
Quantifying Truncation-Related Uncertainties in Unsteady Fluid Dynamics Reduced Order Models

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Abstract :

In this paper, we present a new method to quantify the uncertainty introduced by the drastic dimensionality reduction commonly practiced in the field of computational fluid dynamics, the ultimate goal being to simulate accurate priors for real-time data assimilation. Our key ingredient is a stochastic Navier--Stokes closure mechanism that arises by assuming random unresolved flow components. This decomposition is carried out through Galerkin projection with a proper orthogonal decomposition (POD-Galerkin) basis. The residual velocity fields, model structure, and evolution of coefficients of the reduced order's solutions are used to compute the resulting multiplicative and additive noise's correlations. The low computational cost of these consistent correlation estimators makes them applicable to the study of complex fluid flows. This stochastic POD-reduced order model (POD-ROM) is applied to 2-dimensional and 3-dimensional direct numerical simulations of wake flows at Reynolds 100 and 300, respectively, with uncertainty quantification and forecasting outside the learning interval being the main focus. The proposed stochastic POD-ROM approach is shown to stabilize the unstable temporal coefficients and to maintain their variability under control, while exhibiting an impressively accurate predictive capability.

Keywords : Fluid dynamics, reduced order model, uncertainty quantification, stochastic closure, proper orthogonal decomposition

22 **1. Introduction.** The industrial application of partial differential equations (PDE)-
23 driven processes – fluid dynamics, for instance – can be a daunting task, mainly due to
24 the computational complexity involved with its resolution. This computational burden
25 becomes even excruciatingly difficult to handle when it comes to achieving real-time sim-
26 ulations. To tackle this difficulty, reduced order models (ROM) are commonly employed
27 to speed up deterministic and stochastic design simulations [9, 22, 56], or optimal control
28 problems [19, 36, 45]. The interested community has proposed a plethora of different algo-
29 rithms to reduce the computational cost of stochastic PDEs for uncertainty quantification
30 (UQ) applications [20, 21, 44, 54, 55, 69, 77]. In particular, when some parameters of
31 deterministic or stochastic PDEs are random, the weighted reduced basis (wRB) method
32 [20, 21] helps choosing the best parameters’ value for each new full-order simulation. With
33 the addition of stabilizing terms, [77] applied this method to linear advection-dominated
34 problems, including advection by a random velocity field.

35 In turbulent fluid dynamics, the system’s energy usually spreads out over many degrees
36 of freedom. This prevents low-dimensional approximations of the state vector from being
37 sufficiently accurate, but such a rough approximations can theoretically be sufficient for
38 specific industrial applications, especially when the quantity of interest (QoI) is a spatial
39 average (e.g. lift and drag). However, that multiscale property prevents, in general, the
40 constitution of accurate reduced systems for the dynamics of those low-dimensional state
41 approximations. Indeed, severe modal truncations often usually end up destabilizing the
42 system and overdamping some of the stable coefficients of the reduced order solution [69].

Consequently, to stabilize the ROM, authors commonly introduce an additional deterministic term (typically an eddy viscosity term) [2, 15, 79], along with a possible calibration on available data [12, 23, 80]. This calibration procedure can be extended to the complete set of the ROM's parameters [1, 10, 61, 72]. ROM performances have mainly been evaluated on low Reynolds-number flows (say $Re \leq 100$) [e.g. 10, 75, 80], while for flows at much greater Reynolds numbers, evaluations close to the learning time interval and reduced dynamics for two-dimensional flow observables (e.g. particle image velocimetry) have usually been the norm [e.g. 1, 12, 23, 75]. Long time ROM predictions have been otherwise performed with a substantial number of modes [e.g. 14, 74]. Yet, turbulent flow ROMs remain inexact and uncontrolled in the long run, owing to their intrinsic chaotic nature and the growth of accumulated error along time. Outside the learning time interval, predictions becomes less and less accurate. Moreover, these predictions necessitate accurate initial conditions, forcing and geometric information, which are often poorly known.

Ensemble-based data assimilation – such as particle filters or ensemble Kalman filters – can alleviate these issues by forecasting an ensemble of likely future states of the system, while sequentially constraining them with on-coming measurements [27, 28]. Still, this necessitates accurate quantification of their associated simulation's uncertainties. In this context, the aim is not to reduce the dimensionality of UQ, but rather to quantify the uncertainty introduced by the dimensionality reduction.

Note, UQ is a recurrent issue in applied fluid dynamics, and many strategies have been proposed for incorporating randomness in the physical models through some of their parameters [e.g. 44, 47]. However, the error introduced by these noisy parameters is not *a priori* tied to dimensionality reduction and to the contribution of unresolved components. In particular, in fluid dynamics, random initial conditions have first been widely used for both UQ and predictability studies [e.g. 51]. It was later demonstrated this yields under-dispersive quantification, i.e. it has a tendency to underestimate the error associated to the dimensionality reduction [8, 31, 35, 53].

Alternatively, authors have considered the introduction of additive noises, most likely beginning with the introduction of EDQNM [46, 57]. Without special care, such a strategy often leads to energy conservation loss, stability issues and radical changes of the underlying attractor [17].

The Modified Quasilinear Gaussian (MQG) method [69, 70, 71] approximates the third-order moment to help redistribute the right amount of energy between the coefficients of the reduced solution. Finally, several techniques related to averaging and homogenization theory exploit a time-scale separation hypothesis [34, 43, 53, 58], one of the most notable being the MTV model [49]. This latter approach can reproduce intermittency and extreme events alike, thanks to its correlated additive and multiplicative noises. However, besides potential energy conservation issues, the noise covariance is often not explicit enough, and has to be simplified and estimated using the available data. Interested readers can refer to [64], and references herein, for more detailed reviews on model error specification in coarse-scale computational fluid dynamics (CFD). For ROM UQ, [73] propose distributions and efficient sampling methods for the projection matrices in Galerkin-projection-based dimensionality reduction methods. Although apparently more pertinent than methods based on randomized parameters, the relation of this technique to errors associated to mode truncation and turbulent chaotic behaviour remains unclear.

In this paper, we propose to quantify the uncertainty introduced by modal dimensionality reduction through the so-called dynamics under location uncertainty (LU) [50, 65]. Specifically, we adapt the aforementioned stochastic closure to the Galerkin-projection-based ROM. Inspired from the theoretical works of [11, 52], the LU closure relies on the

92 stochastic transport of the flow variables, together with a decorrelation assumption of
 93 the unresolved fluctuations with respect to the resolved slow/large scales. More precisely,
 94 the residual velocity – i.e. the difference between the usual Navier-Stokes solution \mathbf{v} and
 95 some large-scale velocity component \mathbf{w} – is assumed to be time-uncorrelated at the char-
 96 acteristic time of the large-scale processes. This residual velocity is informally denoted
 97 $\mathbf{v}' = \boldsymbol{\sigma}\dot{\mathbf{B}} = \boldsymbol{\sigma}d\mathbf{B}_t/dt$ where $t \mapsto \boldsymbol{\sigma}\mathbf{B}_t$ is a \mathbf{Q} -Wiener process [26, 62], and hence, Gaus-
 98 sian in nature. Note that this apparent simplified Gaussian assumption leads to, as we
 99 will see, a non-Gaussian multiplicative noise in the dynamics. Spatial correlations of the
 100 residual velocity are then specified through the Hilbert-Schmidt integral operator $\boldsymbol{\sigma}$ with
 101 a C^2 kernel $\check{\boldsymbol{\sigma}}: \bar{\Omega}^2 \rightarrow \mathbb{R}^{d \times d}$:

$$102 \quad (1.1) \quad \boldsymbol{\sigma}(\mathbf{x})d\mathbf{B}_t \triangleq \int_{\Omega} \check{\boldsymbol{\sigma}}(\mathbf{x}, \mathbf{z})d\mathbf{B}_t(\mathbf{z})d\mathbf{z} \quad \forall (\mathbf{x}, t) \in \Omega \times [0, T].$$

103 This operator – or equivalently the spatial covariance of the residual velocity – can be
 104 modeled or learned from data. The review [64] describes some of the many choices that
 105 have been explored in this vein. This includes for instance parametric models based on
 106 fluid velocity self-similarity or brute-force non-parametric covariance estimation from high-
 107 resolution datasets. Here, \mathbf{B}_t is an \mathbb{I}_d -cylindrical Wiener process and $d\mathbf{B}_t/dt$ plays the role
 108 of spatio-temporal white noise. The above definition enables us to characterize the way
 109 physical quantities are transported by the stochastic flow:

$$110 \quad (1.2) \quad d\mathbf{X}_t = \mathbf{w}(\mathbf{X}_t, t)dt + \boldsymbol{\sigma}(\mathbf{X}_t)d\mathbf{B}_t \quad \forall t \in [0, T],$$

111 This resembles the expression for transport in classical fluid dynamics. Material deriva-
 112 tives and other differential operations of fluid dynamics are then derived through the use
 113 of stochastic PDEs (SPDE), in particular, by applying the Itô-Wentzell formula [42] and a
 114 stochastic version of the Reynolds transport theorem [40, 50, 65]. As such, LU models can
 115 be applied to model error quantification [17, 64, 66, 68], to improve large-scale simulations
 116 [6, 7, 40, 66, 68], to reduced order modeling and data analysis [67] or to data assimilation
 117 purposes [16, 81] in geophysical fluid dynamics and CFD. To note, in the geometric me-
 118 chanics community [38, 24], the Stochastic Advection by Lie Transport (SALT) method
 119 has been derived for large-scale modeling and data assimilation [25]. Both frameworks
 120 have been compared, numerically [7, 64] and conceptually, [6, 68], with LU and SALT
 121 exhibiting different conservation properties, namely energy preservation and circulation
 122 conservation, respectively. Applied to a barotropic Quasi-Geostrophic model, LU leads to
 123 improved accuracy when compared to a classical large-scale deterministic framework or to
 124 the circulation conservation stochastic setup [6, 7]. The LU setting also fully captures the
 125 structural deformation of the large-scale flow component by the spatial inhomogeneity of
 126 the small-scales [6]. It is important to note that these properties are independent of the
 127 choice of stochastic integral.

128 In this paper, our focus is to analyse the LU setting to help define efficient, highly
 129 reduced order models for real time data assimilation or control applications. For the
 130 sake of simplicity, we will deal with Proper Orthogonal Decomposition (POD) [48] as
 131 dimensionality reduction technique – where time and space dependency are separated –
 132 but the proposed methodology applies to all types of modal decompositions.

133 In section 2, we introduce the stochastic fluid dynamics closure we will employ through-
 134 out the paper, as well as its algebraic structure, followed by the Galerkin projection of this
 135 SPDE to derive our stochastic ROM, with a brief recall of the principle behind POD-ROMs
 136 in section 3. Several estimations needed to complete our stochastic POD-ROM are detailed
 137 in section 4, as well as the efficient and consistent estimators we exploit to rely both on

138 data and on the closure's physical grounding. In section 5, we discuss the conservative
 139 properties of LU dynamics and of its reduced versions, and finally, section 6 is dedicated
 140 to the numerical evaluation of the UQ capabilities of our ROM.

141 **2. Navier-Stokes model under location uncertainty.** Galerkin projections of Navier-
 142 Stokes equations do not specifically take into account residual velocity contributions, and
 143 thus, nor do they offer a precise quantification of their induced errors. To help remedy this
 144 issue, we propose to directly project SPDEs – i.e. the LU Navier-Stokes representation –
 145 instead of the classical Navier-Stokes equations. The resulting ROM is expected to describe
 146 the same physical system, as we postulate that the solution of the SPDE to be statistically
 147 similar to a large-scale representation of the original (deterministic) equation's solution.

148 **2.1. The random physical model.** Let us denote by Ω an open bounded subset of \mathbb{R}^d ,
 149 $T \in \mathbb{R}_+^*$ and $L^2(\Omega)$ (resp. $\mathbf{L}^2 \triangleq (L^2(\Omega))^d$) the space of square-integrable scalar (resp.
 150 vector) fields on Ω . In the case of incompressible fluids, the LU Navier-Stokes equations
 151 on $\Omega \times [0, T]$ read:

$$152 \quad (2.1) \quad \underbrace{\mathbb{D}_t \mathbf{w}}_{\text{Stochastic transport}} = \underbrace{-\nabla(p \, dt + \mathbf{p}_\sigma d\mathbf{B}_t)}_{\text{Pressure forcing}} + \underbrace{\frac{1}{Re} \Delta(\mathbf{w} dt + \boldsymbol{\sigma} d\mathbf{B}_t)}_{\text{Molecular viscous dissipation}},$$

$$153 \quad (2.2) \quad 0 = \underbrace{\nabla \cdot (\mathbf{w}^* dt + \boldsymbol{\sigma} d\mathbf{B}_t)}_{\text{Mass conservation}},$$

154 where $p + \mathbf{p}_\sigma \frac{d\mathbf{B}_t}{dt}$ informally represents the pressure also decomposed into a large-scale and
 155 a small-scale time-uncorrelated component, Re stands for the Reynolds number, and for
 156 every smooth-enough function $\mathbf{q} : \Omega \times [0, T] \rightarrow \mathbb{R}^d$, we denote:

$$157 \quad (2.3) \quad (\mathbb{D}_t \mathbf{q})_k \triangleq \underbrace{d_t q_k}_{\substack{\triangleq q_k(\mathbf{x}, t+dt) - q_k(\mathbf{x}, t) \\ \text{Time increment}}} + \underbrace{(\mathbf{w}^* dt + \boldsymbol{\sigma} d\mathbf{B}_t) \cdot \nabla q_k}_{\text{Advection}} - \underbrace{\nabla \cdot (\frac{1}{2} \mathbf{a} \nabla q_k)}_{\text{Turbulent diffusion}} dt,$$

$$158 \quad (2.4) \quad \mathbf{w}^* \triangleq \mathbf{w} - \frac{1}{2} (\nabla \cdot \mathbf{a})^T,$$

$$159 \quad (2.5) \quad \mathbf{a} \triangleq \mathbb{E} \{ (\boldsymbol{\sigma} d\mathbf{B}_t) (\boldsymbol{\sigma} d\mathbf{B}_t)^T \} / dt = \boldsymbol{\sigma} \otimes \boldsymbol{\sigma},$$

160 where operator \otimes is defined later on in this section.

