delta t), \]  \hspace{1cm} (35)

where

\[ A := \int_s^t (a_r - a_s) \, dr, \quad B := \int_s^t \sum_{i=1}^{m} (b_{i,r} - b_{i,s}) \, dW_{i,r}, \quad C := C_1 - C_2 - C_3, \]

with

\[ C_1 := \frac{1}{2} \int_s^t \sum_{i=1}^{m} (b_{i,r}(b_{i,r}) - b_{i,s}(b_{i,s})) \, dr, \quad C_2 := \frac{1}{2} \int_s^t \sum_{i=1}^{m} b_{i,s}(b_{i,s})(\Delta W_i)^2 - \Delta t, \quad C_3 := \frac{1}{2} \int_s^t \sum_{i,j=1}^{m} b_{i,s}(b_{j,s}) \Delta W_i \Delta W_j. \]

Applying the triangle and Young’s inequalities to (35) we arrive at

\[ E\left[ \left\| A + B + C \right\|^2_{L^2(\Omega)} \right] \leq 3E\left[ \| A \|^2_{L^2(\Omega)} + \| B \|^2_{L^2(\Omega)} + \| C \|^2_{L^2(\Omega)} + \bar{C}^2(\Delta t)^3 \right]. \]

Using **A2**, the Cauchy–Schwarz inequality and **A1**, we estimate the first term as

\[ E\left[ \left\| A \right\|^2_{L^2(\Omega)} \right] \leq \Delta t E\left[ \int_s^t |a_r - a_s|^2_{L^2(\Omega)} \, dr \right] \leq \frac{\bar{C}^2}{2}(\Delta t)^3. \]

Estimation of the second term is given by

\[ E\left[ \left\| B \right\|^2_{L^2(\Omega)} \right] = \int_\Omega E\left[ \left( \int_s^t \sum_{i=1}^{m} (b_{i,r} - b_{i,s}) \, dW_{i,r} \right)^2 \right] d\Omega \]  \hspace{1cm} (using the Itô isometry)

\[ = E\left[ \int_s^t \left( \int_\Omega \sum_{i=1}^{m} (b_{i,r} - b_{i,s}) \right)^2 \, dr \, d\Omega \right] \]  \hspace{1cm} (the Cauchy–Schwarz inequality leads to)

\[ \leq \Delta t E\left[ \int_s^t \left\| \sum_{i=1}^{m} (b_{i,r} - b_{i,s}) \right\|^2_{L^2(\Omega)} \, dr \right] \leq \frac{\bar{C}^2}{2}(\Delta t)^3 \]  \hspace{1cm} (using **A2**).
To estimate the term $C$ in (35), we use the triangle inequality to get

$$E\left|C\right|_{L^2(\Omega)}^2 \leq E\left|C_1\right|_{L^2(\Omega)}^2 + \left|C_2\right|_{L^2(\Omega)}^2 + \left|C_3\right|_{L^2(\Omega)}^2,$$

and then separately estimate each term on the right hand side.

Applying the Cauchy–Schwarz inequality and A4 to $C_1$, we get the following estimation

$$E\left|C_1\right|_{L^2(\Omega)}^2 \leq \frac{\Delta t}{2} \int_{\Omega} \left\| \sum_{i=1}^{m} (b_{i,r}(b_{i,s}) - b_{i,s}(b_{i,s})) \right\|_{L^2(\Omega)}^2 d\Omega \leq \frac{\tilde{C}_2^2}{8} (\Delta t)^3.$$

The term $C_2$ is estimated as

$$E\left|C_2\right|_{L^2(\Omega)}^2 = \int_{\Omega} \left( \frac{1}{2} \sum_{i=1}^{m} (b_{i,s}(b_{i,s})) ( (\Delta W_i)^2 - \Delta t)^2 \right) \frac{1}{4} \int_{\Omega} \sum_{i=1}^{m} (b_{i,s}(b_{i,s}))^2 E \left[ (\Delta W_i)^4 - 2(\Delta W_i)^2 \Delta t + (\Delta t)^2 \right] d\Omega \leq \frac{\tilde{C}_2^2}{2} (\Delta t)^2 \quad \text{(using A3)}.$$

Using A3 for $C_3$ leads to

$$E\left|C_3\right|_{L^2(\Omega)}^2 = \frac{1}{4} \int_{\Omega} \sum_{i,j} (b_{i,s}(b_{i,s}))^2 E \left[ (\Delta W_i)^2 \right] E \left[ (\Delta W_j)^2 \right] d\Omega \leq \frac{(\Delta t)^2}{4} \left\| \sum_{i=1}^{m} (b_{i,s}(b_{i,s})) \right\|_{L^2(\Omega)}^2 \leq \frac{\tilde{C}_2^2}{4} (\Delta t)^2.$$

Finally, we arrive at the following estimation

$$E\left|A + B + C\right|_{L^2(\Omega)}^2 \leq C^* \left( (\Delta t)^2 + (\Delta t)^3 \right) \leq C^* (\Delta t)^2, \quad C^* > 0,$$

which proves the theorem. \hfill \Box

**Remark.** Conditions A1-A5 are satisfied and SPDE (31) is well-posed for sufficiently large $p$ for all $T > 0$ if the stochastic QG equation (19) has a solution in $W^{2p,2}$ such that $E \left[ \sup_{t \in [0,T]} \left\| q_i \right\|_{W^{2p,2}}^2 \right] < \infty, \ i = 1, 2.$

### 3.2.3 Initial conditions

The choice of the initial condition for the stochastic QG model is important, especially in the context of uncertainty quantification and data assimilation, for it significantly influences the evolution of the flow as well as its further predictability. A straightforward approach based on a random perturbation of the true solution (which is $q^a$ in our case) at time $t = 0.0$ can lead to the injection of unphysical perturbations into flow dynamics which, in turn, can result in a unphysical solution. Therefore, in order to perform uncertainty quantification tests, presented in Section 4, we need a number of independent realizations of the initial condition that are physically consistent with the flow dynamics. To this end, we start at time $t = -t^*$ with the true solution $q^a$ of the deterministic model and run it until $t_0 = 0$ with independent realizations of the Brownian noise $W$ (see Section 4 for details) to produce independent samples from the initial condition. As a result, the ensemble of stochastic solutions (also referred to as ensemble members) “covers” the true deterministic solution at time $t_0$.

