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# Quantifying truncation-related uncertainties in unsteady fluid dynamics reduced order models \*

Valentin Resseguier $^{\dagger}$ , Agustin M. Picard $^{\dagger}$ , Etienne Mémin $^{\ddagger}$ , and Bertrand Chapron $^{\S}$ 

Abstract. In this paper, we present a new method to quantify the uncertainty introduced by the drastic 56 dimensionality reduction commonly practiced in the field of computational fluid dynamics, the 7 ultimate goal being to simulate accurate priors for real-time data assimilation. Our key ingredient 8 is a stochastic Navier-Stokes closure mechanism that arises by assuming random unresolved 9 flow components. This decomposition is carried out through Galerkin projection with a Proper 10 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 11 12multiplicative and additive noise's correlations. The low computational cost of these consistent 13 correlation estimators makes them applicable to the study of complex fluid flows. This stochastic 14 POD-ROM is applied to 2D and 3D DNS wake flows at Reynolds 100 and 300, respectively, with 15Uncertainty Quantification (UQ) and forecasting outside the learning interval being the main 16focus. The proposed stochastic POD-ROM approach is shown to stabilize the unstable temporal 17coefficients and to maintain their variability under control, while exhibiting an impressively accurate predictive capability. 18

Key words. Fluid dynamics, reduced order model, uncertainty quantification, stochastic closure, proper
 orthogonal decomposition

21 AMS subject classifications. 60H35, 65M60, 65M75, 76M35, 93B11

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2

3 4

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

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

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<sup>&</sup>lt;sup>†</sup>Lab, SCALIAN DS, Rennes, France (valentin.resseguier@scalian.com).

<sup>&</sup>lt;sup>‡</sup>Fluminance team, Inria, Rennes, France .

<sup>&</sup>lt;sup>§</sup>LOPS, Ifremer, Plouzané, France.

Consequently, to stabilize the ROM, authors commonly introduce an additional determin-43 istic term (typically an eddy viscosity term) [2, 15, 79], along with a possible calibration on 44 available data [12, 23, 80]. This calibration procedure can be extended to the complete set 45of the ROM's parameters [1, 10, 61, 72]. ROM performances have mainly been evaluated on 46 low Reynolds-number flows (say  $Re \leq 100$ ) [e.g. 10, 75, 80], while for flows at much greater 47 Reynolds numbers, evaluations close to the learning time interval and reduced dynamics 48 for two-dimensional flow observables (e.g. particle image velocimetry) have usually been 49the norm [e.g. 1, 12, 23, 75]. Long time ROM predictions have been otherwise performed 50 with a substantial number of modes [e.g. 14, 74]. Yet, turbulent flow ROMs remain inexact 52 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 53 less and less accurate. Moreover, these predictions necessitate accurate initial conditions, 5455forcing 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 62 been proposed for incorporating randomness in the physical models through some of their 63 parameters [e.g. 44, 47]. However, the error introduced by these noisy parameters is not a64 65 *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 66 both UQ and predictability studies [e.g. 51]. It was later demonstrated this yields under-67 dispersive quantification, i.e. it has a tendency to underestimate the error associated to 68 the dimensionality reduction [8, 31, 35, 53]. 69

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-74order moment to help redistribute the right amount of energy between the coefficients of 75the reduced solution. Finally, several techniques related to averaging and homogenization 76 theory exploit a time-scale separation hypothesis [34, 43, 53, 58], one of the most notable 77 78 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 79 potential energy conservation issues, the noise covariance is often not explicit enough, 80 and has to be simplified and estimated using the available data. Interested readers can 81 refer to [64], and references herein, for more detailed reviews on model error specification in 82 coarse-scale computational fluid dynamics (CFD). For ROM UQ, [73] propose distributions 83 and efficient sampling methods for the projection matrices in Galerkin-projection-based 84 dimensionality reduction methods. Although apparently more pertinent than methods 85 86 based on randomized parameters, the relation of this technique to errors associated to 87 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-projectionbased ROM. Inspired from the theoretical works of [11, 52], the LU closure relies on the

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

102 (1.1) 
$$\boldsymbol{\sigma}(\boldsymbol{x}) \mathrm{d}\boldsymbol{B}_t \stackrel{\Delta}{=} \int_{\Omega} \boldsymbol{\breve{\sigma}}(\boldsymbol{x}, \boldsymbol{z}) \mathrm{d}\boldsymbol{B}_t(\boldsymbol{z}) \mathrm{d}\boldsymbol{z} \quad \forall (\boldsymbol{x}, t) \in \Omega \times [0, T].$$