161 Throughout this paper, we consider various linear integral operators defined on some
 162 subspace $\mathbf{D} \subset \mathbf{L}^2$. Denoted $\boldsymbol{\eta}$, each of those operators can be defined through a matrix
 163 kernel $\check{\boldsymbol{\eta}}$ of $(L^2(\Omega^2))^{d \times d}$ as follows:

$$164 \quad (2.6) \quad (\boldsymbol{\eta} \boldsymbol{\xi})(\mathbf{x}) \triangleq \int_{\Omega} \underbrace{\check{\boldsymbol{\eta}}(\mathbf{x}, \mathbf{z})}_{\substack{\text{kernel} \\ \text{of } \boldsymbol{\eta}}} \boldsymbol{\xi}(\mathbf{z}) d\mathbf{z} \quad \forall \boldsymbol{\xi} \in \mathbf{D} \subset \mathbf{L}^2, \forall \mathbf{x} \in \Omega.$$

165 Two first examples of such operator are $\boldsymbol{\sigma}$ encoding the small-scale velocity component
 166 spatial correlations (defined in (1.1)) and \mathbf{p}_σ encoding the small-scale pressure component
 167 spatial correlations. For two such linear integral operators $\boldsymbol{\eta}$ and $\boldsymbol{\theta}$, we note:

$$168 \quad (2.7) \quad (\boldsymbol{\eta} \otimes \boldsymbol{\theta})(\mathbf{x}) \triangleq \int_{\Omega} \check{\boldsymbol{\eta}}(\mathbf{x}, \mathbf{z}) \check{\boldsymbol{\theta}}^T(\mathbf{x}, \mathbf{z}) d\mathbf{z} \quad \forall \mathbf{x} \in \Omega.$$

169 Theoretical foundations to analyze SPDEs are outside the scope of this paper. Inter-
 170 ested readers may refer to [30, 52] for deeper insights. Here, we focus on the stochastic

Physical meaning	Notation	Full-order term	Property	ROM term
Molecular viscous dissipation	\mathbf{L}	$\frac{1}{Re}\Delta$	symmetric, < 0	\mathbf{l}
Turbulent diffusion	\mathbf{F}_{dif}	$\nabla \cdot (\frac{1}{2}\mathbf{a}\nabla\bullet)$	symmetric, < 0	$\check{\mathbf{f}}_{\text{dif}}$
Advecting velocity correction	\mathbf{F}_{adv}	$\frac{1}{2}(\nabla \cdot \mathbf{a})\nabla$	skew-symmetric (if $\nabla \cdot (\nabla \cdot \mathbf{a})^T = 0$)	$\check{\mathbf{f}}_{\text{adv}}$
Usual advection	$\mathbf{C}(\mathbf{w}, \bullet)$	$-(\mathbf{w} \cdot \nabla)$	skew-symmetric (if $\nabla \cdot \mathbf{w} = 0$)	\mathbf{c}
Advection by the residual velocity	$\mathbf{Gd}\mathbf{B}_t$	$-(\boldsymbol{\sigma}\text{d}\mathbf{B}_t \cdot \nabla)$	skew-symmetric noise (if $\nabla \cdot \boldsymbol{\sigma} = 0$)	$\boldsymbol{\alpha}\text{d}\mathbf{B}_t$
Molecular viscous dissipation of the residual velocity	$\mathbf{Hd}\mathbf{B}_t$	$\frac{1}{Re}\Delta\boldsymbol{\sigma}\text{d}\mathbf{B}_t$	additive noise	$\boldsymbol{\theta}\text{d}\mathbf{B}_t$
Pressure gradient	$\text{d}\mathbf{P}$	$-\nabla(p\text{d}t + \mathbf{p}_\sigma\text{d}\mathbf{B}_t)$	Potential field	Included in other terms

Table 1: Terms of LU Navier-Stokes equations and their algebraic properties

171 closure mechanism and its reduced order expression. The stochastic transport operator
 172 \mathbb{D}_t involves the usual terms of the deterministic material derivative, on top of three addi-
 173 tional new terms: an advecting velocity correction (\mathbf{w}^* instead of \mathbf{w}), a heterogeneous and
 174 anisotropic turbulent diffusion, and a multiplicative noise. This last term corresponds to
 175 the advection by the unresolved velocity $\boldsymbol{\sigma}\dot{\mathbf{B}}$. Finally, we can recover the classical Navier-
 176 Stokes equations by setting the residual velocity to zero – i.e. $\boldsymbol{\sigma} = 0$. Let us highlight
 177 that for conserved scalars, this operator corresponds to the material derivative – i.e. the
 178 derivative along the stochastic flow $\text{d}(\mathbf{w}(\mathbf{X}_t, t))$ [65]. This stochastic Navier-Stokes model
 179 is generic, and depending on the application, forces and boundary conditions, it may be
 180 modified accordingly to adjust to any incompressible flow configurations. For compressible
 181 stochastic flows, some new terms appear. Interested readers may refer to [65].

182 In addition to the classical physical assumptions pertaining to the establishment of the
 183 Navier-Stokes equations for incompressible fluids, the main assumption of the LU setting is
 184 to consider the unresolved fluctuation velocity component uncorrelated in time. To note,
 185 the incompressible character of the random fluctuations can be relaxed at the price of
 186 additional terms in the transport operator [65]

187 **2.2. Algebraic structure of the model.** The algebraic properties of the different terms
 188 can be quickly described. We can formally rewrite the velocity evolution law (2.1) for
 189 $t \in [0, T]$ as follows:

$$190 \quad (2.8) \quad \text{d}_t\mathbf{w} = (\text{dM})(\mathbf{w}) \triangleq ((\mathbf{L} + \mathbf{F})(\mathbf{w}) + \mathbf{C}(\mathbf{w}, \mathbf{w}))\text{d}t + (\mathbf{Gd}\mathbf{B}_t)(\mathbf{w}) + (\mathbf{Hd}\mathbf{B}_t) + \text{d}\mathbf{P},$$

191 where table 1 details each term. Operator \mathbf{L} represents the molecular viscosity term,
 192 $\mathbf{F} = \mathbf{F}_{\text{dif}} + \mathbf{F}_{\text{adv}}$, the turbulent diffusion plus the advecting velocity correction, and $\mathbf{Gd}\mathbf{B}_t$,
 193 the advection by the random residual velocity. All of them are linear differential operators,
 194 while \mathbf{C} , the term representing the usual non-linear advection effect, is a bilinear differential
 195 operator. The additive noise $\mathbf{Hd}\mathbf{B}_t$ corresponds to the molecular viscous dissipation of
 196 the time-uncorrelated velocity component, $\boldsymbol{\sigma}\dot{\mathbf{B}}$, while the last term on the right-hand side,

197 dP , is the pressure forcing.

198 Additionally, under suitable boundary conditions, the algebraic structures of the dif-
 199 ferent operators can be further specified. For instance, \mathbf{L} and \mathbf{F}_{dif} are symmetric negative
 200 operators. For the other terms, additional incompressibility conditions are needed. The
 201 mass conservation equation (2.2) implies $\nabla \cdot \boldsymbol{\sigma} = 0^1$, which is actually the case in practice,
 202 either because of the parametric model used for $\boldsymbol{\sigma}$ or because of the incompressibility of
 203 the velocity data used to estimate $\boldsymbol{\sigma}$. Accordingly, $\mathbf{G}d\mathbf{B}_t$ is a skew-symmetric operator.
 204 As a matter of fact, if $(\boldsymbol{\zeta}, \boldsymbol{\xi}) \triangleq \int_{\Omega} \boldsymbol{\zeta} \cdot \boldsymbol{\xi}$ denotes the scalar product of \mathbf{L}^2 , for every $\boldsymbol{\zeta}$ and
 205 $\boldsymbol{\xi}$ in the Sobolev space $H_0^1(\Omega) = \{\mathbf{f} \in \mathbf{L}^2 : \int_{\Omega} \|\nabla \mathbf{f}^T\|^2 < \infty; \mathbf{f}|_{\partial\Omega} = 0\}$ (with partial
 206 derivative taken in the weak sense and $\|\bullet\|$ stands for the Euclidean norm on $\mathbb{R}^{d \times d}$), an
 207 integration by parts gives:

$$208 \quad (2.9) \quad (\boldsymbol{\zeta}, (\mathbf{G}d\mathbf{B}_t)(\boldsymbol{\xi})) = - \sum_{k=1}^d \int_{\Omega} \zeta_k (\boldsymbol{\sigma} d\mathbf{B}_t \cdot \nabla) \xi_k = - \sum_{k=1}^d \int_{\Omega} \zeta_k \nabla \cdot (\boldsymbol{\sigma} d\mathbf{B}_t \xi_k),$$

$$209 \quad (2.10) \quad = \sum_{k=1}^d \int_{\Omega} (\boldsymbol{\sigma} d\mathbf{B}_t \cdot \nabla \zeta_k) \xi_k = -((\mathbf{G}d\mathbf{B}_t)(\boldsymbol{\zeta}), \boldsymbol{\xi}).$$

210 The mass conservation equation also implies $\nabla \cdot \mathbf{w}^* = 0$ which may or may not be the
 211 case in practice. If $\nabla \cdot \mathbf{w} = 0$, operator \mathbf{C} is skew-symmetric with respect to the second
 212 argument – i.e. $\mathbf{g} \mapsto \mathbf{C}(\mathbf{f}, \mathbf{g})$ is skew-symmetric – whereas \mathbf{F}_{adv} is skew-symmetric if the
 213 drift correction $\mathbf{w}^* - \mathbf{w} = -\frac{1}{2}(\nabla \cdot \mathbf{a})^T$ is divergence-free.

214 Moreover, the turbulent diffusion \mathbf{F}_{dif} is related to the random skew-symmetric operator
 215 $\mathbf{G}d\mathbf{B}_t$. Indeed, for every process $\boldsymbol{\xi}$ in $H^2(\Omega) = \{\mathbf{f} \in \mathbf{L}^2 : \frac{\partial \mathbf{f}}{\partial x_i}, \frac{\partial \partial \mathbf{f}}{\partial x_i \partial x_j} \in \mathbf{L}^2, 1 \leq i, j \leq d\}$,

$$216 \quad (2.11) (\mathbf{F}_{\text{dif}}(\boldsymbol{\xi}))_k \triangleq \nabla \cdot (\frac{1}{2} \mathbf{a} \nabla \xi_k) = \nabla \cdot (\frac{1}{2} (\boldsymbol{\sigma} \otimes \boldsymbol{\sigma}) \nabla \xi_k) = \frac{1}{2} (\boldsymbol{\sigma}^T \nabla)^T (\otimes (\boldsymbol{\sigma}^T \nabla)^T \xi_k),$$

$$217 \quad (2.12) \quad = \frac{1}{2} \mathbf{G} (\otimes \mathbf{G}(\xi_k)) = (\frac{1}{2} \mathbf{G} (\otimes \mathbf{G}(\boldsymbol{\xi})))_k = (-\frac{1}{2} \mathbf{G}^* (\otimes \mathbf{G}(\boldsymbol{\xi})))_k,$$

218 where \mathbf{G}^* denotes the adjoint of \mathbf{G} . It also shows that $\mathbf{F}_{\text{dif}}(\mathbf{w})dt = \frac{1}{2}d \langle \mathbf{G}(\mathbf{w}), \mathbf{B}_t \rangle$, where
 219 $\langle \mathbf{g}, \mathbf{h} \rangle$ denotes the quadratic covariation of any functions \mathbf{g} and \mathbf{h} . The diffusion term
 220 explicitly appears when working with the Itô stochastic integral and is only implicitly
 221 taken into account with Stratonovich integral [6, 68].

222 As discussed in more detail in section 5, these algebraic properties make the LU Navier-
 223 Stokes model – and to a certain extent, its reduced order versions – conservative (up to
 224 molecular viscosity and boundary conditions effects).

225 **3. Galerkin projection.** To sample good priors for future Bayesian estimation algo-
 226 rithms, we aim at deriving a computationally efficient fluid dynamics ROM able to quantify
 227 its own errors with respect to the true fluid dynamics (i.e. the Navier-Stokes equations).
 228 As previously mentioned, standard Galerkin techniques – even with the best determinis-
 229 tic closures – are hardly capable of such a goal as they were not originally designed for
 230 it. Hence, we propose to perform Galerkin projections on the LU Navier-Stokes model
 231 instead, and to study its appropriateness for this sort of tasks.

232 **3.1. A ROM with correlated additive and multiplicative noise.** Let \mathbf{v} be the real
 233 velocity field (i.e. the Navier-Stokes equations' solution) and $\boldsymbol{\phi}_0$, a background velocity
 234 field, typically the velocity temporal mean $\bar{\mathbf{v}} \triangleq \frac{1}{T} \int_0^T \mathbf{v}$. To reduce the state space dimen-
 235 sion, we project the fluid velocity anomaly, $\mathbf{v} - \boldsymbol{\phi}_0$, in a subspace spanned by a number of

¹i.e. $\nabla_{\mathbf{x}} \cdot \check{\boldsymbol{\sigma}}(\mathbf{x}, \mathbf{z}) = 0, \forall (\mathbf{x}, \mathbf{z}) \in \Omega^2$

236 orthonormal spatial modes $(\phi_i)_{1 \leq i \leq n}$.

$$237 \quad (3.1) \quad \mathbf{v}(\mathbf{x}, t, \omega) = \underbrace{\sum_{i=0}^n b_i(t, \omega) \phi_i(\mathbf{x})}_{\triangleq \mathbf{w}^R} + \underbrace{\text{Residual}}_{\triangleq \mathbf{v}'} \quad \forall (\mathbf{x}, t) \in \Omega \times [0, T],$$

238 where $b_0 = 1$ and $\phi_0 = \bar{\mathbf{v}}$ by convention. The associated temporal coefficients, b_i , are
 239 possibly random and depend on a realization ω of a sample space $\check{\Omega}$ whereas the reduced
 240 basis functions ϕ_i , are assumed to be deterministic and stationary.

241 As typically done while working with ROMs, we aim at specifying the evolution of the
 242 projected velocity field \mathbf{w}^R . A standard technique for that is the Galerkin projection of
 243 the physical PDE – here, the Navier-Stokes equations – onto the reduced basis' functions
 244 ϕ_i , where the resolved component \mathbf{w}^R is approximated by the solution of these projected
 245 equations. Mode truncation can create many problems. For moderately turbulent to
 246 turbulent flows and small dimension n , a closure model to handle the truncated modes
 247 is unavoidable. With the LU setting – described in section 2 – an elegant stochastic
 248 alternative for this problem can be derived. Accordingly, we will (i) assume that the
 249 residual velocity \mathbf{v}' is time-uncorrelated and is denoted $\sigma d\mathbf{B}_t/dt$ and (ii) approximate the
 250 resolved component \mathbf{w}^R to a realization of the solution of the Galerkin projection of the
 251 stochastic Navier-Stokes representation (2.1)-(2.2). The former hypothesis is a debatable
 252 choice with respect to some ROM's applications whose pertinence and limitations will be
 253 discussed further in section 4.5.