The next experiment is to study for how long this property holds. To this end, we introduce the following function

$$\tilde{T}_S := \frac{1}{|T|} \int_T \tilde{\theta}(q^a) \, dt, \quad \tilde{\theta}(q^a) = \begin{cases} 1 & \text{if } q^a \in S, \\ 0 & \text{if } q^a \notin S, \end{cases}$$

which represents the time period spent by the true deterministic solution, $q^a$, within the spread of stochastic solutions $S$. The behavior of the function $\tilde{T}_S$ for the whole computational domain is given in Figure 5.
Figure 5: Shown is the time $T$ spent by the true deterministic velocity $V^a$, stream function $\psi^a$, and potential vorticity $q^a$ within the spread of stochastic solutions $S$ over the time period $T = [-1,0]$ hour and $T = [-16,0]$ hour for the heterogeneous and homogeneous flow. The stochastic spread (consisting of 100 independent samples from the initial condition) has been computed with the stochastic QG model (19) using the first 64 leading EOFs, which capture 96% of the flow variability (see Section 4). The blue color in the colorbar corresponds to $T = 0$ (the stochastic spread never captures the true deterministic solution over the time period $T$). The red color in the colorbar corresponds to $T = 1$ (the stochastic spread always captures the true deterministic solution over the time period $T$). As mentioned above, the potential vorticity $q^a$ is computed as the solution of the elliptic equation (22) with the stream function $\psi^a$, where $\psi^a$ is computed by spatially averaging the high-resolution stream function $\psi_f$ over the coarse grid cell $G^c = 129 \times 65$. The true velocity $V^a$ is computed by differentiating the stream function $\psi^a$. As the plot shows, the spread of stochastic solutions captures the true values of $V^a$, $\psi^a$, and $q^a$ for both heterogeneous and homogeneous flow equally well. For both the heterogeneous and homogeneous flow regime, the length of the time interval $T$ has a minor influence on the behavior of the stochastic spread (compare the top and bottom row in the Figure) thus ensuring a better coverage of the true solution with the stochastic spread over longer time. The region along the upper and lower boundary is not properly covered by the spread, because the boundary layer dynamics is difficult to capture on the coarse grid. However, the area of the boundary region is very small compared to the area of the whole domain, and therefore it has a negligible effect on the uncertainty quantification results.
In order to compute the function \( \tilde{T}_S \), we start at time \( t^* = -1 \) hour with the true solution \( q^a(t^*) \) and run the stochastic QG model \( (19) \) until \( t_0 = 0 \) with 100 independent realizations of the Brownian noise \( W \), and with the first 64 leading EOFs, which capture 96% of the total variance (see Section 4). As seen in Figure 5, the spread of stochastic solutions \( S \) captures the true deterministic velocity \( V^a \), stream function \( \psi^a \), and potential vorticity \( q^a \) for both heterogeneous and homogeneous flow, and over short and long time intervals \( T \) equally well except the neighbourhood of the upper and lower boundary. This boundary layer dynamics is difficult to capture on the coarse grid, because of the low resolution. However, the boundary layer is very small with respect to the whole domain, and so its contribution to uncertainty quantification results is miniscule. Overall, we have shown that the stochastically advected deterministic initial condition provides a solid basis for uncertainty quantification tests (given in Section 4) as well as for data assimilation, which will be the object of future research.

4 Calibration of eigenvectors

We present a methodology for modelling the difference between passive, infinitesimal Lagrangian particles advected by the high-resolution deterministic velocity field \( u \) computed on the fine grid \( G^f = 2049 \times 1025 \) and its coarsened counterpart \( \bar{u} \) computed on the coarse grid \( G^c = 129 \times 65 \) by differentiating the coarse-grain stream function \( \psi^a \). The stream function is computed by spatially averaging the high-resolution stream function \( \psi^f \) over the coarse grid cell \( G^c \). Based on this difference, we compute Empirical Orthogonal Functions (EOFs) [Preisendorfer, 1988; Hannachi et al., 2007] and evaluate how the accuracy of the deterministic flow dynamics reconstructed from the leading EOFs and their corresponding Principal Components (PCs) depends on the number of EOF-PC pairs. We also perform uncertainty quantification tests for the stochastic differential equation for Lagrangian particles (36) and the stochastic QG model (19), and study how the number of EOF-PC pairs and size of the ensemble of stochastic solutions (referred to as ensemble members) affect the width of the stochastic spread.

4.1 Measuring the Lagrangian evolution

In the stochastic GFD framework, stochastic PDEs are derived from the starting assumption that (averaged) fluid particles satisfy the equation

\[
\frac{d}{dt} \bar{x}(a,t) = \bar{u}(\bar{x}(a,t), t) \, dt + \sum_{i=1}^{N_l} \xi_i(\bar{x}(a,t)) \circ dW_i,
\]

where \( a \) is the Lagrangian label. The assumption (36) leads to, for example, the stochastic QG equation

\[
\frac{d}{dt} \bar{q}^l(x,t) + (\bar{u}^l(x,t) \, dt + \sum_{i=1}^{N_l} \xi_i^l(x,t) \circ dW_i^l(t)) \cdot \nabla \bar{q}^l(x,t) = F^l \, dt, \quad l = 1, 2,
\]

with \( F^l \) being the right hand side of (20). This is the system of stochastic PDEs that we actually solve. That is, equation (36) is not explicitly solved but describes the motion of fluid particles under the stochastic PDE solution.

The goal of the stochastic PDE is to model the coarse-grained components of a deterministic PDE that exhibits rapidly fluctuating components. The derivation of deterministic fluid dynamics starts from the equation

\[
\frac{d}{dt} x(a,t) = u(x(a,t), t) \, dt.
\]

After defining an averaged trajectory \( \bar{x}(a,t) \), we write

\[
x(a,t) = \bar{x}(a,t) + \xi(\bar{x}(a,t), t/\epsilon^2),
\]

on the assumption that the fluctuations in \( \xi \) are faster than those in \( \bar{x} \); this scale separation is parameterised by the small parameter \( \epsilon \). Thus the deterministic equation for \( \bar{x} \) is

\[
\frac{d}{dt} \bar{x}(a,t) = u(\bar{x}(a,t) + \xi(\bar{x}(a,t), t/\epsilon^2)) \, dt - \xi(\bar{x}(a,t), t/\epsilon^2) \, dt.
\]

If \( \xi \) has a fast dependency on \( t \) and has a stationary invariant measure, then according to homogenisation theory [Cotter et al., 2017] we may average this equation over the invariant measure (subject to a centring condition) to
get an effective equation
\[ \frac{d\hat{x}(a, t)}{dt} = \bar{u}(\hat{x}(a, t), t) + \sum_{i=1}^{\infty} \xi_i(\hat{x}(a, t)) \circ dW_i(t) + \mathcal{O}(\epsilon). \]

After truncation of this sum, we recover equation (36).