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,  $B_t$  is an  $\mathbb{I}_d$ -cylindrical Wiener process and  $dB_t/dt$  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 (1.2) 
$$d\boldsymbol{X}_t = \boldsymbol{w}(\boldsymbol{X}_t, t)dt + \boldsymbol{\sigma}(\boldsymbol{X}_t)d\boldsymbol{B}_t \quad \forall t \in [0, T],$$

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 of stochastic PDEs (SPDE), in particular, by applying the Ito-Wentzell formula [42] and a 113 stochastic version of the Reynolds transport theorem [40, 50, 65]. As such, LU models can 114 be applied to model error quantification [17, 64, 66, 68], to improve large-scale simulations 115[6, 7, 40, 66, 68], to reduced order modeling and data analysis [67] or to data assimilation 116 purposes [16, 81] in geophysical fluid dynamics and CFD. To note, in the geometric me-117 chanics community [38, 24], the Stochastic Advection by Lie Transport (SALT) method 118 has been derived for large-scale modeling and data assimilation [25]. Both frameworks 119120 have been compared, numerically [7, 64] and conceptually, [6, 68], with LU and SALT exhibiting different conservation properties, namely energy preservation and circulation 121 122conservation, respectively. Applied to a barotropic Quasi-Geostrophic model, LU leads to improved accuracy when compared to a classical large-scale deterministic framework or to 123the circulation conservation stochastic setup [6, 7]. The LU setting also fully captures the 124 structural deformation of the large-scale flow component by the spatial inhomogeneity of 125the small-scales [6]. It is important to note that these properties are independent of the 126 choice of stochastic integral. 127

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

In section 2, we introduce the stochastic fluid dynamics closure we will employ throughout the paper, as well as its algebraic structure, followed by the Galerkin projection of this SPDE to derive our stochastic ROM, with a brief recall of the principle behind POD-ROMs in section 3. Several estimations needed to complete our stochastic POD-ROM are detailed in section 4, as well as the efficient and consistent estimators we exploit to rely both on data and on the closure's physical grounding. In section 5, we discuss the conservative properties of LU dynamics and of its reduced versions, and finally, section 6 is dedicated to the numerical evaluation of the UQ capabilities of our ROM.

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

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

152 (2.1)  

$$\underbrace{\mathbb{D}_{t}\boldsymbol{w}}_{\text{Stochastic}} = \underbrace{-\boldsymbol{\nabla}\left(p\,\,\mathrm{d}t + \boldsymbol{p}_{\sigma}\mathrm{d}\boldsymbol{B}_{t}\right)}_{\text{Pressure}} + \underbrace{\frac{1}{Re}\Delta\left(\boldsymbol{w}\mathrm{d}t + \boldsymbol{\sigma}\mathrm{d}\boldsymbol{B}_{t}\right)}_{\text{Molecular viscous}},$$
153 (2.2)  

$$0 = \underbrace{\boldsymbol{\nabla}\cdot\left(\boldsymbol{w}^{*}\mathrm{d}t + \boldsymbol{\sigma}\mathrm{d}\boldsymbol{B}_{t}\right)}_{\text{Mass conservation}},$$

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

157 (2.3) 
$$(\mathbb{D}_t \boldsymbol{q})_k \stackrel{\triangle}{=} \underbrace{\operatorname{d}_t q_k}_{\substack{\substack{\alpha \in \mathbf{x}, t+\mathrm{d}t \end{pmatrix} - q_k(\boldsymbol{x}, t) \\ \text{Time increment}}} + \underbrace{\underbrace{(\boldsymbol{w}^* \mathrm{d}t + \boldsymbol{\sigma} \mathrm{d}\boldsymbol{B}_t) \cdot \boldsymbol{\nabla} q_k}_{\text{Advection}} - \underbrace{\boldsymbol{\nabla} \cdot \left(\frac{1}{2}\boldsymbol{a}\boldsymbol{\nabla} q_k\right)}_{\text{Turbulent}}_{\text{diffusion}} \mathrm{d}t,$$

158 (2.4)  $\boldsymbol{w}^* \stackrel{\triangle}{=} \boldsymbol{w} - \frac{1}{2} \left( \boldsymbol{\nabla} \cdot \boldsymbol{a} \right)^T,$ 