254 To obtain this stochastic ROM, the SPDE (2.8) is first projected onto the divergence-
 255 free function space through the non-local Leray operator $\mathcal{P} = \mathbb{I}_d - \nabla \nabla^T \Delta^{-1}$. This projec-
 256 tion, which requires the resolution of a Poisson equation is used to simplify the system by
 257 removing the pressure term. Since divergence-free solution is considered (see section 3.2),
 258 the resolved velocity component w^R is naturally incompressible and we get

$$259 \quad (3.2) \quad \mathcal{P} d_t \mathbf{w}^R = d_t \mathbf{w}^R, \quad \mathcal{P} \mathbf{L}(\mathbf{w}^R) = \mathbf{L}(\mathbf{w}^R), \quad \mathcal{P} d\mathbf{P} = 0.$$

260 Moreover, $\mathcal{P}(\mathbf{H}d\mathbf{B}_t) = (\mathbf{H}d\mathbf{B}_t)$ because of the necessary incompressibility of the Brow-
 261 nian term in the continuity equation (2.2)². Then, the resulting SPDE is projected onto
 262 each of the reduced basis' functions:

$$263 \quad (3.3) \quad db_i = (\phi_i, d_t \mathbf{w}^R) = (d\mathbf{M}_i^R)(\mathbf{b}) \triangleq (\phi_i, \mathcal{P}(d\mathbf{M})(\mathbf{w}^R)), \quad 1 \leq i \leq n,$$

264 where $\mathbf{b} = (b_i)_{0 \leq i \leq n}$ and

$$265 \quad (d\mathbf{M}_i^R)(\mathbf{b}) = \sum_{p=0}^n \underbrace{(\phi_i, \mathbf{L}(\phi_p))}_{\triangleq l_{pi}} b_p dt + \sum_{p=0}^n \underbrace{(\phi_i, \mathcal{P}\mathbf{F}(\phi_p))}_{\triangleq \check{f}_{pi}} b_p dt + \sum_{p,q=0}^n \underbrace{(\phi_i, \mathcal{P}\mathbf{C}(\phi_p, \phi_q))}_{\triangleq c_{pqi}} b_p b_q dt$$

$$266 \quad (3.4) \quad + \underbrace{(\phi_i, (\mathbf{H}d\mathbf{B}_t))}_{\triangleq (\theta_{i\bullet} d\mathbf{B}_t)} + \sum_{p=0}^n \underbrace{(\phi_i, \mathcal{P}(\mathbf{G}d\mathbf{B}_t)(\phi_p))}_{\triangleq (\alpha_{pi\bullet} d\mathbf{B}_t)} b_p, \quad 1 \leq i \leq n.$$

267 The terms $(\alpha_{pi\bullet} d\mathbf{B}_t)_{1 \leq p, i \leq n}$ and $((\theta_{i\bullet} + \alpha_{0i\bullet}) d\mathbf{B}_t)_{1 \leq i \leq n}$ correspond to a Gaussian skew-
 268 symmetric matrix and a Gaussian vector respectively, both with correlated coefficients.
 269 If the functions ϕ_i were spatial Fourier modes associated with small wave-numbers, the
 270 ROM (3.3) would represent a (stochastic) Large-Eddy-Simulation-like model expressed in
 271 Fourier space and \mathbf{b} would be the set of Fourier coefficients of the solution. Hereafter, we
 272 will solely focus on the POD.

²which is coherent with the fact that $\nabla \cdot \mathbf{v}' = 0$ from (3.1) because $\nabla \cdot \mathbf{v} = 0$.

273 **3.2. Proper Orthogonal Decomposition.** In the POD framework, the reduced basis'
 274 functions are computed through a set of velocity snapshots $(\mathbf{v}_{\text{obs}}(\bullet, t_i))_{0 \leq i \leq N-1}$. More
 275 precisely, they are a solution to the constrained optimization problem:

$$276 \quad (3.5) \quad \underset{(\phi_i)_{1 \leq i \leq n}}{\text{Maximize}} \sum_{i=1}^n \overline{(\phi_i, \mathbf{v}_{\text{obs}} - \bar{\mathbf{v}})^2} \quad \text{subject to} \quad (\phi_i, \phi_j) = \delta_{ij}, \quad 1 \leq i, j \leq n.$$

277 Reduced basis functions ϕ_i are thus the n orthonormal functions which can best explain
 278 the snapshots' temporal variability. Similarly to a principal component analysis (PCA),
 279 the solutions of this optimization problem are the eigenfunctions of the velocity anomalies'
 280 $(\mathbf{v}_{\text{obs}} - \bar{\mathbf{v}})$ spatial covariance. Numerically, this matrix is extremely large, and we generally
 281 opt to solve the dual problem instead: we seek the eigenvalue decomposition of the velocity
 282 anomalies' temporal covariance:

$$283 \quad (3.6) \quad C_{ij}^v = ((\mathbf{v}_{\text{obs}} - \bar{\mathbf{v}})(\bullet, t_i), (\mathbf{v}_{\text{obs}} - \bar{\mathbf{v}})(\bullet, t_j)), \quad 0 \leq i, j \leq N-1.$$

284 This method is often referred to as the snapshot method. In the POD framework, the
 285 mode $\phi_0 = \bar{\mathbf{v}}$ is set to the time averaged velocity, and the temporal coefficients energies
 286 $\overline{b_i^2}$ are denoted λ_i . Furthermore, if the snapshots describe a divergence-free velocity field
 287 \mathbf{v}_{obs} , the spatial bases ϕ_i are divergence-free as well.

288 **4. Estimations of subgrid terms.** To close our stochastic ROM (3.3)-(3.4), we need
 289 to estimate the variance tensor \mathbf{a} (involved in the ROM matrix $\check{\mathbf{f}} = \check{\mathbf{f}}_{\text{dif}} + \check{\mathbf{f}}_{\text{adv}}$ defined in
 290 table 1 and in equation (3.4) under the braces) as well as the ROM noise variances and
 291 correlations. Firstly, if we recall that $b_0 = 1$, we note that:

$$292 \quad (4.1) \quad (\alpha_{\bullet i} \bullet d\mathbf{B}_t)^T \mathbf{b} + (\theta_{i \bullet} \bullet d\mathbf{B}_t) = \sum_{k=1}^n (\alpha_{ki \bullet} \bullet d\mathbf{B}_t) b_k + ((\theta_{i \bullet} + \alpha_{0i \bullet}) \bullet d\mathbf{B}_t), \quad 1 \leq i \leq n.$$

293 The multiplicative and additive noises of the ROM correspond to the first and second term
 294 of the right-hand side, respectively. To simplify notations, we write:

$$295 \quad (4.2) \quad \tilde{\alpha}_{pi \bullet} = \alpha_{pi \bullet} + \delta_{p0} \theta_{i \bullet}, \quad 1 \leq i \leq n, \quad 0 \leq p \leq n.$$

296 To fully specify the ROM, the following correlations must be estimated:

$$297 \quad (4.3) \quad \begin{cases} \mathbf{a}(\mathbf{x}) &= \mathbb{E} \{ (\boldsymbol{\sigma}(\mathbf{x}) d\mathbf{B}_t) (\boldsymbol{\sigma}(\mathbf{x}) d\mathbf{B}_t)^T \} / dt \quad \forall \mathbf{x} \in \Omega, \\ \Sigma_{pi, qj}^\alpha &= \mathbb{E} \{ (\tilde{\alpha}_{pi \bullet} \bullet d\mathbf{B}_t) (\tilde{\alpha}_{qj \bullet} \bullet d\mathbf{B}_t) \} / dt, \quad 1 \leq i, j \leq n, \quad 0 \leq p, q \leq n. \end{cases}$$

298 **4.1. The curse of dimensionality.** Computing correlations of Gaussian noises $(\tilde{\alpha} d\mathbf{B}_t)$
 299 involves the two-point quadratic cross-variation tensor of the small-scale velocity:

$$300 \quad (4.4) \quad \mathbf{Q}(\mathbf{x}, \mathbf{y}) = \mathbb{E} \{ (\boldsymbol{\sigma}(\mathbf{x}) d\mathbf{B}_t) (\boldsymbol{\sigma}(\mathbf{y}) d\mathbf{B}_t)^T \} / dt \quad \forall \mathbf{x}, \mathbf{y} \in \Omega.$$

301 The coefficients (i, j) of the covariance matrix of the Gaussian vector $(\boldsymbol{\theta} d\mathbf{B}_t)$ can be ex-
 302 pressed as follows:

$$303 \quad (4.5) \quad \mathbb{E} \{ (\theta_{i \bullet} \bullet d\mathbf{B}_t) (\theta_{j \bullet} \bullet d\mathbf{B}_t) \} = \mathbb{E} \{ (\phi_i, \nu \nabla^2 \boldsymbol{\sigma} d\mathbf{B}_t) (\nu \nabla^2 \boldsymbol{\sigma} d\mathbf{B}_t, \phi_j) \},$$

$$304 \quad (4.6) \quad = \iint_{\Omega^2} \phi_i(\mathbf{x})^T \nu^2 \nabla_x^2 \nabla_y^2 \mathbf{Q}(\mathbf{x}, \mathbf{y}) dt \phi_j(\mathbf{y}) d\mathbf{x} d\mathbf{y}.$$

305 Since, by definition, $\forall \mathbf{x} \in \Omega$, $\mathbf{a}(\mathbf{x}) = \mathbf{Q}(\mathbf{x}, \mathbf{x})$, the whole stochastic ROM is closed by
 306 specifying the tensor \mathbf{Q} . In practice, this tensor is often heterogeneous – i.e. $\boldsymbol{\sigma} \mathbf{B}_t$ is

307 non-stationary in space. Thus, its spatially-discrete version is expected to be so large
 308 that its estimation or even its storage becomes prohibitive. To overcome this difficulty,
 309 a first strategy is to assume a model structure for the covariance as per [41, 66, 64, 68].
 310 If the small-scale velocity is observed, other techniques can be considered. Indeed, one
 311 can build a POD representation of the small-scale velocity $\sigma \dot{\mathbf{B}}$, learned from available
 312 snapshots or realizations as in [7, 24, 64, 68]. Depending on the desired accuracy for the
 313 noise representation, a great number of modes would have to be estimated and the number
 314 of coefficients involved in the ROM can quickly grow out of control. Here, we rely on
 315 a method specifically devised for this kind of ROM frameworks: the noise structure is
 316 again learned from observed residual velocity snapshots, but without passing through the
 317 covariance \mathbf{Q} . It enables us to directly estimate the correlations of the random ROM's
 318 coefficients, as it will be explained later on.

319 **4.2. Variance tensor estimation.** Considering the variance tensor \mathbf{a} stationary leads
 320 to a simple estimator through time averaging as in [67]:

$$321 \quad (4.7) \quad \hat{\mathbf{a}} = \Delta t \overline{\mathbf{v}'_{\text{obs}} (\mathbf{v}'_{\text{obs}})^T},$$

322 where

$$323 \quad (4.8) \quad \mathbf{v}'_{\text{obs}} = \mathbf{v}_{\text{obs}} - \mathbf{w}_{\text{obs}}^R = \mathbf{v}_{\text{obs}} - \sum_{i=0}^n b_i^{\text{obs}} \phi_i,$$

324 is the observed POD's residual velocity. Since $\mathbf{a} dt = d \langle \sigma \mathbf{B}, (\sigma \mathbf{B})^T \rangle$, the estimator (4.7)
 325 is consistent thanks to the quadratic covariation definition.

326 **4.3. Noise correlation estimation.** Besides the variance tensor, there are $n^2(n+1)^2$
 327 correlations to estimate according to (4.3). For any function ξ in $H^2(\Omega)$, let us introduce
 328 the linear functional:

$$329 \quad (4.9) \quad K_{jq}[\xi] \triangleq (\phi_j, -\mathcal{P}[(\xi \cdot \nabla) \phi_q] + \delta_{q0} \nu \Delta \xi), \quad 1 \leq j \leq n, \quad 0 \leq q \leq n.$$

330 Using this notation, the noise's covariance can be estimated as follows:

$$331 \quad (4.10) \quad \widehat{\Sigma_{pi,qj}^{\alpha}} = \frac{\Delta t}{\lambda_p^{\text{obs}}} K_{jq} \left[\overline{b_p^{\text{obs}} \left(\frac{\Delta b_i^{\text{obs}}}{\Delta t} \right)'' \mathbf{v}'_{\text{obs}}} \right], \quad 1 \leq i, j \leq n, \quad 0 \leq p, q \leq n,$$

332 where $b_0^{\text{obs}} = \lambda_0^{\text{obs}} = 1$ and for $1 \leq i \leq n$,

$$333 \quad (4.11) \quad b_i^{\text{obs}} = (\phi_i, \mathbf{v}_{\text{obs}}),$$

$$334 \quad (4.12) \quad \lambda_i^{\text{obs}} = \overline{(b_i^{\text{obs}})^2},$$

$$335 \quad (4.13) \quad \left(\frac{\Delta b_i^{\text{obs}}}{\Delta t} \right)'' = \left(\frac{\Delta b_i^{\text{obs}}}{\Delta t} \right)' - \overline{\left(\frac{\Delta b_i^{\text{obs}}}{\Delta t} \right)'},$$

$$336 \quad (4.14) \quad \left(\frac{\Delta b_i^{\text{obs}}}{\Delta t} \right)' = \left(\frac{\Delta b_i^{\text{obs}}}{\Delta t} \right) - \left((\mathbf{b}^{\text{obs}})^T (\mathbf{l} + \check{\mathbf{f}})_{\bullet i} + (\mathbf{b}^{\text{obs}})^T \mathbf{c}_{\bullet \bullet i} \mathbf{b}^{\text{obs}} \right),$$

$$337 \quad (4.15) \quad \left(\frac{\Delta b_i^{\text{obs}}}{\Delta t} \right) (t_k) = \frac{b_i^{\text{obs}}(t_k + \Delta t) - b_i^{\text{obs}}(t_k)}{\Delta t}, \quad 0 \leq k \leq N - 1.$$

338 To ensure the noise's covariance matrix to have the desired symmetric non-negative struc-
 339 ture, we only keep the symmetric part of the estimated tensor (4.10) and set its possible
 340 negative eigenvalues to zero. The part inside the functional K_{jq} in the estimator (4.10)
 341 is inspired from [32], where products of martingale time increments are projected onto

342 orthogonal functions of $L^2([0, T])$. For ROMs with a small number of dimensions n , the
 343 estimator's computational cost is remarkably low as the observed coefficients of the reduced
 344 solution \mathbf{b}^{obs} were already computed by the method of snapshots (see section 3.2). Hence,
 345 the computational cost for $b_p^{\text{obs}} \left(\frac{\Delta b_i^{\text{obs}}}{\Delta t} \right)''$ is negligible and the part inside K_{jq} only involves
 346 a projection of the residual velocity along the time dimension. Finally, the $n(n+1)$ differ-
 347 ential operators K_{jq} are computed only on $n(n+1)$ functions that do not depend on the
 348 time variable.

349 We prove the consistency of this estimator in Appendix A by capitalising on the
 350 quadratic covariation's definition and the orthogonality of the observed temporal coeffi-
 351 cients b_i^{obs} . In addition, this can also be extended to non-orthogonal coefficients by solving
 352 the linear system engendered by the matrix $(\overline{b_p b_k})_{pk}$.

353 **4.4. Noise dimension reduction.** Using the Cholesky decomposition $\boldsymbol{\sigma}^\alpha$ of the noise
 354 covariance tensor:

$$355 \quad (4.16) \quad \Sigma_{pi,qj}^\alpha = \sum_{lk} \sigma_{pi,lk}^\alpha \sigma_{qj,lk}^\alpha, \quad 1 \leq i, j \leq n, \quad 0 \leq p, q \leq n,$$

356 and $O(n^2)$ independent white noises, one can sample realizations of the ROM Gaussian
 357 noise terms $\tilde{\boldsymbol{\alpha}} d\mathbf{B}_t$. However, $\boldsymbol{\sigma}^\alpha$ has $O(n^4)$ coefficients, while the ROM works with only
 358 n modes and involves – leaving the noise terms aside – $O(n^3)$ coefficients. Therefore, we
 359 propose to reduce the noise dimension through a tensorial PCA of $\boldsymbol{\Sigma}^\alpha$, eventually only
 360 keeping the n first eigenvectors. This leads to the following sampling strategy:

$$361 \quad (4.17) \quad \tilde{\boldsymbol{\alpha}} d\mathbf{B}_t \approx \sum_{k=1}^n \tilde{\boldsymbol{\alpha}}_k^R d\beta_t^{(k)},$$

362 where $(\tilde{\boldsymbol{\alpha}}_k^R)_k \in \mathbb{R}^{(n+1) \times n}$ are the matrix forms of the first n eigenvectors (weighted by the
 363 corresponding eigenvalues' square roots) and $(\beta^{(k)})_k$ are n independent one-dimensional
 364 Brownian motions. Since $\tilde{\boldsymbol{\alpha}} d\mathbf{B}_t$ is a multiplicative noise and the temporal coefficients b_i
 365 have various amplitudes $\sqrt{\lambda_i}$, the covariance matrix $\boldsymbol{\Sigma}^\alpha$ is adequately re-normalized by the
 366 amplitudes $\sqrt{\lambda_i}$ before applying the PCA.