We assume that \( u(x, t) \) can be modelled well with a fine grid simulation, whilst \( \bar{u}(\hat{x}, t) \) can be modelled on a coarse grid simulation. Then, we wish to estimate \( \xi \), using data from \( u(x, t) \) in order to simulate \( \bar{u}(x, t) \).

Methodology is as follows. We spin up a fine grid solution from \( t = -T_{\text{spin}} \) to \( t = 0 \) (till some statistical equilibrium is reached), then record velocity time series from \( t = 0 \) to \( t = M\Delta t \), where \( \Delta t = k\delta t \), and \( \delta t \) is the fine grid timestep. We define \( X^0_{ij} \) as coarse grid points.

For each \( m = 0, 1, \ldots, M - 1 \), we

1. Solve \( \hat{X}_{ij}(t) = u(X_{ij}(t), t) \) with initial condition \( X_{ij}(m\Delta t) = X^0_{ij} \), where \( u(x, t) \) is the solution from the fine grid simulation.
2. Compute \( \bar{u}_{ij}(t) \) by spatially averaging \( u(x, t) \) over the coarse grid cell size around gridpoint \((i, j)\).
3. Compute \( \bar{X}_{ij} \) by solving \( \hat{X}_{ij}(t) = \bar{u}_{ij}(t) \) with the same initial condition.
4. Compute the difference \( \Delta X^m_{ij} = \hat{X}_{ij}((m + 1)\Delta t) - X_{ij}((m + 1)\Delta t) \), which measures the error between the fine and coarse trajectory.

Having obtained \( \Delta X^m_{ij} \), we would like to extract the basis for the noise. This amounts to a Gaussian model of the form
\[ \frac{\Delta X^m_{ij}}{\sqrt{\Delta t}} = \Delta X_{ij} + \sum_{k=1}^{N_i} \xi_{k_{ij}} \Delta W^k_m, \]
where \( \Delta W^k_m \) are independent and identically distributed normal random variables with mean zero and variance one.

We estimate \( \xi \) by minimising
\[ E \left[ \left( \sum_{i,j,m} \frac{\Delta X^m_{ij}}{\sqrt{\Delta t}} - \Delta X_{ij} - \sum_{k=1}^{N_i} \xi_{k_{ij}} \Delta W^k_m \right)^2 \right], \]
where the choice of \( N \) can be informed by using EOFs.

Our choice of Empirical Orthogonal Function analysis is based on the capability of this method for extracting spatially coherent, temporally uncorrelated and statistically significant modes of transient variability from multivariable time series. In particular, this method is efficient for dimensionality reduction, compression and spatio-temporal variability analysis of atmospheric and oceanic data. Generally speaking, one can use different flow decomposition methods instead of EOF analysis (e.g. Dynamic Mode Decomposition (DMD) [Schmid, 2010], Optimized DMD [Chen et al., 2012], Singular Spectrum Analysis [Elsner and Tsonis, 1996], etc.), and analyse how they affect the parameterisation, but such a study would be beyond the scope of this paper.

### 4.2 Validity of the approximation

Having computed EOFs and their corresponding PCs, we can analyze how the coarse-grid solution
\[ X^c(t) := \bar{X}^c(t) + \Delta X(t), \]
depends on the number of EOF-PC pairs (denoted by \( \xi \) and \( P \)), which approximates the difference \( \Delta X := \mathbf{x} - \bar{X}^c \) defined as
\[ \Delta X(t) \approx \sum_{i=1}^{N_i} \xi_i(\bar{X}^c(t)) P_i(t). \]

Here, \( \mathbf{x} \) is the solution of the deterministic equation (37) with \( \mathbf{u} \) being the high-resolution velocity, and \( \bar{X}^c(t) \) is the solution of the deterministic equation
\[ \frac{d\bar{X}^c(t)}{dt} = \mathbf{u}(\bar{X}^c(t), t) \, dt, \]
(40)
with the spatially averaged velocity $\bar{u}$.

In this section, we solve ODE (40) with the velocity $\mathbf{u}$ computed from the high-resolution heterogeneous flow (Figure 2). However, it is important to note that the results presented here are qualitatively independent of flow dynamics, and hence they are equally valid for both heterogeneous and homogeneous flows. In order to solve equation (40), we use the classical 4-stage Runge–Kutta method [Hairer et al., 1993] given by the Butcher tableau (41).

\[
\begin{array}{cccc}
0 & & & \\
\frac{1}{2} & 0 & \frac{1}{2} & \\
\frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{2} & \\
1 & 0 & 0 & 1 & \\
\end{array}
\]

(41)

We present the results in Figure 6. We remark that in this case Lagrangian particles move freely within the flow, i.e. they are not remapped every time step $\Delta t$ as in Section 4.3. It is also worth noting that we computed the relative error $\delta$ for $\Delta \mathbf{X}$ including both the time-mean and fluctuating component, since excluding the time-mean would result in a much higher error.

![Figure 6](image)

Figure 6: Dependence of the $L^2$-norm relative error of Lagrangian path separations $\delta = ||\mathbf{x} - \mathbf{x}^c||_{L^2}/||\mathbf{x}||_{L^2}$ on the number of leading EOF-PC pairs used in approximation (39) is shown. Here $\mathbf{x}$ (see equation (37)) and $\mathbf{x}^c$ (see equation (40)) are the positions of Lagrangian particles freely advected by the high-resolution velocity $\mathbf{u}$ computed on the fine-grid $G^f = 2049 \times 1025$, and its coarse-grained analogue $\mathbf{u}^c$ computed on the coarse grid $G^c = 129 \times 65$ by differentiating the coarse-grain stream function $\psi^a$, respectively. The EOFs and their corresponding PCs, used in this test, capture 96% of the flow variability and have been computed over the period of $T = [0, 70]$ days. The time period is not a critical parameter; it has been chosen so as to demonstrate how accurately the solution can be approximated by a given number of EOF-PC pairs. Our results show that using more EOF-PC pairs in computing the positions of Lagrangian particles $\mathbf{x}^c$, tends to increase the accuracy of the solution $\mathbf{x}^c$.