159 (2.5) 
$$\boldsymbol{a} \stackrel{\triangle}{=} \mathbb{E}\left\{ \left(\boldsymbol{\sigma} \mathrm{d} \boldsymbol{B}_{t}\right) \left(\boldsymbol{\sigma} \mathrm{d} \boldsymbol{B}_{t}\right)^{T} \right\} / \mathrm{d} t = \boldsymbol{\sigma} \circledast \boldsymbol{\sigma},$$

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

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

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

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

168 (2.7) 
$$(\boldsymbol{\eta} \circledast \boldsymbol{\theta})(\boldsymbol{x}) \stackrel{\Delta}{=} \int_{\Omega} \boldsymbol{\breve{\eta}}(\boldsymbol{x}, \boldsymbol{z}) \, \boldsymbol{\breve{\theta}}^{\mathrm{T}}(\boldsymbol{x}, \boldsymbol{z}) d\boldsymbol{z} \quad \forall \boldsymbol{x} \in \Omega.$$

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	L	$\frac{1}{Re}\Delta$	symmetric, $< 0$	l
dissipation		<i>Re</i>		
Turbulent	$F_{ m dif}$	$\mathbf{ abla}\cdot (rac{1}{2} oldsymbol{a} \mathbf{ abla}ullet)$	symmetric, $< 0$	$reve{f}_{ m dif}$
diffusion				
Advecting velocity	$F_{ m adv}$	$rac{1}{2} \left( oldsymbol{ abla} \cdot oldsymbol{a}  ight) oldsymbol{ abla}$	skew-symmetric	$oldsymbol{\check{f}}_{ ext{adv}}$
correction		2	(if $\boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} \cdot \boldsymbol{a})^T = 0$ )	
Usual	$oldsymbol{C}(oldsymbol{w},ullet)$	$-(\boldsymbol{w} \cdot \boldsymbol{\nabla})$	skew-symmetric	c
advection			(if $\boldsymbol{\nabla} \cdot \boldsymbol{w} = 0$ )	
Advection by the	$oldsymbol{G} \mathrm{d} oldsymbol{B}_t$	$-(\boldsymbol{\sigma}\mathrm{d}\boldsymbol{B}_t\cdot\boldsymbol{ abla})$	skew-symmetric	$oldsymbol{lpha} \mathrm{d}oldsymbol{B}_t$
residual velocity			noise	
			(if $\boldsymbol{\nabla} \cdot \boldsymbol{\sigma} = 0$ )	
Molecular viscous	$oldsymbol{H}\mathrm{d}oldsymbol{B}_t$	$rac{1}{Re}\Delta oldsymbol{\sigma} \mathrm{d}oldsymbol{B}_t$	additive	$oldsymbol{ heta}{ ext{d}} oldsymbol{B}_t$
dissipation of the			noise	
residual velocity				
Pressure	$\mathrm{d} oldsymbol{P}$	$-\boldsymbol{\nabla}\left(p\mathrm{d}t+\boldsymbol{p}_{\sigma}\mathrm{d}\boldsymbol{B}_{t}\right)$	Potential	Included in
gradient			field	other terms

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

closure mechanism and its reduced order expression. The stochastic transport operator 171 $\mathbb{D}_t$  involves the usual terms of the deterministic material derivative, on top of three addi-172tional new terms: an advecting velocity correction ( $w^*$  instead of w), a heterogeneous and 173anisotropic turbulent diffusion, and a multiplicative noise. This last term corresponds to 174175the advection by the unresolved velocity  $\sigma B$ . Finally, we can recover the classical Navier-Stokes equations by setting the residual velocity to zero – i.e.  $\sigma = 0$ . Let us highlight 176that for conserved scalars, this operator corresponds to the material derivative - i.e. the 177 derivative along the stochastic flow d  $(\boldsymbol{w}(\boldsymbol{X}_t, t))$  [65]. This stochastic Navier-Stokes model 178is generic, and depending on the application, forces and boundary conditions, it may be 179modified accordingly to adjust to any incompressible flow configurations. For compressible 180 stochastic flows, some new terms appear. Interested readers may refer to [65]. 181