367 It is important to note that the methodology described here is different from a more
 368 usual methodology based on PCA decomposition of the residual velocity \mathbf{v}' keeping n
 369 modes and assuming that the corresponding temporal coefficients $(b_i)_{n+1 \leq i \leq 2n}$ are time-
 370 decorrelated. The complexity of the final ROM is the same in both methodologies but our
 371 ROM maximizes the noise's variance instead of the residual velocity's variance. Thus, our
 372 proposed method is better suited in terms of ROM UQ.

373 **4.5. Time down-sampling rate.** Under the LU Navier-Stokes model hypothesis, the
 374 unresolved term of the velocity field corresponds to a noise uncorrelated in time. This
 375 assumption is consistent with the fact that the higher-order coefficients of the reduced order
 376 solution often tend to have shorter correlation time in fluid dynamics systems. However,
 377 in practice, this assumption is not found to be true, and it is a recurrent issue for the data-
 378 driven modeling of systems combining fast and slowly evolving components [4, 5, 59, 60].
 379 Consequently, a time down-sampling scheme is proposed to force the noise terms to be as
 380 decorrelated as possible.

381 By assuming that the spatially averaged covariance function has a Gaussian form with
 382 a standard deviation equals to the correlation time τ , a simple expression allows us to

383 compute it. For a given unresolved velocity correlation matrix we write:

$$384 \quad (4.18) \quad C_{ij}^{v'} = (\mathbf{v}'_{\text{obs}}(\bullet, t_i), \mathbf{v}'_{\text{obs}}(\bullet, t_j)) = C_{ij}^v - \sum_{k=1}^n b_k^{\text{obs}}(t_i) b_k^{\text{obs}}(t_j), \quad 0 \leq i, j \leq N-1,$$

385 and its associated stationary covariance function

$$386 \quad (4.19) \quad \text{Cov}_s(t_p) = \frac{1}{N-p} \sum_{q=0}^{N-1-p} C_{q,q+p}^{v'}, \quad 0 \leq p \leq N-1.$$

387 We propose the following correlation time estimation:

$$388 \quad (4.20) \quad \hat{\tau} = \sqrt{2 \frac{\overline{\text{Cov}_s^2}}{(\frac{\Delta \text{Cov}_s}{\Delta t})^2}},$$

389 using a forward Euler temporal discretization of the stationary covariance:

$$390 \quad (4.21) \quad \frac{\Delta \text{Cov}_s}{\Delta t}(t_p) \triangleq \frac{\text{Cov}_s(t_p + \Delta t) - \text{Cov}_s(t_p)}{\Delta t}, \quad 0 \leq p \leq N-1.$$

391 These estimations follow over-simplified assumptions known to have a restricted validity.
 392 Experimentally, they still systematically provide the best simulation results when compared
 393 to other more complex estimators (whose derivation is outside the scope of this paper).
 394 Moreover, with a white unresolved velocity with a dirac stationary covariance function,
 395 we obtain $\hat{\tau} = dt$. This result is exactly what we would expect from a white unresolved
 396 velocity, to prevent an overly aggressive down-sampling.

397 Before computing the estimations presented in sections 4.2, 4.3 and 4.4, we use this
 398 estimated correlation time $\hat{\tau}$ to down-sample both the entire dataset and the observed
 399 coefficients of the reduced order solution, leaving us with a time step $\Delta t \approx \hat{\tau}$. On top of
 400 the considerable gain in accuracy, this time down-sampling reduces the amount of data to
 401 process, and hence, makes the off-line ROM building process faster.

402

403 Having estimated and specified all of the stochastic ROM's parameters in equations
 404 (3.3) and (3.4), it is now possible to forecast ensembles of realizations of the ROM through
 405 Monte-Carlo simulations. Before presenting numerical results, we discuss some important
 406 properties of LU models and of their reduced order versions.

407 **5. Kinetic energy budget.** First, the conservative properties of the LU Navier-Stokes
 408 representation are recalled, followed by a proof that by combining Galerkin projections and
 409 the advecting velocity correction compressibility, an intrinsic energy dissipation appears.

410 **5.1. Full-order model budget.** As derived in [65, 68], since the pressure does not
 411 influence the energy budget, by neglecting the molecular viscosity, the divergence of \mathbf{w} and
 412 boundary conditions effects, and by applying Itô's lemma, the expression for the kinetic
 413 energy budget writes:

$$414 \quad (5.1) \quad \frac{d}{dt} \left(\frac{1}{2} \|\mathbf{w}\|_{L^2}^2 \right) = \underbrace{\left(-\frac{1}{2} \mathbf{G}^* (\otimes \mathbf{G}(\mathbf{w})), \mathbf{w} \right)}_{\text{Loss by diffusion}} + \underbrace{\frac{1}{2} \|\mathbf{G}(\mathbf{w})\|_{\text{HS}}^2}_{\text{Energy flux from the noise}} = 0 \quad \forall t \in [0, T],$$

415 where $\|\boldsymbol{\xi}\|_{L^2}^2 = (\boldsymbol{\xi}, \boldsymbol{\xi})$ is the squared norm of L^2 and

$$416 \quad (5.2) \quad \|\boldsymbol{\eta}\|_{\text{HS}}^2 = \iint_{\Omega^2} \sum_{i,j=1}^d \tilde{\eta}_{i,j}^2(\mathbf{x}, \mathbf{z}) d\mathbf{x} d\mathbf{z}$$

417 is the squared Hilbert-Schmidt norm of the integral operator $\boldsymbol{\eta}$. This enables us to state
 418 that the energy is conserved for each realization of the stochastic process, and as a direct
 419 consequence of this, the energy intake of the noise and the dissipation by the turbulent
 420 diffusion must exactly compensate each other. The latter dissipates the kinetic energy of
 421 the mean $\|\mathbb{E}\{\boldsymbol{w}\}\|_{\mathbf{L}^2}^2$, while the former only releases random energy $\|\boldsymbol{w} - \mathbb{E}\{\boldsymbol{w}\}\|_{\mathbf{L}^2}^2$
 422 into the system. Thus, the time-uncorrelated component of the velocity field drains energy from
 423 the mean field to the random component of \boldsymbol{w} .

424 We can also express this energy transfer with the expectation of equation (5.1):

$$425 \quad (5.3) \quad \frac{d}{dt} \int_{\Omega} \text{Var}(\boldsymbol{w}) = \frac{d}{dt} \mathbb{E} \|\boldsymbol{w} - \mathbb{E}\{\boldsymbol{w}\}\|_{\mathbf{L}^2}^2 = -\frac{d}{dt} \|\mathbb{E}\{\boldsymbol{w}\}\|_{\mathbf{L}^2}^2 \quad \forall t \in [0, T].$$

426 Besides the physical relevance of energy conservation, variance inflation and its relation
 427 to the mean field are also of primary interest for data assimilation or ensemble forecasting
 428 issues.

429 **5.2. Reduced-order model budget.** Following (5.1), the full-order LU Navier-Stokes
 430 model (2.1)-(2.2) conserves the kinetic energy, up to molecular viscosity and boundary
 431 condition effects. With reduced order models, the advecting velocity correction is expected
 432 however to create either energy compression or dilation, and the mode truncation, to
 433 introduce a small energy leak. The ROM (3.3) does not exactly solve the global LU Navier-
 434 Stokes model (2.1)-(2.2) but the Galerkin projection of the divergence-free component of
 435 equation (2.1) :

$$436 \quad (5.4) \quad d_t \boldsymbol{w}^R = \sum_{i=0}^n db_i \boldsymbol{\phi}_i = \sum_{i=1}^n (d\mathbb{M}_i^R)(\boldsymbol{b}) \boldsymbol{\phi}_i = \Pi_{\phi} [\mathcal{P}(d\mathbb{M})(\boldsymbol{w}^R)] \quad \forall t \in [0, T],$$

437 where Π_{ϕ} is the projection onto the reduced subspace. Specifically, for any function $\boldsymbol{\zeta} \in \mathbf{L}^2$,
 438 the projection Π_{ϕ} is defined as $\Pi_{\phi}[\boldsymbol{\zeta}] \triangleq \sum_{p=1}^n (\boldsymbol{\phi}_p, \boldsymbol{\zeta}) \boldsymbol{\phi}_p$. As previously stated, we can
 439 evaluate the variation of kinetic energy with the Itô formula. The following result is proved
 440 in Appendix B for every $t \in [0, T]$:

$$441 \quad (5.5) \quad \frac{d}{dt} \left(\frac{1}{2} \|\boldsymbol{w}^R\|_{\mathbf{L}^2}^2 \right) = \underbrace{-\frac{1}{2} \|\mathbf{G}(\boldsymbol{w}^R)\|_{\text{HS}}^2}_{\text{Loss by diffusion}} + \underbrace{\frac{1}{2} \|\Pi_{\phi} [(\mathbf{G})(\boldsymbol{w}^R)]\|_{\text{HS}}^2}_{\text{Energy flux from the noise}} - \underbrace{\frac{1}{2} (\nabla \cdot (\nabla \cdot \boldsymbol{a})^T, \|\boldsymbol{w}^R\|^2)}_{\text{Advecting velocity correction compressibility}},$$

$$442 \quad (5.6) \quad = -\frac{1}{2} (\nabla \cdot (\nabla \cdot \boldsymbol{a})^T, \|\boldsymbol{w}^R\|^2) - \underbrace{\frac{1}{2} \|\Pi_{\phi}^{\perp} [(\mathbf{G})(\boldsymbol{w}^R)]\|_{\text{HS}}^2}_{<0},$$

443 where $\|\bullet\|$ stands for the Euclidean norm on \mathbb{R}^d and $\Pi_{\phi}^{\perp} = \mathbb{I}_d - \Pi_{\phi}$ is the projector onto
 444 the orthogonal complement of the space spanned by the reduced basis' functions.

445 The first term of (5.6) corresponds to the fluid compression/dilation created by the
 446 velocity correction $\boldsymbol{w}^* - \boldsymbol{w} = -\frac{1}{2} (\nabla \cdot \boldsymbol{a})^T$. By construction, the ROM meets the incom-
 447 compressible condition – i.e. $\nabla \cdot \boldsymbol{w} = 0$ – but unlike the LU Navier-Stokes model, it does not
 448 satisfy the finite-variation part of the mass conservation (2.2): $\nabla \cdot \boldsymbol{w}^* = 0$. The velocity
 449 correction divergence is associated to turbulence heterogeneity [6, 16, 67], corresponding
 450 to the spatial maxima (positive energy fluxes) and minima (negative energy fluxes) of the
 451 turbulence's kinetic energy $\|\boldsymbol{v}'\|^2$.

452 The second term of (5.6) informs about the energy flux due to mode truncation. The
 453 ROM's subgrid diffusion extracts energy from some temporal coefficients of the reduced
 454 order solution, while the multiplicative noise distributes it to others. These stabilizing and

455 destabilizing effects recreate a large part of the energy fluxes between coefficients of the
 456 reduced solution, otherwise lost in deterministic ROMs. Thus, the uncorrelated velocity
 457 component drains energy from the coefficients of the reduced solution to give it back to
 458 the temporal coefficients of the truncated modes – i.e. modes orthogonal to the reduced
 459 space. This energy flux is exactly characterized by the second term of (5.6). But, our
 460 stochastic ROM cannot transfer energy from the truncated modes to the reduced solution’s
 461 coefficients, as the former cannot be specified due to the truncation.

462 Such a dissipation could be perfectly prevented by considering $-\frac{1}{2}(\Pi_\phi[\mathbf{G}])^*(\otimes\Pi_\phi[\mathbf{G}])$
 463 represented in the ROM by $\left(-\frac{1}{2}\sum_{i=1}^n\Sigma_{pi,qi}^\alpha\right)_{p,q}$ (see equations (B.11) and (B.12) in Ap-
 464 pendix B), instead of the reduced version of the full turbulent diffusion operator
 465 $\left(-\frac{1}{2}(\phi_p, \mathbf{G}^*(\otimes\mathbf{G}(\phi_q)))\right)_{p,q}$. This correction would have been implicit using the Galerkin
 466 projection with Stratonovich calculus. As demonstrated in [6, 64, 68], using Stratonovich
 467 integral, the turbulent dissipation term does not explicitly appear, neither when deriving
 468 the ROM from scratch nor when switching notations after the Galerkin projection. Let us
 469 stress that the modified advection is still present in the Stratonovich form of the LU model.
 470 Changing the ROM notations from Itô to Stratonovich [42], the following correction term
 471 appears:

$$472 \quad (5.7) \quad \frac{1}{2}d\langle \mathbf{b}^T \boldsymbol{\alpha}_{\bullet p \bullet}, \mathbf{B} \rangle = \sum_{q=0}^n \left(\frac{1}{2} \sum_{i=1}^n \Sigma_{ip,qi}^\alpha \right) b_q dt = \sum_{q=0}^n \left(-\frac{1}{2} \sum_{i=1}^n \Sigma_{pi,qi}^\alpha \right) b_q dt.$$

473 In Stratonovich form, the ROM also still implicitly includes the diffusion term ensuing from
 474 the truncature. Notwithstanding, this additional dissipation in (5.6) is not a problem as
 475 it enables the setting of an energy dissipation mechanism representative of a direct energy
 476 cascade in the truncated modes’ coefficients. Hence, for very turbulent flows described by
 477 few modes, the energy leak appears to be necessary as our main concern is to restore energy
 478 fluxes between the coefficients of the reduced order system. Indeed, those energy fluxes
 479 can be very difficult to model correctly in reduced versions of non-linear systems. As an
 480 example, [69] observe that a basis encoding 50% of the energy can lead to a ROM missing
 481 more than 98% of energy transfers. These missing energy fluxes create instabilities in some
 482 coefficients of the reduced solution (missing negative energy fluxes) while overdamping
 483 others (missing positive energy fluxes). Restoring the energy fluxes between coefficients of
 484 the reduced system is a significant challenge LU models tackle through the combination of
 485 multiplicative noise and turbulent diffusion.

486 To note, the noise dimensionality reduction of section 4.4 introduces an additional
 487 energy leak due to the fact that we are only keeping n eigenvectors over $n(n+1)$ in the
 488 noise covariance matrix’s PCA. This introduces another negative energy flux, as the noise
 489 variance is reduced while the dissipation is maintained.

490 **6. Ensemble forecasting.** As a means to measure the performance of the proposed
 491 ROM in UQ scenarios, ensemble simulations were carried out using the data available
 492 from DNS simulations of wake flows at Reynolds 100 and 300, the former being quasi
 493 two dimensional while the latter, fully three dimensional. Wake flows are well-studied,
 494 non-linear, oscillatory flows which are physically produced by a uniform-velocity inflow
 495 facing a solid obstacle – here, a cylinder. Vortices are thus created behind the obstacle and
 496 periodically detach from it.

497 The dynamics, and in particular their intrinsic dimensionality, strongly differ between
 498 Reynolds 100 and 300. Indeed, as illustrated by figure 1, at Reynolds 100, most of the
 499 energy is concentrated in just a few coefficients of the reduced order solution. In contrast,
 500 at Reynolds 300, the two first modes are meaningful for a rough approximation, but energy

501 spreads over many degrees of freedom. The top panels of figures 3 and 7 confirm a strong
502 difference in complexity between the two flows.