As seen in Figure 6, using more EOF-PC pairs to compute the positions of Lagrangian particles tends to increase the accuracy of the approximated solution. This is an expected result, because $\Delta \mathbf{X} \to 0$ as $N_\xi \to DOF$ in inequality (39), where DOF is the number of degree of freedom on the coarse grid $G^c$.

### 4.3 Approximation of the Lagrangian evolution

In contrast with the previous section, we apply EOF analysis to the fluctuating component of $\Delta \mathbf{X} := \mathbf{x}^c - \mathbf{x}$ and perform uncertainty quantification tests for the stochastic differential equation (SDE) (36) by comparing the true deterministic solution with the ensemble of stochastic equations. As the true deterministic solution, we take the solution $\mathbf{x}^c$ of the deterministic equation (40), while the stochastic ensemble is given by a solution $\mathbf{x}$ of SDE (36)
computed for independent realizations of the Brownian noise $W$. The uncertainty quantification tests are carried out for different number of EOFs and the size of the stochastic ensemble. As opposed to the deterministic case, we use the Brownian noise instead of the Principal Components, and Lagrangian particles are remapped to their original positions (the nodes of the Eulerian grid $G^c$) every time step $\Delta t$. The size of the time step is a critical component for uncertainty quantification and data assimilation, and should be chosen so as to lead to a stochastic ensemble which covers the true solution over this time step.

As mentioned before, to solve the deterministic equation (40), we use the Runge–Kutta method with the Butcher tableau (41). The SDE (36) is solved with the stochastic version of the Runge–Kutta method presented by Algorithm 3.

**Algorithm 3** Stochastic Runge–Kutta method

```
for $n = 0, 1, 2, \ldots$ do
    $k_1 = v(t_n, \bar{x}_n)$, $l_1 = \Xi(t_n, \bar{x}_n)$,
    $k_2 = v(t_n + \frac{\Delta t}{2}, \bar{x}_n + \frac{\Delta t}{2}k_1)$, $l_2 = \Xi(t_n + \frac{\Delta W}{2}, \bar{x}_n + \frac{\Delta W}{2}l_1)$,
    $k_3 = v(t_n + \frac{\Delta t}{2}, \bar{x}_n + \frac{\Delta t}{2}k_2)$, $l_3 = \Xi(t_n + \frac{\Delta W}{2}, \bar{x}_n + \frac{\Delta W}{2}l_2)$,
    $k_4 = v(t_n + \Delta t, \bar{x}_n + \Delta t k_3)$, $l_4 = \Xi(t_n + \Delta W, \bar{x}_n + \Delta W l_3)$,

    $\bar{x}_{n+1} = \bar{x}_n + (k_1 + 2(k_2 + k_3) + k_4)\frac{\Delta t}{6} + (l_1 + 2(l_2 + l_3) + l_4)\frac{\Delta W}{6}$. (42)
```

Here $v$ is the velocity vector, and $\{\bar{x}\}_{i=1}^{N_l}$ is the vector of coordinates of Lagrangian particles, with $N_l$ being the number of Lagrangian particles. The stochastic term $\Xi(t, \bar{x})$ is given by

$$
\Xi(t, \bar{x}) := \sum_{k=1}^{N_l} \xi_{k,(x)}(\bar{x}(t)) \Delta W_{k,t}(t), \quad l = 1, 2.
$$

By Taylor expanding the right hand side of (42):

$$
\bar{x}_{n+1} = \bar{x}_n + v(t_n, \bar{x}_n)\Delta t + \Xi(t_n, \bar{x})\Delta W + (\Xi(t_n, \bar{x}) \cdot \nabla \Xi(t_n, \bar{x})) \frac{(\Delta W)^2}{2} + H.O.T.
$$

it can be seen that the stochastic Runge–Kutta method is in Stratonovich form, and thus consistent with SDE (36).