In addition to the classical physical assumptions pertaining to the establishment of the Navier-Stokes equations for incompressible fluids, the main assumption of the LU setting is to consider the unresolved fluctuation velocity component uncorrelated in time. To note, the incompressible character of the random fluctuations can be relaxed at the price of 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 (2.8) 
$$d_t \boldsymbol{w} = (d\mathbb{M})(\boldsymbol{w}) \stackrel{\triangle}{=} ((\boldsymbol{L} + \boldsymbol{F})(\boldsymbol{w}) + \boldsymbol{C}(\boldsymbol{w}, \boldsymbol{w})) dt + (\boldsymbol{G} d\boldsymbol{B}_t)(\boldsymbol{w}) + (\boldsymbol{H} d\boldsymbol{B}_t) + d\boldsymbol{P},$$

where table 1 details each term. Operator L represents the molecular viscosity term,  $F = F_{dif} + F_{adv}$ , the turbulent diffusion plus the advecting velocity correction, and  $GdB_t$ , the advection by the random residual velocity. All of them are linear differential operators, while C, the term representing the usual non-linear advection effect, is a bilinear differential operator. The additive noise  $HdB_t$  corresponds to the molecular viscous dissipation of the time-uncorrelated velocity component,  $\sigma \dot{B}$ , while the last term on the right-hand side, 197 d $\boldsymbol{P}$ , is the pressure forcing.

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

208 (2.9) 
$$(\boldsymbol{\zeta}, (\boldsymbol{G} \mathrm{d}\boldsymbol{B}_t) (\boldsymbol{\xi})) = -\sum_{k=1}^d \int_{\Omega} \zeta_k (\boldsymbol{\sigma} \mathrm{d}\boldsymbol{B}_t \cdot \boldsymbol{\nabla}) \, \xi_k = -\sum_{k=1}^d \int_{\Omega} \zeta_k \boldsymbol{\nabla} \cdot (\boldsymbol{\sigma} \mathrm{d}\boldsymbol{B}_t \xi_k) \,,$$
  
209 (2.10)  $= \sum_{k=1}^d \int_{\Omega} (\boldsymbol{\sigma} \mathrm{d}\boldsymbol{B}_t \cdot \boldsymbol{\nabla}\zeta_k) \, \xi_k = -((\boldsymbol{G} \mathrm{d}\boldsymbol{B}_t) (\boldsymbol{\zeta}), \boldsymbol{\xi}).$ 

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

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

216 
$$(2.11)(\boldsymbol{F}_{\mathrm{dif}}(\boldsymbol{\xi}))_{k} \stackrel{\Delta}{=} \boldsymbol{\nabla} \cdot \left(\frac{1}{2}\boldsymbol{a}\boldsymbol{\nabla}\boldsymbol{\xi}_{k}\right) = \boldsymbol{\nabla} \cdot \left(\frac{1}{2}(\boldsymbol{\sigma} \otimes \boldsymbol{\sigma})\boldsymbol{\nabla}\boldsymbol{\xi}_{k}\right) = \frac{1}{2}\left(\boldsymbol{\sigma}^{T}\boldsymbol{\nabla}\right)^{T}\left(\otimes \left(\boldsymbol{\sigma}^{T}\boldsymbol{\nabla}\right)^{T}\boldsymbol{\xi}_{k}\right),$$

217 (2.12) 
$$= \frac{1}{2} \boldsymbol{G} \left( \circledast \boldsymbol{G}(\boldsymbol{\xi}_k) \right) = \left( \frac{1}{2} \boldsymbol{G} \left( \circledast \boldsymbol{G}(\boldsymbol{\xi}) \right) \right)_k = \left( -\frac{1}{2} \boldsymbol{G}^* \left( \circledast \boldsymbol{G}(\boldsymbol{\xi}) \right) \right)_k,$$

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

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

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

3.1. A ROM with correlated additive and multiplicative noise. Let  $\boldsymbol{v}$  be the real velocity field (i.e. the Navier-Stokes equations' solution) and  $\phi_0$ , a background velocity field, typically the velocity temporal mean  $\overline{\boldsymbol{v}} \stackrel{\triangle}{=} \frac{1}{T} \int_0^T \boldsymbol{v}$ . To reduce the state space dimension, we project the fluid velocity anomaly,  $\boldsymbol{v} - \phi_0$ , in a subspace spanned by a number of

<sup>1</sup>i.e.  $\nabla_{\boldsymbol{x}} \cdot \breve{\boldsymbol{\sigma}}(\boldsymbol{x}, \boldsymbol{z}) = 0, \forall (\boldsymbol{x}, \boldsymbol{z}) \in \Omega^2$ 