503 The ROM's results \mathbf{w}^R will be compared directly to DNS simulations \mathbf{v}_{ref} on a time
504 interval outside intervals on which the ROM's coefficients and basis functions have been
505 estimated.

506 **6.1. Baseline ROMs.** To better appreciate our stochastic ROM's capabilities, results
507 are compared to two different state-of-the-art algorithms.

508 **6.1.1. Deterministic baseline ROM.** The first state-of-art ROM is a prototype of
509 deterministic ROM widely used in fluid dynamics. After a POD-Galerkin on the classical
510 Navier-Stokes equations, the molecular viscosity coefficient $1/Re$ is replaced by an eddy
511 viscosity coefficient $1/Re^{\text{ev}} \geq 1/Re$ [15]:

$$512 \quad (6.1) \quad \frac{d}{dt} b_i = \frac{Re}{Re^{\text{ev}}} \mathbf{b}^T \mathbf{l}_{\bullet i} + \mathbf{b}^T \mathbf{c}_{\bullet \bullet i} \mathbf{b}, \quad 1 \leq i \leq n.$$

513 The eddy viscosity coefficient is typically fitted by least squares using the dataset b^{obs} .
514 Without that correction, some coefficients of the reduced solution might become unstable
515 because of the missing negative energy fluxes due to mode truncation mentioned in 5.2.
516 The eddy viscosity term generally manages to stabilize those coefficients, but this does not
517 always make this data-driven method accurate. In order to emulate that unstable behavior,
518 we also simulate a simple DNS POD-Galerkin with no eddy viscosity model, i.e. the ROM
519 (6.1) with $Re^{\text{ev}} = Re$.

520 **6.1.2. Stochastic baseline ROM.** As a deterministic model, the ROM above can
521 hardly be used for dynamics-error UQ nor ensemble-based data assimilation. As a matter
522 of fact, a simple randomization of the initial conditions are known to usually lead to error
523 underestimation (see section 1). So, to keep things simple, we define a second baseline
524 ROM by adding a white noise term to the first baseline ROM. This constitutes a simple
525 *ad hoc* randomization technique for a given dynamical system through a Gaussian additive
526 forcing. Despite its potential lack of physical relevance, such a strategy is very often
527 adopted in data-assimilation applications [17].

$$528 \quad (6.2) \quad db_i = \left(\frac{Re}{Re^{\text{ev}}} \mathbf{b}^T \mathbf{l}_{\bullet i} + \mathbf{b}^T \mathbf{c}_{\bullet \bullet i} \mathbf{b} \right) dt + \sigma_{i \bullet}^{\text{ev}} d\mathbf{W}_t, \quad 1 \leq i \leq n,$$

529 where $\sigma^{\text{ev}} \in \mathbb{R}^{n \times n}$ is the Cholesky decomposition of the ROM's noise covariance $\Sigma^{\text{ev}} =$
530 $\sigma^{\text{ev}} (\sigma^{\text{ev}})^T$ and $t \mapsto \mathbf{W}_t \in \mathbb{R}^n$ is a vector of n independent Brownian motions. Since no
531 prior physical information is available for these baseline models, the noise's covariance is
532 also learned from data as follows:

$$533 \quad (6.3) \quad \widehat{\Sigma}_{ij}^{\text{ev}} = \Delta t \overline{\left(\frac{\Delta b_i^{\text{obs}}}{\Delta t} \right)''_{\text{ev}} \left(\frac{\Delta b_j^{\text{obs}}}{\Delta t} \right)''_{\text{ev}}}, \quad 1 \leq i, j \leq n,$$

534 where for $1 \leq i \leq n$,

$$535 \quad (6.4) \quad \left(\frac{\Delta b_i^{\text{obs}}}{\Delta t} \right)''_{\text{ev}} = \left(\frac{\Delta b_i^{\text{obs}}}{\Delta t} \right)'_{\text{ev}} - \overline{\left(\frac{\Delta b_i^{\text{obs}}}{\Delta t} \right)'_{\text{ev}}},$$

$$536 \quad (6.5) \quad \left(\frac{\Delta b_i^{\text{obs}}}{\Delta t} \right)'_{\text{ev}} = \left(\frac{\Delta b_i^{\text{obs}}}{\Delta t} \right) - \left(\frac{Re}{Re^{\text{ev}}} (\mathbf{b}^{\text{obs}})^T \mathbf{l}_{\bullet i} + (\mathbf{b}^{\text{obs}})^T \mathbf{c}_{\bullet \bullet i} \mathbf{b}^{\text{obs}} \right).$$

537 As for the LU ROM, the implicit assumption of white noise residual $\left(\frac{\Delta b_i^{\text{obs}}}{\Delta t} \right)''_{\text{ev}}$ may not be
538 valid. Thus, similarly to section 4.5, an optimal down-sampling time step is estimated with
539 $\sum_{k=1}^n \left(\frac{\Delta b_k^{\text{obs}}}{\Delta t} \right)''_{\text{ev}}(t_i) \left(\frac{\Delta b_k^{\text{obs}}}{\Delta t} \right)''_{\text{ev}}(t_j)$ instead of $C_{ij}^{v'}$, before the noise covariance estimation.

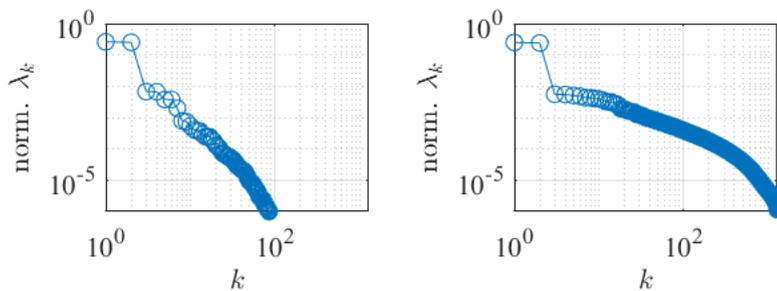


Figure 1: Energies of the reduced solution coefficients normalized by the total solution energy temporal mean $\|\mathbf{v}\|_{L^2}^2$ for the 2D flow at Reynolds 100 (left panel) and the 3D flow at Reynolds 300 (right panel).

540 **6.2. 2D wake flow at Reynolds 100.** Starting with the simpler of the two test cases,
 541 800 seconds of DNS simulation data (about 160 pseudo-periods) were generated for a 2D
 542 wake flow behind a circular cylinder at $Re = 100$. These data were then split into training
 543 and test sets, the former (140 pseudo-periods) being utilized for the construction of the
 544 ROMs, and the latter (20 pseudo-periods), as a reference to which the ROMs will be
 545 compared. Performance will thus be measured through four different metrics: comparison
 546 of temporal coefficients in the time domain, comparison of reconstructed velocity fields in
 547 the spatial domain, global prediction accuracy as measured by the evolution in time of
 548 RMSE, and finally ensemble minimum error.

549 **6.2.1. Temporal coefficients forecast.** The 2-dimensional LU ROM of the Reynolds-
 550 100 flow is simulated 100 times. In figure 2, the coefficients of the reduced solution $b_i^{(k)}$
 551 (where k stands for the k -th simulation) are compared to the coefficients of the reference
 552 solution $b_i^{\text{ref}} = (\phi_i, \mathbf{v}_{\text{ref}})$ (plotted in black). The ensemble mean (in green) follows almost
 553 perfectly the reference's phase, and exhibits a slightly damped magnitude. The damping
 554 effect can be seen as a consequence of the exchange of energy between the mean and the
 555 variance (see equation (5.3)). This interplay is also evidenced by the growth of the confi-
 556 dence interval. The realization we have (randomly) singled-out shows a slowly divergent
 557 behavior.

558 **6.2.2. Velocity forecasts.** Having analyzed the model's forecast capabilities in terms
 559 of the ROM's temporal coefficient, we now focus on the analysis of the velocity fields'
 560 forecast and compare them to the reference – i.e. the projection of full DNS solution onto
 561 the POD basis : $\tilde{\Pi}_\phi[\mathbf{v}_{\text{ref}}] \triangleq \Pi_\phi[\mathbf{v}_{\text{ref}} - \bar{\mathbf{v}}] + \bar{\mathbf{v}} = \sum_{i=0}^n b_i^{\text{ref}} \phi_i$ (with $b_0^{\text{ref}} = 1$). Here, our
 562 goal will be to assess qualitatively the potential limitations of the ROM. Through equation
 563 (3.1), we will compute the velocity fields for the mean, the lowest error realization, and the
 564 prediction generated by the eddy viscosity ROM (6.1) of same dimension. At each time
 565 step, we define the lowest-error realization as follows:

$$566 \quad (6.6) \quad \mathbf{b}^{\min} = \underset{(\mathbf{b}^{(k)})_k}{\operatorname{argmin}} \left\| \mathbf{w}^R - \tilde{\Pi}_\phi[\mathbf{v}_{\text{ref}}] \right\|_{L^2}^2 = \underset{(\mathbf{b}^{(k)})_k}{\operatorname{argmin}} \|\mathbf{b}^{(k)} - \mathbf{b}^{\text{ref}}\|^2.$$

567 We plot in figure 3 the vorticity fields of the ROMs of dimension $n = 8$. A system of
 568 dimension 8 enables us to reproduce fairly well the topology of the velocity fields, and from
 569 figure 2 we conclude that our model's best realization is capable of staying in phase with the
 570 reference, even 50 seconds into the validation set, while the ensemble realization's mean and
 571 the deterministic baseline start losing accuracy. Indeed, the eddies of the latter predictions

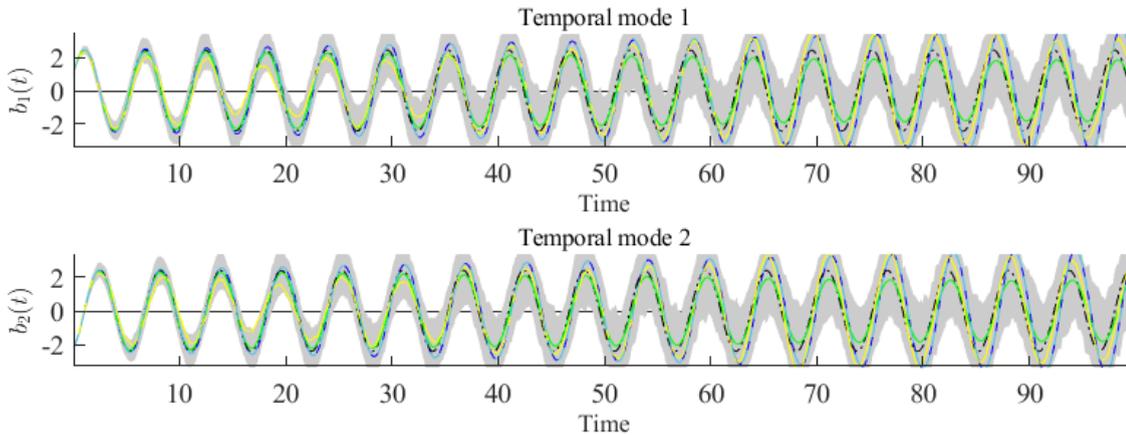


Figure 2: LU POD-ROM forecast for $n = 2$ coefficients of the reduced solution for a 2D wake flow at Reynolds 100: ensemble mean (green line), one random realization (yellow line), confidence interval (gray shade). Blue lines correspond to deterministic ROMs: baseline eddy-viscosity POD-ROM (6.1) (light-blue dashed line) and DNS POD-Galerkin (dark-blue solid line). The dash-dot black plots represent the observed references.

572 are late compared to the reference. This misalignment of eddies is a major type of model
 573 error in CFD, and it is very problematic for data assimilation because misalignment can
 574 hardly be corrected by linear Eulerian algorithms [64]. The LU model's cornerstone is
 575 precisely the random locations of transported quantities, and in particular, the locations
 576 of eddies. This random location idea is encoded in the random flow equation (1.2) and
 577 gave rise to the name "Location Uncertainty" (LU). Here, the LU POD-ROM generates an
 578 ensemble of simulations. Some of them have eddies in advance compared to the mean and
 579 some have late eddies. This variety of eddies' locations allows some ensemble realizations
 580 – in particular the best one – to match the reference's eddies' locations.

581 **6.2.3. Global prediction accuracy.** To compare more precisely the performance of
 582 the proposed ROM, we systematically plot the RMSE, as well as the ensemble's bias,
 583 variance and minimum error. These quantities will also be compared to those obtained by
 584 the stochastic baseline ROM (6.2). This enables us to inspect the UQ capabilities of the
 585 proposed ROM.

586 Although the random energy transfers are a necessary feature when the number of
 587 modes is not large enough, it increases the temporal coefficients' variance while keeping
 588 their biases constant, which yields an increase of the Root Mean Square Error (RMSE) of
 589 the whole ensemble:

$$590 \quad (6.7) \quad \text{RMSE} \triangleq \hat{\mathbb{E}} \left\| \mathbf{w}^R - \tilde{\Pi}_\phi[\mathbf{v}_{\text{ref}}] \right\|_{\mathbf{L}^2}^2 = \left\| \hat{\mathbb{E}}\{\mathbf{w}^R\} - \tilde{\Pi}_\phi[\mathbf{v}_{\text{ref}}] \right\|_{\mathbf{L}^2}^2 + \int_{\Omega} \widehat{\text{Var}}(\mathbf{w}^R).$$

591 In all the following normalized error plots, the blue line corresponds to the solution
 592 computed using a deterministic POD-Galerkin ROMs (with and without eddy viscosity)
 593 and the red one, to the RMSE. The green line represents the ensemble bias, whereas the
 594 magenta line is the error incurred by the ensemble's solution closest to the reference (6.6),
 595 and the gray shade corresponds to $1.96 \times$ the standard-deviation. These quantities are
 596 computed for the whole set of generated realizations. The initial condition is common to
 597 all and the values are normalized by the square root of the solution's energy averaged over
 598 the training set : $\left(\|\bar{\mathbf{v}}\|_{\mathbf{L}^2}^2 + \sum_{i=1}^n \lambda_i \right)^{1/2}$.