Before passing to numerical results, we note that the size of the time step is a critical component for uncertainty quantification and data assimilation. The time step should be short enough that the stochastic ensemble encompasses the true solution. Our experiments show that $\Delta t = 24$ hours properly fulfils this condition. First, we demonstrate that the true deterministic solution $\bar{x}^c$ is enclosed within a cloud of stochastic solutions (also referred as a stochastic spread). To this end, we study how the area of the stochastic cloud (denoted by $A^c$) depends on both the size of the stochastic ensemble, $N_a$, and the number of EOFs. The results are presented in Figures 7 and 8.
Figure 7: Shown is a typical dependence of the area of the stochastic cloud $A^c$ on the size of the stochastic ensemble $\bar{x}$ at the time moments (a) $t = 0$, (b) $t = 50$ hours, (c) $t = 100$ hours, (d) $t = 200$ hours. The left and right column shows the area of the stochastic cloud (marked in grey color) which consists of 100 and 400 ensemble members, respectively. The stochastic ensemble has been computed for the first 64 leading EOFs (96% of the flow variability). The true solution $\bar{x}^c$ is marked with a black dot. The plot represents a typical part of the computational domain of size $[10, 45] \times [45, 65]$ in the first layer, which can be divided into two regions: a fast flow region (the boundary layer along the upper boundary $[10, 45] \times [60, 65]$, the striation occupying the domain $[10, 45] \times [45, 52]$) and a slow flow region $[10, 45] \times (52, 60)$. As it can be seen in the figure, there are two key parameters which influence the size of the stochastic cloud, namely the number of ensemble members and the flow velocity. In particular, the larger the stochastic ensemble is, the wider the cloud becomes. The same is true for the flow velocity: the faster the flow, the larger the stochastic spread. This behavior is expected, since large ensembles or fast flows inevitably increase the variance of the whole stochastic cloud. Clearly, the velocity of the flow contributes much more to the size of the spread than the number of ensemble members (compare the area of the stochastic cloud in the fast and slow region for different number of ensemble members). The most important observation is that the true solution lies within the stochastic cloud almost everywhere. This observation confirms that the parameterisation works well for different flow regimes.
Figure 8: Shown is a typical dependence of the area of the stochastic cloud $A^c$ on the size of the stochastic ensemble $\mathbf{x}$ at the time moments (a) $t = 0$, (b) $t = 50$ hours, (c) $t = 100$ hours, (d) $t = 200$ hours. The left and right column shows the area of the stochastic cloud (marked in grey color) which consists of 100 and 400 ensemble members, respectively; the stochastic ensemble has been computed for the first 128 leading EOFs (99% of the flow variability). The true solution $\hat{\mathbf{x}}^c$ is marked with a black dot. The plot represents a typical part of the computational domain of size $[10, 45] \times [45, 65]$ in the first layer, which can be divided into two regions: a fast flow region (the boundary layer along the upper boundary $[10, 45] \times [60, 65]$ and the striation occupying the domain $[10, 45] \times [45, 52]$) and a slow flow region $[10, 45] \times (52, 60)$. As can be seen in the figure, there are two key parameters which influence the size of the stochastic cloud, namely the number of ensemble members and the flow velocity. In particular, the larger the size of the stochastic ensemble is, the wider the cloud becomes. The same is true for the flow velocity: the faster the flow, the larger the stochastic spread. This is an expected behavior, since large ensembles or fast flows inevitably increases the variance of the whole stochastic cloud. Clearly, the velocity of the flow contributes much more to the size of the spread than the number ensemble members (compare the area of the stochastic cloud in the fast and slow region for different number of ensemble members). As in the previous test with 64 EOFs (see Figure 7), the true solution lies within the stochastic cloud almost everywhere. This result confirms again that the parameterisation works well, with little dependence on the number of EOFs.
Figures 7 and 8 show a typical flow region in the horizontal channel at different time moments and for different number of EOFs and the size of the stochastic ensemble. As seen in the figures, the channel flow can be divided into two regions: a fast flow region (the boundary layer along the upper boundary \([10, 45] \times [60, 65]\) and the striation occupying the domain \([10, 45] \times [45, 52]\)) and a slow flow region \([10, 45] \times (52, 60]\). By comparing Figures 7 and 8, we identify three key parameters which influence the size of the stochastic cloud: the number of EOFs, the size of the stochastic ensemble, and the flow velocity. As Figures 7 and 8 show, the more EOFs are used in the stochastic model, the wider the stochastic spread becomes. The same is true for the size of the stochastic ensemble and the velocity of the flow, namely the stochastic cloud widens as the ensemble size or the flow velocity increases. This behavior is expected, since increasing these parameters offer a better quantification of the uncertainty of the model. The velocity of the flow contributes much more to the size of the spread than the number of ensemble members or EOFs. The results show that regardless of the flow dynamics the true solution \(\hat{x}\) lies within the stochastic cloud almost everywhere. This confirms that the parameterisation works well for a wide range of governing parameters and different flow regimes. Figures 7 and 8 give important insights into how the uncertainty in the stochastic equation (36) behaves with respect to the number of EOFs, the size of the stochastic ensemble, and the flow velocity. Next, we study a more global picture.

To take a more global view, we first divide the flow dynamics into fast (the northern and southern boundary layers, and striations) and slow (flow between the striations) as shown in Figures 9(a) and 9(b), respectively. In terms of the flow velocity, we quantify the flow by the Reynolds number defined as

\[
Re = \mathbf{\nabla} Rd_1/\nu,
\]

where \(\mathbf{\nabla}\) is the maximum time-mean velocity, and \(Rd_1\) is the first baroclinic Rossby deformation radius. We remark that \(Re\) can be defined by using different velocity and length scales (e.g. [Siegel et al., 2001]). Our definition is focused on the mesoscale eddies characterized by the length scale up to \(O(100)\) km and striations. In terms of the Reynolds number, the flow decomposition is given by \(Re_s < 432\) and \(432 \leq Re_f \leq 1440\), where \(Re_s\) and \(Re_f\) are the Reynolds numbers for the slow and fast flow dynamics, respectively.

Before going into detail, it is helpful to introduce the area of the stochastic cloud \(\overline{A}_s\) and \(\overline{A}_f\) averaged over the number of Lagrangian particles in the slow, \(N_{l,s}\), and fast, \(N_{l,f}\), flow region, respectively:

\[
\overline{A}_s(t_k) = \frac{1}{N_{l,s}} \sum_{i=1}^{N_{l,s}} A_{s,i}(t_k), \quad \overline{A}_f(t_k) = \frac{1}{N_{l,f}} \sum_{i=1}^{N_{l,f}} A_{f,i}(t_k),
\]

where \(A_{s,i}\) and \(A_{f,i}\) are the area of the cloud surrounding the \(i\)-th Lagrangian particle belonging to the slow and fast flow, respectively.
We define the $L^2$-error spread for the slow, $\bar{S}_s(t_k)$, and fast, $\bar{S}_f(t_k)$, flow as
\[
\bar{S}_s(t_k) := \left[ \min_{j \in [1, N_s]} \overline{\varepsilon}_{s,j}(t_k), \max_{j \in [1, N_s]} \overline{\varepsilon}_{s,j}(t_k) \right], \quad \bar{S}_f(t_k) := \left[ \min_{j \in [1, N_f]} \overline{\varepsilon}_{f,j}(t_k), \max_{j \in [1, N_f]} \overline{\varepsilon}_{f,j}(t_k) \right],
\]
with mean $L^2$-norm relative errors given by
\[
\overline{\varepsilon}_{s,j}(t_k) := \frac{1}{N_{l,s}} \sum_{i=1}^{N_{l,s}} \frac{\| x_i^s(t_k) - \overline{x}_j^s(t_k) \|^2}{\| x_i^s(t_k) \|^2}, \quad \overline{\varepsilon}_{f,j}(t_k) := \frac{1}{N_{l,f}} \sum_{i=1}^{N_{l,f}} \frac{\| x_i^f(t_k) - \overline{x}_j^f(t_k) \|^2}{\| x_i^f(t_k) \|^2},
\]
where $x_i^s$ is the $i$-th ensemble member.