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

237 (3.1) 
$$\boldsymbol{v}(\boldsymbol{x},t,\omega) = \underbrace{\sum_{i=0}^{n} b_i(t,\omega)\boldsymbol{\phi}_i(\boldsymbol{x})}_{\stackrel{\triangle}{=} \boldsymbol{w}^R} + \underbrace{\operatorname{Residual}}_{\stackrel{\triangle}{=} \boldsymbol{v}'} \quad \forall (\boldsymbol{x},t) \in \Omega \times [0,T],$$

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

As typically done while working with ROMs, we aim at specifying the evolution of the 241projected velocity field  $w^R$ . A standard technique for that is the Galerkin projection of 242 the physical PDE – here, the Navier-Stokes equations – onto the reduced basis' functions 243  $\phi_i$ , where the resolved component  $\boldsymbol{w}^R$  is approximated by the solution of these projected 244equations. Mode truncation can create many problems. For moderately turbulent to 245turbulent flows and small dimension n, a closure model to handle the truncated modes 246is unavoidable. With the LU setting - described in section 2 - an elegant stochastic 247248 alternative for this problem can be derived. Accordingly, we will (i) assume that the residual velocity v' is time-uncorrelated and is denoted  $\sigma dB_t/dt$  and (ii) approximate the 249resolved component  $\boldsymbol{w}^R$  to a realization of the solution of the Galerkin projection of the 250251stochastic Navier-Stokes representation (2.1)-(2.2). The former hypothesis is a debatable choice with respect to some ROM's applications whose pertinence and limitations will be 252discussed further in section 4.5. 253

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

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

Moreover,  $\mathcal{P}(\mathbf{H}d\mathbf{B}_t) = (\mathbf{H}d\mathbf{B}_t)$  because of the necessary incompressibility of the Brownian term in the continuity equation (2.2)<sup>2</sup>. Then, the resulting SPDE is projected onto each of the reduced basis' functions:

263 (3.3) 
$$\mathrm{d}b_i = (\boldsymbol{\phi}_i, \mathrm{d}_t \boldsymbol{w}^R) = (\mathrm{d}\mathbb{M}_i^R)(\boldsymbol{b}) \stackrel{\bigtriangleup}{=} \left(\boldsymbol{\phi}_i, \boldsymbol{\mathcal{P}}(\mathrm{d}\mathbb{M})(\boldsymbol{w}^R)\right), \quad 1 \leqslant i \leqslant n,$$

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

265 
$$(\mathrm{d}\mathbb{M}_{i}^{R})(\boldsymbol{b}) = \sum_{p=0}^{n} \underbrace{\left(\boldsymbol{\phi}_{i}, \boldsymbol{L}(\boldsymbol{\phi}_{p})\right)}_{\triangleq l_{pi}} b_{p} \mathrm{d}t + \sum_{p=0}^{n} \underbrace{\left(\boldsymbol{\phi}_{i}, \boldsymbol{\mathcal{P}F}(\boldsymbol{\phi}_{p})\right)}_{\triangleq \check{f}_{pi}} b_{p} \mathrm{d}t + \sum_{p,q=0}^{n} \underbrace{\left(\boldsymbol{\phi}_{i}, \boldsymbol{\mathcal{P}C}(\boldsymbol{\phi}_{p}, \boldsymbol{\phi}_{q})\right)}_{\triangleq c_{pqi}} b_{p} b_{q} \mathrm{d}t$$

266 (3.4) 
$$+\underbrace{(\boldsymbol{\phi}_i, (\boldsymbol{H} \mathrm{d}\boldsymbol{B}_t))}_{\triangleq(\boldsymbol{\theta}_{i\bullet} \mathrm{d}\boldsymbol{B}_t)} + \sum_{p=0}^{\infty} \underbrace{(\boldsymbol{\phi}_i, \boldsymbol{\mathcal{P}}(\boldsymbol{G} \mathrm{d}\boldsymbol{B}_t)(\boldsymbol{\phi}_p))}_{\triangleq(\boldsymbol{\alpha}_{pi\bullet} \mathrm{d}\boldsymbol{B}_t)} b_p, \quad 1 \leqslant i \leqslant n.$$

The terms  $(\boldsymbol{\alpha}_{pi\bullet} d\boldsymbol{B}_t)_{1 \leq p,i \leq n}$  and  $((\boldsymbol{\theta}_{i\bullet} + \boldsymbol{\alpha}_{0i\bullet}) d\boldsymbol{B}_t)_{1 \leq i \leq n}$  correspond to a Gaussian skewsymmetric matrix and a Gaussian vector respectively, both with correlated coefficients. If the functions  $\boldsymbol{\phi}_i$  were spatial Fourier modes associated with small wave-numbers, the ROM (3.3) would represent a (stochastic) Large-Eddy-Simulation-like model expressed in Fourier space and **b** would be the set of Fourier coefficients of the solution. Hereafter, we will solely focus on the POD.