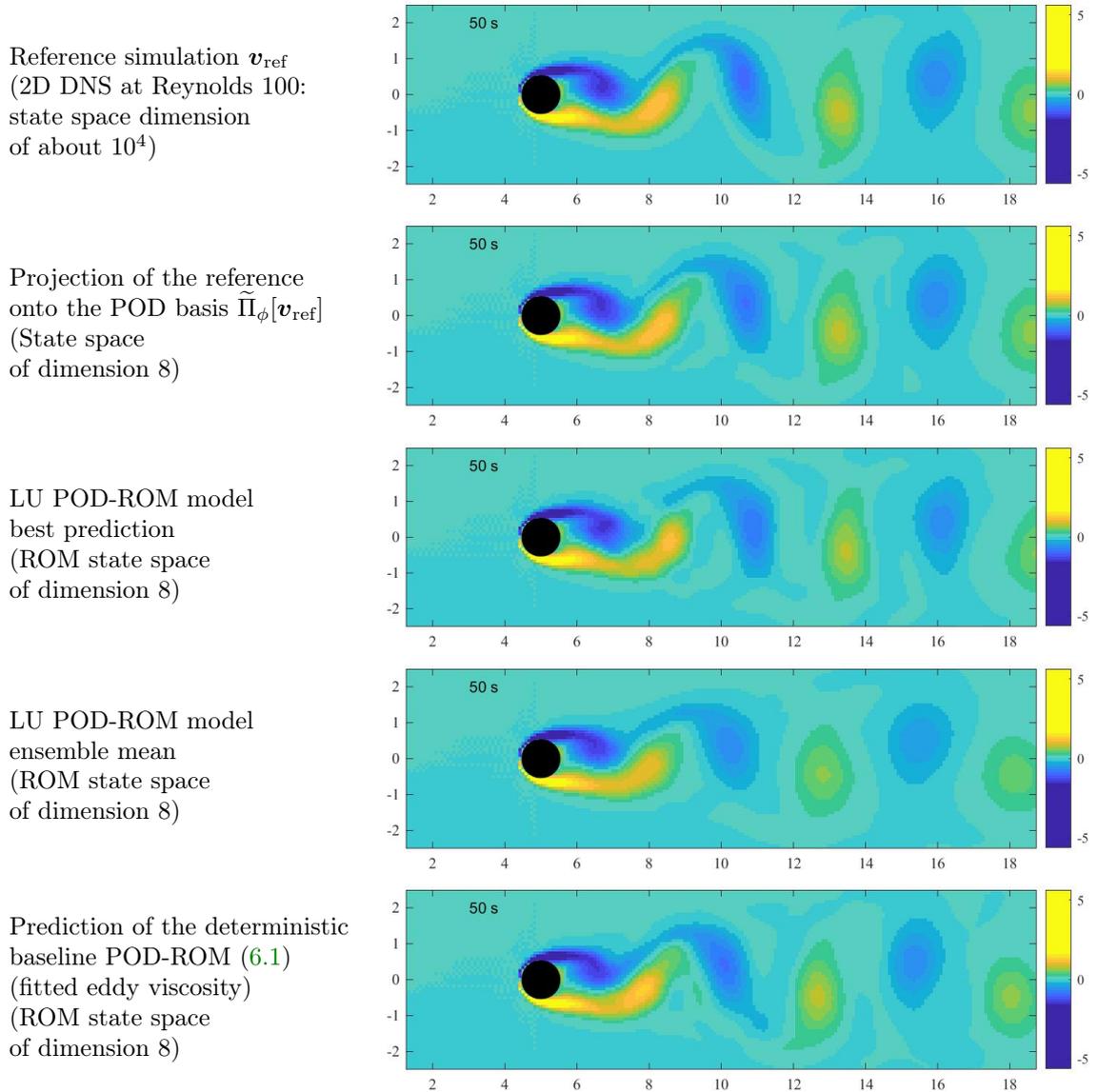


Figure 3: Vorticity fields – 10 vortex shedding cycles after the learning period – from (from top to bottom) the reference simulation \mathbf{v}_{ref} (2D DNS at Reynolds 100: state space dimension of about 10^4), its projection onto the POD basis $\tilde{\Pi}_\phi[\mathbf{v}_{\text{ref}}]$, the LU POD-ROM model’s best prediction, the LU POD-ROM model’s ensemble mean, and the prediction of the deterministic baseline POD-ROM (6.1) (fitted eddy viscosity) (ROM state spaces are of dimension 8). The vorticity is the velocity curl and is the usual and a convenient way of visualizing 2D flows and their vortices.

599 In figure 4, the aforementioned error curves generated by the LU POD-ROM are com-
 600 pared to the stochastic POD with eddy viscosity model (6.2) for $n \in \{2, 4, 8\}$. The LU
 601 POD-ROM’s best realization incurs a rather low error, and for the first two cases, a low
 602 bias too. The same cannot be said for the stochastic eddy viscosity model, which sees its
 603 variance grow out of control at the very beginning of the simulation, making the model’s
 604 predictions diverge almost instantly. This divergence can be explained by the very large
 605 additive noise variance, fitted on the large ROM residuals $\left(\frac{\Delta b_i^{\text{obs}}}{\Delta t}\right)''_{\text{ev}}$ through equation

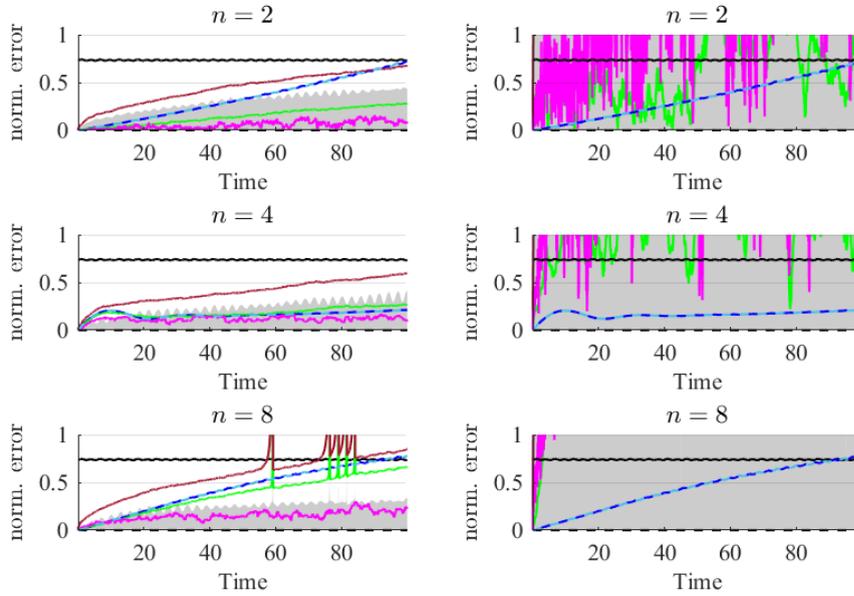


Figure 4: Normalized error for $n = 2, 4$ and 8 coefficients of the reduced solution of a 2D wake flow at Reynolds 100 – with the projection of the DNS onto the POD basis $\tilde{\Pi}_\phi[\mathbf{v}_{\text{ref}}]$ as reference : RMSE (brown line), bias (green line), ensemble minimum error (magenta line) and $1.96 \times$ the standard-deviation (shaded gray) for the LU POD-ROM (left panel) and stochastic baseline POD-ROM (right panel) . Blue lines correspond to deterministic ROMs : baseline eddy-viscosity POD-ROM (6.1) (light-blue dashed line) and DNS POD-Galerkin (dark-blue solid line). The black solid line at the top is the error considering only the time mean velocity, i.e. $b_i = 0, \forall i > 0$.

606 (6.3). This large additive noise hence quickly fills the reduced subspace overwhelming the
 607 physical terms of the reduced dynamics. As for the $n = 8$ simulation, we observe that
 608 the LU POD-ROM differs from the other two simulations by having unstable realizations,
 609 thence the sudden peaks in the bias and mean curves. When a realisation diverges, we
 610 re-sample it uniformly from the other members of the ensemble.

611 Focusing on our stochastic POD-ROM, for any $n \in \{2, 4, 8\}$, even though the ensemble
 612 bias grows as time passes by, the best realization error does not. This is a crucial prop-
 613 erty for a UQ model to have, as this means that an appropriate filtering technique could
 614 eventually retrieve it at each observation, leading to a stable, low error data assimilation
 615 system.

616 **6.3. 3D wake flow at Reynolds 300.** For a more challenging test, a 3D wake flow
 617 behind a circular cylinder at $Re = 300$ was simulated, constructing the ROM just like
 618 in the case of the wake flow at Reynolds 100. The 440 seconds of DNS simulation data
 619 (about 88 vortex shedding pseudo-periods) were split into training (80 vortex shedding
 620 pseudo-periods) and test sets (8 pseudo-periods). Similarly, the ROM was subjected to
 621 the same benchmarks as before, with the equivalent eddy-viscosity UQ-enabled model for
 622 comparison. As it is a more complex flow, we expect the different temporal coefficients to
 623 be harmonically richer and to capture as much of the small-scale interactions as possible,
 624 but yet not to be able to fully reproduce the intricacies of the DNS-simulated flow.

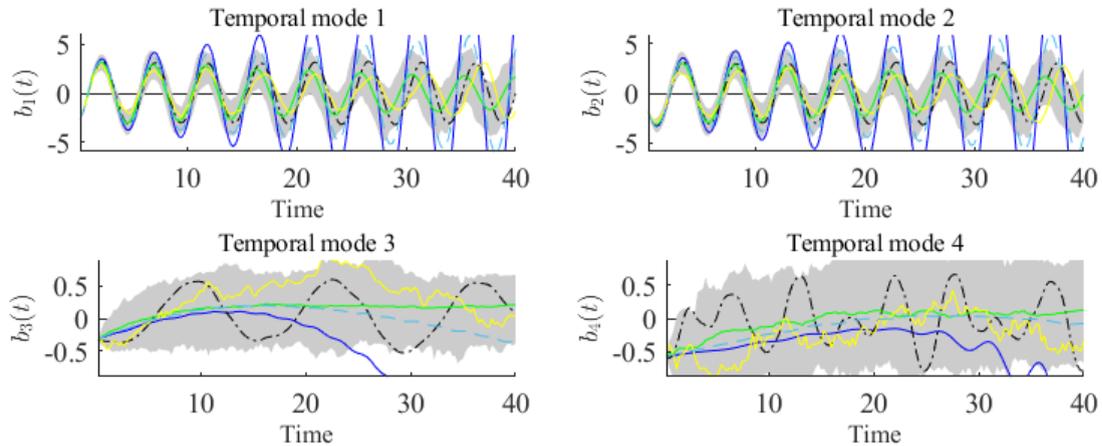


Figure 5: LU POD-ROM forecast for $n = 4$ coefficients of the reduced solution of a 3D wake flow at Reynolds 300: ensemble mean (green line), one random realization (yellow line), confidence interval (gray shade). Blue lines correspond to deterministic ROMs: baseline eddy-viscosity POD-ROM (6.1) (light-blue dashed line) and DNS POD-Galerkin (dark-blue solid line). The dash-dot black plots represent the observed references.

625 **6.3.1. Temporal coefficients forecast.** This new scenario being fully 3D and more
 626 complex, the advantages of the proposed model are clear. This can be seen from the
 627 temporal coefficient forecasts, where the proposed LU stochastic ROM manages to stabilize
 628 the system while the deterministic PODs starts diverging after 5 seconds (i.e. before
 629 one complete vortex shedding), as evidenced by the first temporal coefficients in figure
 630 5. Intermittency probably fools the learning procedure of the eddy viscosity method and
 631 makes it less robust and not adapted to the test set. In contrast, the LU learning procedure
 632 – section 4 – shows a greater degree of robustness and leads to more accurate results. It
 633 is also interesting to note how the random energy contribution increases with the order
 634 of the temporal coefficient in the form of ensemble variance. This is attributed to energy
 635 transfers between temporal coefficients, facilitated by the interplay of multiplicative noise
 636 and turbulent diffusion. This effect is in fact amplified in the 8-dimension ROM in figure 6,
 637 where the temporal coefficients’ means get more damped as the amount of random energy
 638 in the system increases. This energy dissipation mechanism helps the system to remain
 639 bounded, unlike its deterministic counterparts.

640 Interestingly enough, in the $n = 8$ dimension ROM, even when the ensemble variance
 641 increases with the temporal coefficient order, coefficients 5, 6, 7 and 8 of the random
 642 realization (yellow line) also attempt to follow the right reference amplitude and variability,
 643 as it can be observed in figure 6.

644 **6.3.2. Velocity forecasts.** As in the previous case, we now analyze qualitatively the
 645 performance of our proposed method in terms of velocity field predictions.

646 As can be observed from figure 7, the best prediction remains stable and manages
 647 to stay close to the theoretically optimal solution in 8-dimensions on a period of four
 648 shedding cycles after the learning period. Conversely, the baseline model starts to diverge,
 649 as evidenced by the red zones inside the vortices. This result is quite impressive as, even if
 650 the mean velocity field is not as close to the reference as one would like, it still reveals the
 651 potential of a method combining our model with a data assimilation technique to retrieve
 652 the best realization and provide corrections on the fly.

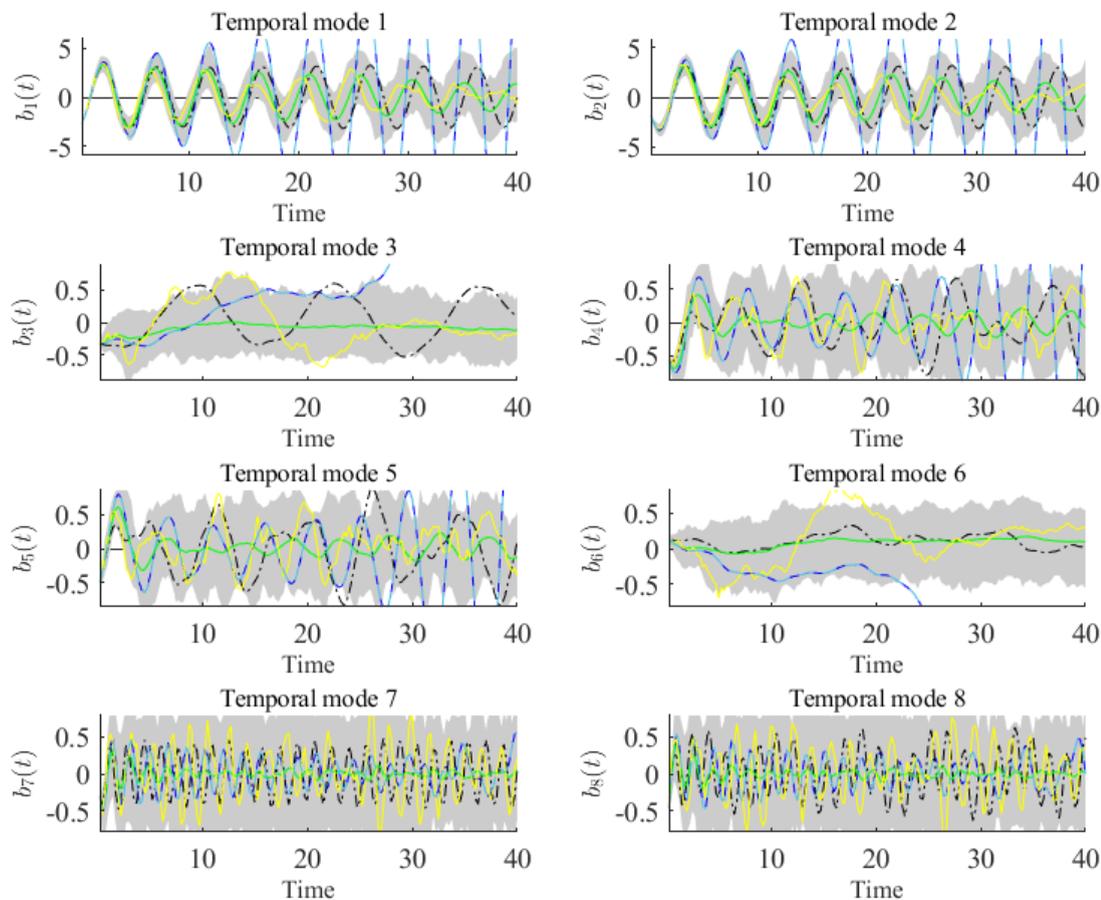


Figure 6: LU POD-ROM forecast for $n = 8$ coefficients of the reduced solution of a 3D wake flow at Reynolds 300: ensemble mean (green line), one random realization (yellow line), confidence interval (gray shade). Blue lines correspond to deterministic ROMs: baseline eddy-viscosity POD-ROM (6.1) (light-blue dashed line) and DNS POD-Galerkin (dark-blue solid line). The dash-dot black plots represent the observed references.