We also introduce the mean $L^2$-norm relative errors
\[
e_s(t_k) := \frac{1}{N_{l,s}} \sum_{i=1}^{N_{l,s}} \frac{\| x_i^s(t_k) - \overline{x}_i^s(t_k) \|^2}{\| x_i^s(t_k) \|^2}, \quad e_f(t_k) := \frac{1}{N_{l,f}} \sum_{i=1}^{N_{l,f}} \frac{\| x_i^f(t_k) - \overline{x}_i^f(t_k) \|^2}{\| x_i^f(t_k) \|^2}
\]
to compute the error between the solution $\overline{x}^c$ of equation (40) (the true solution in the uncertainty quantification context) for which Lagrangian particles are advected by spatially averaged velocity $\overline{u}$ and the deterministic solution $x$ of equation (37) for which Lagrangian particles are moved by the high-resolution velocity $u$. The time index $k = k_s \cup k_f$ is split into a training period $k_s = [0, 299]$ days (the period over which the EOFs have been computed) and a forecast period $k_f = [300, 365]$ days. $N_l = N_{l,s} \cup N_{l,f}$ is the total number of Lagrangian particles. The subdivision of the time intervals into the training and forecast subintervals allows us to study how the parameterisation performs after the training period, where there is no data available for computing EOFs. The dependence of the averaged area of the stochastic cloud for the slow and fast flow regions on the number of EOFs and the size of the stochastic ensemble is presented in Figure 10.

Figure 10: Shown is the dependence of the averaged area of the stochastic cloud for the slow, $\overline{A}_s^c$, and fast, $\overline{A}_f^c$, flow regions on the number of EOFs, $N_\xi$, and the size of the stochastic ensemble $N_a$. The results presented in the figure are in good agreement with the analysis of instantaneous snapshots (see Figures 7 and 8). In particular, the averaged area of the stochastic cloud $\overline{A}_s^c$ is significantly influenced by the three parameters we identified for the case of instantaneous flows: the number of EOFs, the size of the stochastic ensemble, and the flow velocity. More importantly, the qualitative behavior of $\overline{A}$ is similar to those of $A^c$ (the area of the stochastic ensemble associated with a given Lagrangian particle). Namely, as the size of the stochastic ensemble, $N_a$, increases so does the area of the cloud (for example, compare the red and brown lines for which the ensemble size is $N_a = 100$ and $N_a = 400$, respectively). The increase in the number of EOFs, $N_\xi$, also leads to a larger area of the cloud (for instance, compare the red and magenta lines for which $N_\xi = 64$ and $N_\xi = 128$, respectively). The same is true for the flow velocity: the faster the flow, the larger the stochastic cloud (compare the red and blue lines which corresponds to the fast and slow velocity region, respectively). The most important observation here is that we can estimate the contribution of each parameter to the parameterisation. The size of the stochastic ensemble and the number of EOFs have rather small effects on the area of the stochastic cloud. The most significant contribution comes from the velocity of the flow. Namely, the size of the stochastic cloud for fast flows is always larger than that for slow flows (compare the upper four curves with the lower four curves in the plot).
Upon analysing the results presented in Figure 10, we have found that the averaged area of the stochastic cloud $\overline{A}$ significantly depends on the number of EOFs, the size of the stochastic ensemble, and the flow velocity. This dependence is qualitatively the same as that for the area of the stochastic ensemble, $A^c$, associated with a given Lagrangian particle (see Figures 7 and 8). In particular, as the size of the stochastic ensemble or the number of EOFs increases so does the area of the cloud. These results stay the same for the stochastic QG model studied in Section 4.4. With respect to the flow velocity, we observe that the faster the flow is, the larger the stochastic cloud becomes. As seen in Figure 10, the size of the stochastic ensemble and the number of EOFs have a smaller effect on the area of the stochastic cloud. The major contribution comes from the velocity of the flow.

Having studied the influence of different parameters on the area of the stochastic cloud, we can now perform uncertainty quantification tests, as presented in Figure 11.
Figure 11: Shown is the dependence of the $L^2$-error spread for the slow, $\bar{S}_s(t_k)$, and fast, $\bar{S}_f(t_k)$, flow, and the mean $L^2$-norm relative error $e_s^r(t_k)$ and $e_f^r(t_k)$ on the number of EOFs, $N_\xi$, and the size of the stochastic ensemble $N_a$. The presented results show that the $L^2$-norm relative error between the true solution $\tilde{x}_c$ for which Lagrangian particles are advected by spatially averaged velocity $\bar{u}$ (see equation (40)) and the deterministic solution $x$ for which Lagrangian particles are moved by the high-resolution velocity $u$ (see equation (37)) is small over the whole time interval for both slow and fast flows. Moreover, this error is also enclosed within the spread of stochastic solutions over the whole time interval. Most importantly, the error remains small not only over the training interval, but also over the forecast interval. This confirms that the leading EOFs properly capture the spatial structure of the flow, and the parameterization performs equally well for both fast and slow flows. Along with the uncertainty quantification results, we can ask the question: “How does the stochastic spread depend on the number of EOFs, the size of the ensemble, and the flow dynamics?” As seen in the figure, the presented results are in good agreement with the ones in Figure 10. The stochastic spread is significantly influenced by the number of EOFs, the size of the stochastic ensemble, and the flow velocity. More specifically, the spread widens as the number of EOFs, $N_\xi$, increases (compare the red and magenta spreads (Figures (a) and (b)) for which $N_\xi = 64$ and $N_\xi = 128$, respectively). As the size of the stochastic ensemble, $N_a$, grows, so does the spread (compare the red and brown spreads (Figures (a) and (c)) for which the ensemble size is $N_a = 100$ and $N_a = 400$, respectively). The velocity of the flow has a much more noticeable effect on the spread: the faster the flow, the wider the stochastic spread (compare the red and blue spread (Figure a) which corresponds to the fast and slow velocity region, respectively). Thus, we conclude that the stochastic ensemble and the number of EOFs have a smaller effect on the width of the stochastic spread, and the major contribution is given by the velocity of the flow, as also confirmed by the results in Figure 10.

The uncertainty quantification results presented in Figure 11 show that the $L^2$-norm relative error between the true solution $\tilde{x}_c$ (computed for the spatially averaged velocity $\bar{u}$, equation (40)) and the deterministic solution $x$ (computed for the high-resolution velocity $u$, equation (37)) is small and contained in the spread of stochastic solutions over the whole time interval for both slow and fast flows. Moreover, the error remains small not only within the training interval but also within the forecast interval. The results in Figure 11 are in good agreement
with the ones presented in Figure 10. In particular, the spread gets wider, upon increasing either the number of EOFs, or the size of the stochastic ensemble. In addition, the faster the flow is, the wider the stochastic spread becomes. However, the stochastic ensemble and the number of EOFs have a smaller effect on the width of the stochastic spread, compared with the velocity of the flow, as also confirmed by the results in Figure 10. Overall, we conclude that the leading EOFs properly capture the spatial structure of the flow, and the parameterization performs equally well for both fast and slow flows.