<sup>&</sup>lt;sup>2</sup>which is coherent with the fact that  $\nabla \cdot \boldsymbol{v}' = 0$  from (3.1) because  $\nabla \cdot \boldsymbol{v} = 0$ .

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

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

277 Reduced basis functions  $\phi_i$  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  $(v_{obs} - \overline{v})$  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 (3.6) 
$$C_{ij}^{v} = \left( (\boldsymbol{v}_{\text{obs}} - \overline{\boldsymbol{v}}) \left( \bullet, t_{i} \right), \left( \boldsymbol{v}_{\text{obs}} - \overline{\boldsymbol{v}} \right) \left( \bullet, t_{j} \right) \right), \quad 0 \leq i, j \leq N-1.$$

This method is often referred to as the snapshot method. In the POD framework, the mode  $\phi_0 = \overline{v}$  is set to the time averaged velocity, and the temporal coefficients energies  $\overline{b_i^2}$  are denoted  $\lambda_i$ . Furthermore, if the snapshots describe a divergence-free velocity field  $v_{\text{obs}}$ , the spatial bases  $\phi_i$  are divergence-free as well.

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

292 (4.1) 
$$(\boldsymbol{\alpha}_{\bullet i \bullet} \mathrm{d}\boldsymbol{B}_t)^T \boldsymbol{b} + (\boldsymbol{\theta}_{i \bullet} \mathrm{d}\boldsymbol{B}_t) = \sum_{k=1}^n (\boldsymbol{\alpha}_{ki \bullet} \mathrm{d}\boldsymbol{B}_t) b_k + ((\boldsymbol{\theta}_{i \bullet} + \boldsymbol{\alpha}_{0i \bullet}) \mathrm{d}\boldsymbol{B}_t), \quad 1 \leq i \leq n.$$

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

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

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

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

4.1. The curse of dimensionality. Computing correlations of Gaussian noises  $(\tilde{\alpha} dB_t)$ involves the two-point quadratic cross-variation tensor of the small-scale velocity:

300 (4.4) 
$$\boldsymbol{Q}(\boldsymbol{x},\boldsymbol{y}) = \mathbb{E}\left\{ \left(\boldsymbol{\sigma}(\boldsymbol{x})\mathrm{d}\boldsymbol{B}_{t}\right) \left(\boldsymbol{\sigma}(\boldsymbol{y})\mathrm{d}\boldsymbol{B}_{t}\right)^{T} \right\} / \mathrm{d}t \quad \forall \boldsymbol{x}, \boldsymbol{y} \in \Omega.$$

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

303 (4.5) 
$$\mathbb{E}\left\{\left(\boldsymbol{\theta}_{i\bullet}\mathrm{d}\boldsymbol{B}_{t}\right)\left(\boldsymbol{\theta}_{j\bullet}\mathrm{d}\boldsymbol{B}_{t}\right)\right\}=\mathbb{E}\left\{\left(\boldsymbol{\phi}_{i},\nu\boldsymbol{\nabla}^{2}\boldsymbol{\sigma}\mathrm{d}\boldsymbol{B}_{t}\right)\left(\nu\boldsymbol{\nabla}^{2}\boldsymbol{\sigma}\mathrm{d}\boldsymbol{B}_{t},\boldsymbol{\phi}_{j}\right)\right\},$$

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

Since, by definition,  $\forall x \in \Omega$ , a(x) = Q(x, x), the whole stochastic ROM is closed by specifying the tensor Q. In practice, this tensor is often heterogeneous – i.e.  $\sigma B_t$  is

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

4.2. Variance tensor estimation. Considering the variance tensor a stationary leads to a simple estimator through time averaging as in [67]:

321 (4.7) 
$$\widehat{\boldsymbol{a}} = \Delta t \ \overline{\boldsymbol{v}'_{\text{obs}} \left(\boldsymbol{v}'_{\text{obs}}\right)^T},$$

322 where

323 (4.8) 
$$\boldsymbol{v}_{\rm obs}' = \boldsymbol{v}_{\rm obs} - \boldsymbol{w}_{\rm obs}^R = \boldsymbol{v}_{\rm obs} - \sum_{i=0}^n b_i^{\rm obs} \boldsymbol{\phi}_i,$$