653 **6.3.3. Global prediction accuracy.** Just like in the two-dimensional flow, the error
 654 curves are plotted and compared to the results obtained with the stochastic eddy viscosity
 655 model (6.2). The curves in figure 8 evidence the predictive power of our proposed model: it
 656 is capable of great stability and accuracy even after 40 seconds while the deterministic and
 657 eddy viscosity models prove to be quite unstable by rapidly diverging. These properties are
 658 showcased by the bias and mean curves that converge to the zero-temporal-coefficient error
 659 curve instead of growing in an unbounded manner, while still having at least one realization
 660 with relatively low error that could eventually be identified through data assimilation
 661 techniques.

662 **7. Conclusion.** This paper proposed a stochastic ROM derived from a stochastic fluid
 663 dynamics modelling standpoint, called dynamics under location uncertainty (LU), which
 664 formulates unresolved small-scale parameterization through SPDEs. The stochastic ROM
 665 is obtained through a classical POD-Galerkin projection of these SPDEs, and the basis
 666 functions are defined from a high-resolution deterministic simulation of the target flow.
 667 The resulting model bears similarities with the Navier-Stokes equations, but also encom-
 668 passes an advection velocity correction, a turbulent diffusion and a skew-symmetric multi-

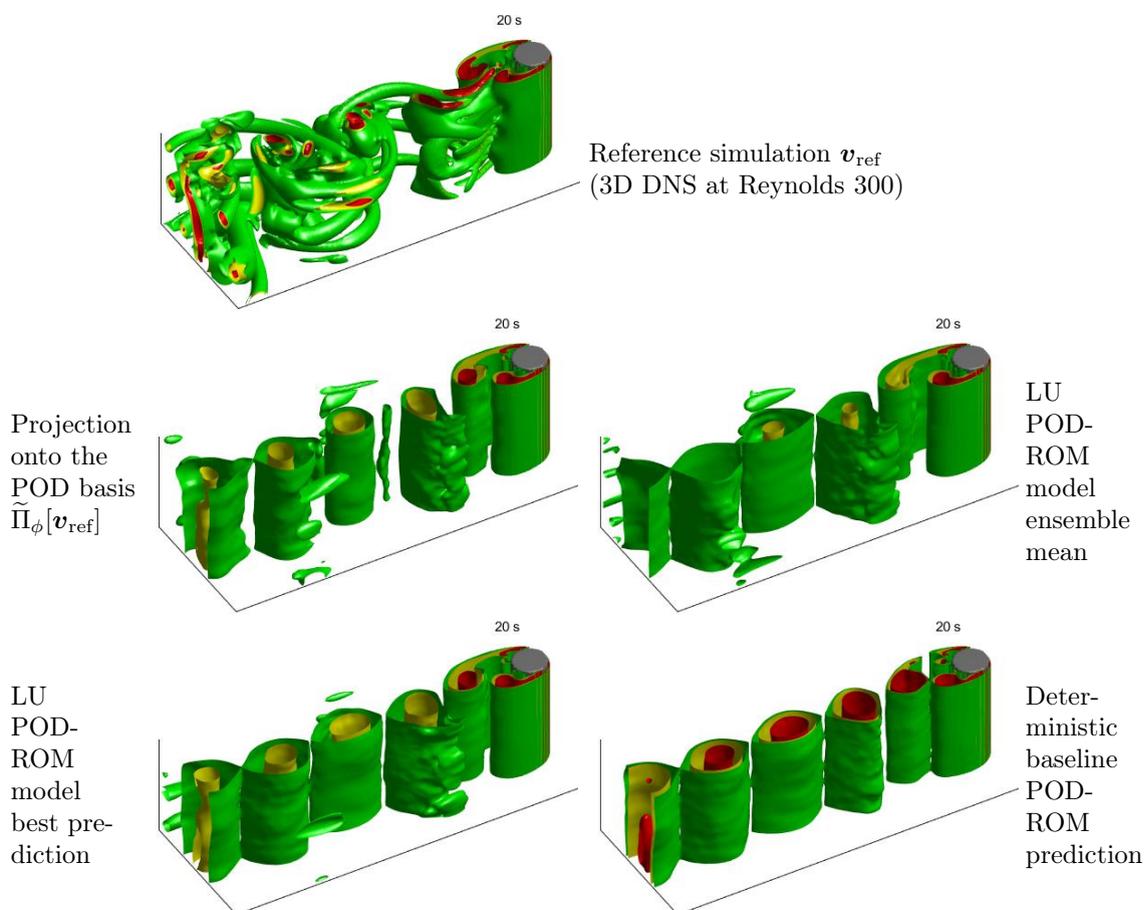


Figure 7: Q-criterion iso-surfaces – 4 vortex shedding cycles after the learning period – from (from left to right and from top to bottom) the reference simulation \mathbf{v}_{ref} (3D DNS at Reynolds 300: state space dimension of about 10^7), its projection onto the POD basis $\tilde{\Pi}_\phi[\mathbf{v}_{\text{ref}}]$, the LU POD-ROM model’s ensemble mean, the LU POD-ROM model’s best prediction, and the prediction of the deterministic baseline POD-ROM (6.1) (fitted eddy viscosity) (POD-ROM state spaces are of dimension 8). The Q-criterion [39] is a quadratic function of the velocity gradient and is the usual and a convenient way for visualizing 3D flows and their vortices.

669 plicative noise terms. From the statistics of the POD’s residuals – i.e. the data component
 670 orthogonal to the POD’s modes – these new terms can be fully characterized.

671 The implementation necessitates additional off-line computations on top of the classical
 672 POD-Galerkin procedure: estimations of a variance tensor and of the reduced multiplicative
 673 noise’s covariance matrix. The former, proportional to the point-wise $d \times d$ covariance
 674 matrix of POD’s residual, is readily computed. The latter can constitute a formidable
 675 computational challenge. Moreover, with a fully data-driven method, the risk of over-
 676 fitting is very high. To circumvent these issues, an intermediate solution is proposed
 677 with an easy-to-compute estimator, along with consistency proofs under the LU setting
 678 assumptions. Since the latter may not always be met – specifically, the time decorrelation
 679 assumption of the POD residual – measures are taken to enforce them on the model, as
 680 part of its constitutive steps. Namely, to force the decorrelation – and in doing so, improve
 681 the accuracy of the estimators and the ROM as a whole – a down-sampling of the dataset

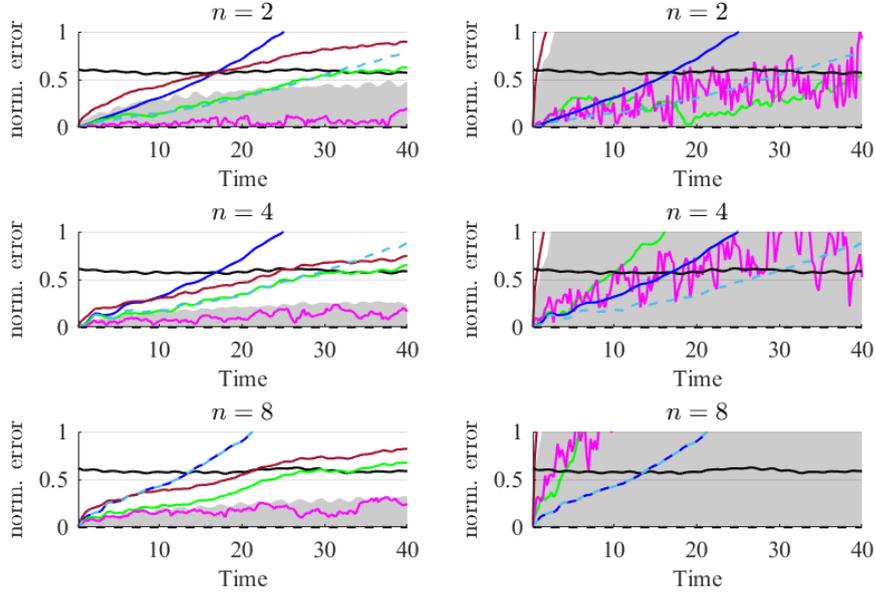


Figure 8: Normalized error for $n = 2, 4$ and 8 coefficients of the reduced solution of a 3D wake flow at Reynolds 300 – with the projection of the DNS onto the POD basis $\tilde{\Pi}_\phi[\mathbf{v}_{\text{ref}}]$ as reference : RMSE (red line), bias (green line), ensemble minimum error (magenta line) and $1.96 \times$ the standard-deviation (shaded gray) for the LU POD-ROM (left panel) and stochastic baseline POD-ROM (right panel) . Blue lines correspond to deterministic ROMs: baseline eddy-viscosity POD-ROM (6.1) (light-blue dashed line) and DNS POD-Galerkin (dark-blue solid line). The black solid line at the top is the error considering only the time mean velocity, i.e. $b_i = 0, \forall i > 0$.

682 is applied at a rate equal to the residual’s correlation time. Finally, in order to restrict the
 683 number of coefficients needed to characterize the ROM to the usual $O(n^3)$, a technique to
 684 reduce the dimensionality of the noise covariance matrix is also proposed.

685 The conservative properties of the LU closure are discussed, and we demonstrate that,
 686 when performing Galerkin projections of the $\text{It}\bar{o}$ form of LU SPDEs, we end up forfeiting
 687 these properties. In the reduced order version, two energy fluxes appear: the first one is
 688 attributed to the possible advecting velocity correction divergence, whilst the second one
 689 is negative and is directly associated with mode truncation. We argue that this energy
 690 loss is understandable, and even desirable, with an interplay between noise and turbulent
 691 diffusion to maintain non-linear energy fluxes between coefficients of the reduced solution
 692 despite mode truncation.

693 Numerical comparisons are performed between our stochastic ROM and state-of-the-art
 694 deterministic and stochastic ROMs. As test cases, we chose a two-dimensional wake flow
 695 at Reynolds 100 with few degrees of freedom, and a more complex three-dimensional wake
 696 flow at Reynolds 300 with many more degrees of freedom. Deterministic Navier-Stokes sim-
 697 ulations stood for references and all of the ROMs were initialized with their values, and the
 698 forecasts, compared to them. For the stochastic ROMs, ensembles of 100 realizations were
 699 simulated. The state-of-the-art stochastic ROM’s solutions quickly diverged in time, whilst
 700 the temporal coefficients of our ROM proved to be neither unstable nor over-damped. The
 701 LU POD-ROM solution’s biases were even found to be smaller than those of each of the

702 other stochastic ROMs' that we have considered. Moreover, at any given moment, the LU
703 POD-ROM ensembles managed to remain very close to the reference, suggesting that they
704 could be efficient priors for Bayesian inverse problems.

705

706 Following this work, we have applied the LU POD-ROM with unknown initial condi-
707 tions in conjunction with particle filter algorithms to estimate velocity flows in real-time
708 from few local measurements [63].

709 Finally, when working at very large Reynolds numbers, DNS simulations are no longer
710 an option, but LES (Large Eddy Simulation), DDES (Delayed Detached Eddy Simulation)
711 and RANS (Reynolds Averaged Navier Stokes) can still provide useful data to build ROMs,
712 at the cost of some approximation error. To tackle this, the closure mechanism's estima-
713 tion procedure may be adjusted to address the small-scale velocity statistics neglected by
714 LES-like approaches. Another approach that we are currently exploring is to consider the
715 Galerkin projection on a LU version of LES and DDES. Non-polynomial terms of LES and
716 DDES complicate the dimensional reduction, but discrete empirical interpolation methods
717 (DEIM) [18] may be able to handle it. As illustrated in this paper, our stochastic closure
718 naturally prevents truncation-induced instabilities, and we expect a similar behavior at
719 higher Reynolds. If the proposed in-house stabilization is not sufficient, existing stabilisa-
720 tion and/or data-driven methods [33, 37, 77] could be added. Furthermore, CFD outputs
721 may also be at a resolution different from the resolution of the measurements. Hence, de-
722 pending on the relative precision of CFD and measurements, there could be an additional
723 or a missing very-small-scale residual turbulence in the assimilated measures. Accordingly,
724 we will need a simple statistical model for this very-small-scale turbulence and include
725 its effects in the observation model through either an additional "measurement noise" or
726 additional smoothing.

727 Besides, in realistic applications, Reynolds number, initial and boundary conditions, as
728 well as a plethora of other parameters, are often only approximately known. So, combina-
729 tions with other state-of-the-art dimensionality reduction methods are most likely neces-
730 sary. Typically, we could use wRB [20, 21, 77] for uncertain mean inflow (Reynolds number
731 and angle of attack) and a reduced pressure equation [75, 76] for time dependent boundary
732 conditions. Our new implementation of LU terms in the ITHACA-FV library [75, 76] will
733 surely aid on these practical aspects.

734 Nevertheless, note that a wRB method to simulate random velocity effect [77] does not
735 directly apply to the purpose of the current paper. Indeed, we try to quantify the uncer-
736 tainty induced by the dimensional reduction of the deterministic Navier-Stokes equations
737 and not to reduce the dimension of an uncertainty quantification problem. The random
738 residual velocity can hardly be considered a wRB parameter because we do not choose
739 its value. There is only one "realization" and this is the one given by the deterministic
740 Navier-Stokes equations. We could specify some statistics for the random residual veloc-
741 ity and simulate the stochastic Navier-Stokes equations (2.1)-(2.2) but this would make
742 our method much more complex, much more CPU demanding, and could possibly lead to
743 over-fitting. Moreover, that random velocity is a residual, and thus, its statistics depend
744 on the reduced dimension n . That would also greatly complicate the wRB algorithm.

745 Finally, relying purely on data can offer the advantage of directly tackling very high
746 Reynolds number configurations. It would require us to filter noisy measurements, and
747 most likely, to rely on simplified (often 2D) data-driven models [1, 13, 29, 78]. From
748 this latter point of view, modeling under location location offers a great flexibility which
749 might be of great interest. As a matter of fact, the LU formalism enables us to derive
750 random dynamics close to the data but still based on stochastic transport principles [3].

751 The noise parameters can be updated online from incoming data and simulations. A full
 752 characterization of the noise dynamics through statistical learning procedures would then
 753 probably enable us to devise advanced data-driven models that are able to handle even
 754 more complex situations.