4.4 Application of EOFs to the stochastic QG equations

The Lagrangian evolution studied in the previous section demonstrates encouraging results. However, it cannot guarantee that the application of EOFs to the stochastic QG equations (19) is equally beneficial. Therefore, this section focuses on uncertainty quantification for the stochastic QG model. Here, we impose more stringent restrictions upon the parameterisation (compared to those given in Section 3.2.3). In particular, we analyse how long the true deterministic solution remains within the stochastic ensemble one standard deviation, not within the whole stochastic ensemble as in Sections 3.2.3 and 4.3. In other words, we study how the function

\[ \tilde{T}_{S_\sigma} = \frac{1}{|T|} \int T \delta(q^o) \, dt, \quad \delta(q^o) = \begin{cases} 1 & \text{if } q^o \in S_\sigma, \\ 0 & \text{if } q^o \notin S_\sigma, \end{cases} \]

depends on the number of EOFs and the size of the stochastic ensemble. As in Section 3.2.3, \( \tilde{T}_{S_\sigma} \) is a time period spent by the true deterministic solution, \( q^o \), within the stochastic ensemble one standard deviation \( S_\sigma = [S - \sigma(S), S + \sigma(S)] \), where \( \sigma(S) \) is the standard deviation of \( S \). The results are presented in Figures 12 and 13.
Figure 12: Shown is the dependence of $\tilde{T}_{S_\sigma}$ on the number of EOFs $N_\xi$ and size of the stochastic ensemble $N_a$ over the time period $T = [0, 24]$ hours for the heterogeneous flow ($\mu = 4 \times 10^{-8} \text{s}^{-1}$) presented in Figure 2. The blue color in the colorbar corresponds to $\tilde{T}_{S_\sigma} = 0$ (the stochastic spread never captures the true deterministic solution over the time period $T$). The red color in the colorbar corresponds to $\tilde{T}_{S_\sigma} = 1$ (the stochastic spread always captures the true deterministic solution over the time period $T$). As seen, the smoother the field is, the longer the true deterministic solution, $q^a$, remains within the spread of stochastic solutions (see, for example, Figure (a) showing the stream function $\psi_1$, velocity $V_1$, and potential vorticity (PV) $q_1$). Obviously, the stream function is enclosed within the spread for a longer period of time compared to the velocity and PV, while the spread captures the velocity for a longer time than PV. Besides, using more EOFs (compare Figures (a) and (b) for which $N_\xi = 1$ (23% of the flow variability) and $N_\xi = 2$ (42% of the flow variability) leading EOFs, respectively) leads to a better coverage of the true solution with the spread. Surprisingly, using even more EOFs does not lead to significantly better results; for example, compare Figures (b) and (c) which present the uncertainty quantification results for $N_\xi = 2$ (42% of the flow variability) and $N_\xi = 4$ (60% of the flow variability) leading EOFs, respectively. The same conclusion holds for the size of the stochastic ensemble: the larger the size of the ensemble, the longer the spread captures the true solution (compare Figures (a) and (d) for which $N_a = 100$ and $N_a = 200$, respectively). However, using more ensemble members does not results in a much better coverage of the true solution with the stochastic spread (compare Figures (d) and (e) for which $N_\xi = 200$ and $N_\xi = 400$, respectively). The uncertainty quantification results presented here are in good qualitative agreement with the Lagrangian simulations given in Section 4.3. Thus, we conclude that uncertainty quantification tests for Lagrangian simulations can be used to qualitatively quantify uncertainty for the stochastic QG model. This observation allows to significantly reduce computational resources needed for uncertainty quantification tests, since Lagrangian simulations are computationally much less intensive than those of the stochastic QG model.
Figure 13: Shown is the dependence of $\tilde{T}_{\sigma}$ on the number of EOFs $N_{\xi}$ and size of the stochastic ensemble $N_a$ over the time period $T = [0, 24]$ hours for the homogenous flow ($\mu = 4 \times 10^{-7} \text{ s}^{-1}$) presented in Figure 3. The blue color in the colorbar corresponds to $\tilde{T}_{\sigma} = 0$ (the stochastic spread never captures the true deterministic solution over the time period $T$). The red color in the colorbar corresponds to $\tilde{T}_{\sigma} = 1$ (the stochastic spread always captures the true deterministic solution over the time period $T$). As for the heterogeneous flow, the smoother the field is, the longer the true deterministic solution, $q$, remains within the spread of stochastic solutions (see Figure (a) showing the stream function $\psi_1$, velocity $V_1$, and potential vorticity $q_1$). The stream function is enclosed within the spread for longer compared to the velocity and PV, while the spread captures the velocity for a longer time period than PV. Using more EOFs (compare Figures (a) and (b) for which $N_{\xi} = 1$ (15% of the flow variability) and $N_{\xi} = 2$ (28% of the flow variability) leading EOFs, respectively) leads to a better coverage of the true solution with the spread. As in the heterogeneous case, using even more EOFs does not lead to significantly better results; compare Figures (b) and (c) which present the uncertainty quantification results for $N_{\xi} = 2$ (28% of the flow variability) and $N_{\xi} = 4$ (48% of the flow variability) leading EOFs, respectively. The same conclusion holds for the size of the stochastic ensemble: the larger the size of the ensemble, the longer the spread captures the true solution (compare Figures (a) and (d) for which $N_a = 100$ and $N_a = 200$, respectively). However, using more ensemble members does not result in a much better coverage of the true solution with the stochastic spread (compare Figures (d) and (e) for which $N_a = 200$ and $N_a = 400$, respectively). The uncertainty quantification results for the homogeneous flow are qualitatively the same as for the heterogeneous flow presented in Figure 13. Thus, the parameterisation was found to perform equally well for both homogeneous and heterogeneous flows.
As seen in Figures 12 and 13, the uncertainty quantification results are qualitatively the same for the heterogeneous and homogeneous flow. In particular, the smoother the field is, the longer the true deterministic solution, $q^a$, remains enclosed within the spread of stochastic solutions. In both cases, the stream function $\psi_1$ is enclosed within the spread for a longer period of time compared to the velocity $V_1$ and potential vorticity $q_1$, while the spread captures the velocity for a longer time than the potential vorticity. Moreover, using more EOFs results in a better coverage of the true solution with the stochastic spread. However, we found that for both the heterogeneous and homogeneous flow, using more than two leading EOFs does not lead to significantly better results. The same conclusion holds for the size of the stochastic ensemble: the larger the size of the ensemble, the longer the spread captures the true solution, but using more than 200 ensemble members does not result in a much better coverage of the true solution with the stochastic spread. Overall, we conclude that the proposed parameterisation performs equally well for both simpler homogeneous flows and more complex heterogeneous ones. The uncertainty quantification results presented here are in good qualitative agreement with the Lagrangian simulations given in Section 4.3. Thus, uncertainty quantification tests in the Lagrangian framework can be used to qualitatively quantify uncertainty for the stochastic QG model. This important observation allows to use Lagrangian simulations which are computationally much less intensive than those of the stochastic QG model.