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

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

329 (4.9) 
$$K_{jq}[\boldsymbol{\xi}] \stackrel{\triangle}{=} (\boldsymbol{\phi}_j, -\boldsymbol{\mathcal{P}}\left[(\boldsymbol{\xi} \cdot \boldsymbol{\nabla}) \, \boldsymbol{\phi}_q\right] + \delta_{q0} \, \nu \Delta \boldsymbol{\xi}), \quad 1 \leq j \leq n, \quad 0 \leq q \leq n.$$

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

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

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

333 (4.11) 
$$b_i^{\text{obs}} = (\boldsymbol{\phi}_i, \boldsymbol{v}_{\text{obs}}),$$

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

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

336 (4.14) 
$$\left(\frac{\Delta b_i^{\text{obs}}}{\Delta t}\right)^T = \left(\frac{\Delta b_i^{\text{obs}}}{\Delta t}\right) - \left(\left(\boldsymbol{b}^{\text{obs}}\right)^T (\boldsymbol{l} + \boldsymbol{\breve{f}})_{\bullet i} + \left(\boldsymbol{b}^{\text{obs}}\right)^T \boldsymbol{c}_{\bullet \bullet i} \boldsymbol{b}^{\text{obs}}\right),$$

$$\left(\Delta b_i^{\text{obs}}\right) = b_i^{\text{obs}}(t_k + \Delta t) - b_i^{\text{obs}}(t_k)$$

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

To ensure the noise's covariance matrix to have the desired symmetric non-negative structure, we only keep the symmetric part of the estimated tensor (4.10) and set its possible negative eigenvalues to zero. The part inside the functional  $K_{jq}$  in the estimator (4.10) is inspired from [32], where products of martingale time increments are projected onto orthogonal functions of  $L^2([0,T])$ . For ROMs with a small number of dimensions n, the estimator's computational cost is remarkably low as the observed coefficients of the reduced solution  $\boldsymbol{b}^{\text{obs}}$  were already computed by the method of snapshots (see section 3.2). Hence, the computational cost for  $b_p^{\text{obs}} \left(\frac{\Delta b_p^{\text{obs}}}{\Delta t}\right)''$  is negligible and the part inside  $K_{jq}$  only involves a projection of the residual velocity along the time dimension. Finally, the n(n+1) differential operators  $K_{jq}$  are computed only on n(n+1) functions that do not depend on the time variable.

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

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

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

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

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

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 corresponding eigenvalues' square roots) and  $(\beta^{(k)})_{k}$  are *n* independent one-dimensional Brownian motions. Since  $\tilde{\boldsymbol{\alpha}} d\boldsymbol{B}_{t}$  is a multiplicative noise and the temporal coefficients  $b_{i}$ have various amplitudes  $\sqrt{\lambda_{i}}$ , the covariance matrix  $\boldsymbol{\Sigma}^{\boldsymbol{\alpha}}$  is adequately re-normalized by the amplitudes  $\sqrt{\lambda_{i}}$  before applying the PCA.

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

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

By assuming that the spatially averaged covariance function has a Gaussian form with a standard deviation equals to the correlation time  $\tau$ , a simple expression allows us to 383 compute it. For a given unresolved velocity correlation matrix we write:

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

385 and its associated stationary covariance function

386 (4.19) 
$$\operatorname{Cov}_{s}(t_{p}) = \frac{1}{N-p} \sum_{q=0}^{N-1-p} C_{q,q+p}^{v'}, \quad 0 \leq p \leq N-1.$$

387 We propose the following correlation time estimation:

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

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

390 (4.21) 
$$\frac{\Delta \operatorname{Cov}_s}{\Delta t}(t_p) \stackrel{\triangle}{=} \frac{Cov_s(t_p + \Delta t) - Cov_s(t_p)}{\Delta t}, \quad 0 \le p \le N - 1$$

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

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

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

5. Kinetic energy budget. First, the conservative properties of the LU Navier-Stokes representation are recalled, followed by a proof that by combining Galerkin projections and 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  $\boldsymbol{w}$  and 412 boundary conditions effects, and by applying Itō's lemma, the expression for the kinetic 413 energy budget writes:

414 (5.1) 
$$\frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{1}{2} \|\boldsymbol{w}\|_{\boldsymbol{L}^{2}}^{2}\right) = \underbrace{\left(-\frac{1}{2}\boldsymbol{G}^{*}\left(\circledast\boldsymbol{G}(\boldsymbol{w})\right),\boldsymbol{w}\right)}_{\mathrm{Loss by diffusion}} + \underbrace{\frac{1}{2} \|\boldsymbol{G}(\boldsymbol{w})\|_{\mathrm{HS}}^{2}}_{\mathrm{Form the noise}} = 0 \quad \forall t \in [0,T],$$

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

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

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

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

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

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.