755 **Appendix A. Estimation formulas.** In this appendix, we consider a full probability
 756 space (A, \mathcal{F}, P) , and a filtration of σ -algebra $\{\mathcal{F}_t\}_{t \geq 0}$. For the Hilbert space $H^2(\Omega)$, we
 757 understand $\mathcal{H}^2 = \mathcal{H}^2(0, T; \Omega, \mathcal{F})$ as the space of strongly measurable, $\{\mathcal{F}_t\}_{t \geq 0}$ adapted
 758 processes $\mathbf{u} : \mathbb{R}^d \times [0, T] \rightarrow \mathbb{R}^d$ such that $(\mathbf{x} \mapsto \mathbf{u}(\mathbf{x}, t))$ belong to $H^2(\Omega)$ for every $t \in [0, T]$
 759 and

$$760 \quad (A.1) \quad \|\mathbf{u}\|_{\mathcal{H}^2}^2 = \mathbb{E} \int_0^T \|\mathbf{u}(\bullet, t)\|_{H^2(\Omega)}^2 dt < \infty.$$

761 Similarly, we can define $\mathcal{L}^2(0, T; \Omega, \mathcal{F})$ from \mathbf{L}^2 and its norm. We recall below a classical
 762 proposition related to quadratic variation process:

763 *Proposition: Stochastic integration and quadratic variations.* If \mathbf{M} is a continuous mar-
 764 tingale and $\mathbf{X} \in \mathcal{L}^2(0, T; \Omega, \mathcal{F})$, then there exists a unique bounded continuous martingale
 765 $\int_0^t \mathbf{X} d\mathbf{M}$ such that for every continuous martingale \mathbf{N} (with zero initial condition)

$$766 \quad (A.2) \quad \left\langle \int_0^t \mathbf{X} d\mathbf{M}, \mathbf{N} \right\rangle = \int_0^t \mathbf{X} d\langle \mathbf{M}, \mathbf{N} \rangle.$$

767 As stated in the introduction, we assume that the operator $\boldsymbol{\sigma}$ is Hilbert-Schmidt and
 768 that its kernel $\check{\boldsymbol{\sigma}} : \bar{\Omega}^2 \rightarrow \mathbb{R}^{d \times d}$ is C^2 over the compact bounded set $\bar{\Omega}^2$. Therefore,

$$769 \quad (A.3) \quad \|\boldsymbol{\sigma} \mathbf{B}\|_{\mathcal{H}^2}^2 \leq \max_{i,j} \sup_{\bar{\Omega}^2} \left(\|\check{\boldsymbol{\sigma}}\|^2 + \|\partial_{x_i} \check{\boldsymbol{\sigma}}\|^2 + \|\partial_{x_i} \partial_{x_j} \check{\boldsymbol{\sigma}}\|^2 \right) |\Omega^2| T < \infty,$$

770 where $\|\bullet\|$ stands for the Euclidean norm on $\mathbb{R}^{d \times d}$ and $|\Omega^2|$ the Lebesgue measure of Ω^2 .
 771 As such, $((\mathbf{x}, t) \mapsto \boldsymbol{\sigma}(\mathbf{x}) \mathbf{B}_t)$ belong to \mathcal{H}^2 . In particular, $(\mathbf{x} \mapsto \boldsymbol{\sigma}(\mathbf{x}) \mathbf{B}_t)$ belong to $H^2(\Omega)$
 772 for every $t \in [0, T]$ and $\partial_{x_i} \boldsymbol{\sigma}, \partial_{x_i} \partial_{x_j} \boldsymbol{\sigma}$ are also Hilbert-Schmidt for every $1 \leq i, j \leq d$.
 773 Additionally, we assume that the POD modes ϕ_i belong to $H^2(\Omega)$ and have bounded
 774 gradients.

775 After defining boundary conditions, \mathcal{P} and \mathbf{K} are well defined on $H^1(\Omega)$ and $H^2(\Omega)$
 776 respectively. Then, for every $\boldsymbol{\zeta} \in H^1(\Omega)$, $\|\mathcal{P}\boldsymbol{\zeta}\|_{L^2} \leq \|\boldsymbol{\zeta}\|_{L^2}$ since \mathcal{P} is a projection and
 777 then, for every $\boldsymbol{\xi} \in H^2(\Omega)$, by Cauchy-Schwarz and triangular inequalities:

$$778 \quad (A.4) \quad |K_{jq}(\boldsymbol{\xi})| \leq \|\phi_j\|_{L^2} (\|\nabla \phi_q^T\|_{\infty} + \nu) \|\boldsymbol{\xi}\|_{H^2(\Omega)},$$

779 where $\|\nabla \phi_i^T\|_{\infty} = \sup_{\Omega} \|\nabla \phi_i^T\| < \infty$. The bound above gives the continuity of \mathbf{K} on
 780 $H^2(\Omega)$. We also assume that the observed coefficients of the reduced solution $b_i^{\text{obs}} =$
 781 $(\phi_i, \mathbf{v}_{\text{obs}})$ are continuous semi-martingales and solutions of the ROM (3.3)-(3.4). From
 782 there, the orthogonality of the coefficients of the reduced solution yields, for $1 \leq i, j \leq n$
 783 and $0 \leq p, q \leq n$:

$$784 \quad (A.5) \quad \int_0^T b_p d\langle b_i, \int_0^t (\tilde{\alpha}_{qj} \bullet d\mathbf{B}_s) \rangle = \int_0^T \sum_{k=0}^n b_p d\langle \int_0^t (\tilde{\alpha}_{ki} \bullet d\mathbf{B}_s) b_k, \int_0^t \tilde{\alpha}_{qj} \bullet d\mathbf{B}_s \rangle,$$

$$785 \quad (A.6) \quad = \sum_{k=0}^n \left(\int_0^T b_p b_k \right) \Sigma_{ki, qj}^{\alpha},$$

$$786 \quad (A.7) \quad = T \lambda_p \Sigma_{pi, qj}^{\alpha}.$$

787 Now, let us note that for $1 \leq j \leq n$ and $0 \leq q \leq n$:

$$788 \quad (\text{A.8}) \quad \tilde{\alpha}_{qj} \bullet d\mathbf{B}_s = (\phi_j, -\mathcal{P} [(\sigma d\mathbf{B}_s \cdot \nabla) \phi_q] + \delta_{q0} \nu \Delta \sigma d\mathbf{B}_s) = d(K_{jq} [\sigma \mathbf{B}]).$$

789 Then, with the definition of the quadratic covariation and the increment notation $\Delta \xi(t_k) =$
790 $\xi(t_{k+1}) - \xi(t_k)$, we obtain the estimator's expression and its consistency for every $1 \leq i, j \leq$
791 n and $0 \leq p, q \leq n$:

$$792 \quad (\text{A.9}) \quad \Sigma_{pi,qj}^\alpha = \frac{1}{\lambda_p T} \int_0^T b_p d\langle b_i, \int_0^t (\tilde{\alpha}_{qj} \bullet d\mathbf{B}_s) \rangle,$$

$$793 \quad (\text{A.10}) \quad = \frac{1}{\lambda_p T} \int_0^T b_p d\langle b_i, K_{jq} [\sigma \mathbf{B}] \rangle,$$

$$794 \quad (\text{A.11}) \quad = \frac{1}{\lambda_p T} \mathbb{P}\text{-}\lim_{\Delta t \rightarrow 0} \sum_{t_k=0}^T b_p(t_k) (\Delta b_i)(t_k) K_{jq} [\sigma \Delta \mathbf{B}_{t_k}],$$

$$795 \quad (\text{A.12}) \quad = K_{jp} \left[\frac{1}{\lambda_p T} \mathbb{P}\text{-}\lim_{\Delta t \rightarrow 0} \sum_{t_k=0}^T b_p(t_k) (\Delta b_i)(t_k) \sigma \Delta \mathbf{B}_{t_k} \right],$$

796 where the continuity of the operator K_{jp} on $H^2(\Omega)$ enabled us to switch the limit in prob-
797 ability and the operator K_{jp} . The martingale flow increments $\sigma \Delta \mathbf{B}_{t_k}$ are approximated
798 by $\mathbf{v}'(\bullet, t_k) \Delta t$. In practice, for each $1 \leq i \leq n$ we can replace Δb_i by

$$799 \quad (\text{A.13}) \quad \Delta b_i'' = \Delta b_i' - \overline{\Delta b_i'},$$

800 where

$$801 \quad (\text{A.14}) \quad \Delta b_i' = \Delta b_i - \left(\mathbf{b}^T (\mathbf{l} + \check{\mathbf{f}}) \bullet_i + \mathbf{b}^T \mathbf{c}_{\bullet\bullet i} \mathbf{b} \right) \Delta t.$$

802 Mathematically, this is still correct for very large values of T . Indeed,

803 $\frac{\Delta b_i'}{T} = \frac{b_i'(T+\Delta T) - b_i'(0)}{T} \Delta t \xrightarrow{T \rightarrow \infty} 0$ and $b_i' - b_i$ has finite variations. Thus, $b_i'' - b_i$ approaches a
804 finite variation process (for large T). Numerically, this formulation improves the accuracy
805 of the model as it allows us to remove the smooth-in-time part of Δb_i , thus minimizing
806 estimation error as well.

807 **Appendix B. Energy dissipation.**

808 On top of assumptions of Appendix A, we neglect the viscosity ($\mathbf{L} = 0$) and assume
809 zero Dirichlet boundary conditions for the reduced basis' functions and for $\mathbf{x} \mapsto \sigma(\mathbf{x}) \mathbf{B}_t$
810 for every $t \in [0, T]$. Note that these fields are divergence-free (since they are learned
811 from a set of incompressible velocity fields). As such, we have: $\forall i \leq n$, $\|\mathbf{G}(\phi_i)\|_{\text{HS}}^2 \leq$
812 $\|\nabla \phi_i^T\|_\infty^2 \|\sigma\|_{\text{HS}}^2 < \infty$, i.e. $\mathbf{G}(\phi_i)$ is Hilbert-Schmidt. This makes $\mathbf{G}(\mathbf{w}^R)$ and $\Pi_\phi [\mathbf{G}(\mathbf{w}^R)]$
813 also Hilbert-Schmidt.

814 Using the projected Navier-Stokes model (5.4), for every $t \in [0, T]$ we can formally
815 remove the orthogonal projection by moving it into the divergence-free functions space \mathcal{P}
816 through integration by parts:

$$817 \quad (\text{B.1}) \quad d_t \mathbf{w}^R = \sum_{i=1}^n (\phi_i, \mathcal{P}(d\mathbb{M})(\mathbf{w}^R)) \phi_i = \sum_{i=1}^n (\mathcal{P} \phi_i, (d\mathbb{M})(\mathbf{w}^R)) \phi_i,$$

$$818 \quad (\text{B.2}) \quad = \sum_{i=1}^n (\phi_i, (d\mathbb{M})(\mathbf{w}^R)) \phi_i = \Pi_\phi [(C(\mathbf{w}^R, \mathbf{w}^R) + F(\mathbf{w}^R)) dt + (G d\mathbf{B}_t)(\mathbf{w}^R)].$$

819 Then, upon applying the Itô formula to the local kinetic energy we obtain

$$820 \quad (\text{B.3}) \quad d\left(\frac{1}{2}\|\mathbf{w}^R\|_{L^2}^2\right) = \int_{\Omega} \left(d_t(\mathbf{w}^R)^T \mathbf{w}^R + \frac{1}{2}d_t\langle(\mathbf{w}^R)^T, \mathbf{w}^R\rangle\right) \quad \forall t \in [0, T].$$

821 To remove the (orthogonal) projection operator Π_{ϕ} from the first term, we exploit its
822 symmetry, and afterwards, the fact that \mathbf{w}^R is already in the reduced subspace:

$$823 \quad (\text{B.4}) \quad \int_{\Omega} d_t(\mathbf{w}^R)^T \mathbf{w}^R = (\Pi_{\phi} [(d\mathbb{M})(\mathbf{w}^R)], \mathbf{w}^R),$$

$$824 \quad (\text{B.5}) \quad = ((d\mathbb{M})(\mathbf{w}^R), \Pi_{\phi} [\mathbf{w}^R]),$$

$$825 \quad (\text{B.6}) \quad = ((d\mathbb{M})(\mathbf{w}^R), \mathbf{w}^R),$$

$$826 \quad (\text{B.7}) \quad = (((\mathbf{F}_{\text{dif}} + \mathbf{F}_{\text{adv}})(\mathbf{w}^R) + \mathbf{C}(\mathbf{w}^R, \mathbf{w}^R))dt + (\mathbf{G}d\mathbf{B}_t)(\mathbf{w}^R), \mathbf{w}^R),$$

$$827 \quad = \underbrace{\left(-\frac{1}{2}\mathbf{G}^* (\otimes \mathbf{G}(\mathbf{w}^R)), \mathbf{w}^R\right) dt}_{\text{from } (\mathbf{F}_{\text{dif}}(\mathbf{w}^R), \mathbf{w}^R) \text{ using (2.12)}} + \underbrace{\left(\frac{1}{2}((\nabla \cdot \mathbf{a})\nabla)\mathbf{w}^R, \mathbf{w}^R\right)}_{\text{from } (\mathbf{F}_{\text{adv}}(\mathbf{w}^R), \mathbf{w}^R)}$$

$$828 \quad (\text{B.8}) \quad + \underbrace{(\mathbf{C}(\mathbf{w}^R, \mathbf{w}^R)dt + (\mathbf{G}d\mathbf{B}_t)(\mathbf{w}^R), \mathbf{w}^R)}_{=0 \text{ by skew-symmetry of } \xi \mapsto \mathbf{C}(\mathbf{w}^R, \xi) \text{ and } \mathbf{G}d\mathbf{B}_t},$$

$$829 \quad (\text{B.9}) \quad = \frac{1}{2}\|\mathbf{G}(\mathbf{w}^R)\|_{\text{HS}}^2 - \frac{1}{2}(\nabla \cdot (\nabla \cdot \mathbf{a})^T, \|\mathbf{w}^R\|^2),$$

830 where the second term comes from integration by parts. Besides, the Itô term of the energy
831 budget is straightforward to compute from equation (B.2):

$$832 \quad (\text{B.10}) \quad \int_{\Omega} \frac{1}{2}d_t\langle(\mathbf{w}^R)^T, \mathbf{w}^R\rangle = \frac{1}{2}\|\Pi_{\phi} [(\mathbf{G})(\mathbf{w}^R)]\|_{\text{HS}}^2 dt,$$

$$833 \quad (\text{B.11}) \quad = \sum_{p,q=0}^n \left(\frac{1}{2} \int_{\Omega} \Pi_{\phi} [\mathbf{G}(\phi_p)] \otimes \Pi_{\phi} [\mathbf{G}(\phi_q)]\right) b_p b_q dt.$$

834 From the definition of the projection operator Π_{ϕ} and using the extended notation $(\boldsymbol{\eta} \otimes \boldsymbol{\theta}) \triangleq$
835 $\int_{\Omega} \check{\boldsymbol{\eta}}(z) \check{\boldsymbol{\theta}}^T(z) dz$, we can express the above quadratic operator with the noise statistics as
836 follows:

$$837 \quad (\text{B.12}) \quad \int_{\Omega} \Pi_{\phi} [\mathbf{G}(\phi_p)] \otimes \Pi_{\phi} [\mathbf{G}(\phi_q)] = \sum_{i=1}^n (\phi_i, \mathbf{G}(\phi_p)) \otimes (\phi_i, \mathbf{G}(\phi_q)) = \sum_{i=1}^n \Sigma_{pi, qi}^{\alpha}.$$

838 Finally, by orthogonality, the kinetic energy budget (B.3) simplifies to:

$$839 \quad (\text{B.13}) \quad \frac{d}{dt} \left(\frac{1}{2}\|\mathbf{w}^R\|_{L^2}^2\right) = \frac{1}{2}\|\mathbf{G}(\mathbf{w}^R)\|_{\text{HS}}^2 - \frac{1}{2}(\nabla \cdot (\nabla \cdot \mathbf{a})^T, \|\mathbf{w}^R\|^2) - \frac{1}{2}\|\Pi_{\phi} [\mathbf{G}(\mathbf{w}^R)]\|_{\text{HS}}^2,$$

$$840 \quad (\text{B.14}) \quad = -\frac{1}{2}\|\Pi_{\phi}^{\perp} [\mathbf{G}(\mathbf{w}^R)]\|_{\text{HS}}^2 - \frac{1}{2}(\nabla \cdot (\nabla \cdot \mathbf{a})^T, \|\mathbf{w}^R\|^2),$$

841 where $\Pi_{\phi}^{\perp} = \mathbb{I}_d - \Pi_{\phi}$ is the projector into the orthogonal complement of the reduced
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