Another important question we study is to quantify how the uncertainty in the initial stochastic condition is propagated by the deterministic QG model and compare these uncertainty quantification results with the stochastic case. For doing so, we start the deterministic QG model from the stochastic initial condition at time $t = 0$ (see Section 3.2.3 for details) and run it for each independent realization of the Brownian noise $W$, and compare the behavior of the deterministic spread (denoted by $T_{S_d}$) for the deterministic QG model with the stochastic spread for the stochastic QG model (denoted by $\tilde{T}_{S_o}$). The results of this simulation for the heterogeneous and homogeneous flow are given in Figures 14 and 15, respectively.
Figure 14: Shown is the spread $\tilde{T}_{S_\sigma}$ for the stochastic QG model (top row) and spread $T_{S_\sigma}$ for the deterministic QG model (bottom row) for the heterogeneous flow ($\mu = 4 \times 10^{-8} \text{ s}^{-1}$). The stochastic spread $\tilde{T}_{S_\sigma}$ has been computed for one leading EOF with 100 independent realizations of the Brownian noise over the time period $T = [0, 24]$ hours. The deterministic spread $T_{S_\sigma}$ has been computed with the deterministic QG model started at $t = 0$ and run from the stochastic initial condition (see Section 3.2.3 for details) with 100 independent realizations of the Brownian noise over the same period of time. The blue color in the colorbar indicates that the spread never captures the true deterministic solution over the time period $T$, while the red one indicates that the stochastic spread always captures the true deterministic solution over the time period $T$. As seen in the plot, the true deterministic solution, $q^o$, remains enclosed within the stochastic spread much longer than within the deterministic spread (compare either the stream function $\psi_1$, velocity $V_1$, or potential vorticity $q_1$ for the stochastic spread (top row) and deterministic spread (bottom row)). Moreover, if we compare the deterministic and stochastic spreads at individual grid points we find that many more points in the domain are captured by the stochastic spread than by the deterministic one. Thus, we conclude for data assimilation that the proposed stochastic parameterisation would be preferable to the deterministic QG model.
Figure 15: Shown is the spread $\tilde{T}_{S_{\sigma}}$ for the stochastic QG model (top row) and spread $T_{S_{\sigma}}$ for the deterministic QG model (bottom row) for the homogeneous flow ($\mu = 4 \times 10^{-7} \text{s}^{-1}$). The stochastic spread $\tilde{T}_{S_{\sigma}}$ has been computed for one leading EOF with 100 independent realizations of the Brownian noise over the time period $T = [0, 24]$ hours. The deterministic spread $T_{S_{\sigma}}$ has been computed with the deterministic QG model started at $t = 0$ and run from the stochastic initial condition (see Section 3.2.3 for details) with 100 independent realizations of the Brownian noise over the same period of time. The blue color in the colorbar indicates that the spread never captures the true deterministic solution over the time period $T$, while the red one indicates that the stochastic spread always captures the true deterministic solution over the time period $T$. As seen in the plot, the true deterministic solution, $q^{a}$, remains enclosed within the stochastic spread much longer than within the deterministic spread (compare either the stream function $\psi_1$, velocity $V_1$, or potential vorticity $q_1$ for the stochastic spread (top row) and deterministic spread (bottom row)). As for the heterogeneous flow (Figure 14), the stochastic spread captures much more individual grid points in the domain than the deterministic spread. Thus, we have found that for data assimilation the proposed parameterisation would be preferable to the deterministic QG model; not only for heterogeneous flows, but also for homogeneous flows.

In summary, by comparing the uncertainty quantification results for the heterogeneous flow (Figure 14) and homogeneous flow (Figure 15), we have found that the stochastic spread captures the true deterministic solution $q^{a}$ (computed on the coarse grid $G^c$) for much longer times and for much more individual grid points in the computational domain. Therefore, for data assimilation, the proposed parameterisation would be considerably more preferable than the deterministic QG model; not only for heterogeneous flows (Figure 14), but also for homogeneous ones (Figure 15). Overall, we conclude that the parameterisation of the stochastic QG model is robust to large variations of the flow dynamics and governing parameters, and can be equally well applied to both homogeneous and heterogeneous flows.

5 Conclusion and future work

In this paper we have introduced a stochastic parameterisation for unresolved eddy motions in a two-layer quasi-geostrophic channel model with forcing and dissipation. The parameterisation is based upon the idea of “transport noise”, which models the modifications to the velocity field due to unresolved dynamics. This model assumes that the transport of large scale components is accurate, but that the velocity field used to transport these components is missing contributions from unresolved scales. We first introduced a time-integration scheme for the stochastic PDE, shown that it is in Stratonovich form, and proved its consistency as $\Delta t \to 0$. Then we described a procedure for extracting stochastic forcing by post-processing high resolution simulations, and demonstrated the procedure
by using uncertainty quantification experiments for both the SDE and stochastic QG model for homogeneous and heterogeneous flow dynamics. The results show that the proposed parameterisation is efficient and effective for both homogeneous and heterogeneous flows, and they lay the solid foundation for data assimilation.

In future work, we intend to use this approach as the basis for data assimilation algorithms, to investigate the assimilation of data from a high-resolution deterministic model into a low-resolution stochastic model. We also intend to examine the derivation of “prognostic” parameterisations where the stochastic forcing patterns are determined from the coarse model itself using physical principles, rather than the “diagnostic” parameterisations of this paper where they are determined from high resolution simulations. The diagnostic approach proposed in this paper will provide important insight by comparing the diagnosed forcing with the state of the stochastic model.

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