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

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

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

441 (5.5) 
$$\frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{1}{2} \|\boldsymbol{w}^{R}\|_{\boldsymbol{L}^{2}}^{2}\right) = \underbrace{-\frac{1}{2} \left\|\boldsymbol{G}(\boldsymbol{w}^{R})\right\|_{\mathrm{HS}}^{2}}_{\mathrm{Loss by diffusion}} + \underbrace{\frac{1}{2} \left\|\Pi_{\phi}\left[(\boldsymbol{G})(\boldsymbol{w}^{R})\right]\right\|_{\mathrm{HS}}^{2}}_{\mathrm{Energy flux from the noise}} - \underbrace{\frac{1}{2} \left(\boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} \cdot \boldsymbol{a})^{T}, \|\boldsymbol{w}^{R}\|^{2}\right)}_{\mathrm{Advecting velocity correction}},$$
  
442 (5.6) 
$$= -\frac{1}{2} \left(\boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} \cdot \boldsymbol{a})^{T}, \|\boldsymbol{w}^{R}\|^{2}\right) \underbrace{-\frac{1}{2} \left\|\Pi_{\phi}\left[(\boldsymbol{G})(\boldsymbol{w}^{R})\right]\right\|_{\mathrm{HS}}^{2}}_{<0},$$

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.

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

The second term of (5.6) informs about the energy flux due to mode truncation. The ROM's subgrid diffusion extracts energy from some temporal coefficients of the reduced order solution, while the multiplicative noise distributes it to others. These stabilizing and destabilizing effects recreate a large part of the energy fluxes between coefficients of the reduced solution, otherwise lost in deterministic ROMs. Thus, the uncorrelated velocity component drains energy from the coefficients of the reduced solution to give it back to the temporal coefficients of the truncated modes – i.e. modes orthogonal to the reduced space. This energy flux is exactly characterized by the second term of (5.6). But, our stochastic ROM cannot transfer energy from the truncated modes to the reduced solution's coefficients, as the former cannot be specified due to the truncation.

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

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

In Stratonovich form, the ROM also still implicitly includes the diffusion term ensuing from 473 474 the truncature. Notwithstanding, this additional dissipation in (5.6) is not a problem as it enables the setting of an energy dissipation mechanism representative of a direct energy 475 cascade in the truncated modes' coefficients. Hence, for very turbulent flows described by 476few modes, the energy leak appears to be necessary as our main concern is to restore energy 477 fluxes between the coefficients of the reduced order system. Indeed, those energy fluxes 478can be very difficult to model correctly in reduced versions of non-linear systems. As an 479example, [69] observe that a basis encoding 50% of the energy can lead to a ROM missing 480481 more than 98% of energy transfers. These missing energy fluxes create instabilities in some coefficients of the reduced solution (missing negative energy fluxes) while overdamping 482others (missing positive energy fluxes). Restoring the energy fluxes between coefficients of 483 the reduced system is a significant challenge LU models tackle through the combination of 484 multiplicative noise and turbulent diffusion. 485

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

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

The dynamics, and in particular their intrinsic dimensionality, strongly differ between Reynolds 100 and 300. Indeed, as illustrated by figure 1, at Reynolds 100, most of the energy is concentrated in just a few coefficients of the reduced order solution. In contrast, 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  $\boldsymbol{w}^R$  will be compared directly to DNS simulations  $\boldsymbol{v}_{ref}$  on a time 504 interval outside intervals on which the ROM's coefficients and basis functions have been 505 estimated.

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

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

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

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

6.1.2. Stochastic baseline ROM. As a deterministic model, the ROM above can 520 hardly be used for dynamics-error UQ nor ensemble-based data assimilation. As a matter 521of fact, a simple randomization of the initial conditions are known to usually lead to error 522523underestimation (see section 1). So, to keep things simple, we define a second baseline ROM by adding a white noise term to the first baseline ROM. This constitutes a simple 524adhoc randomization technique for a given dynamical system through a Gaussian additive 525forcing. Despite its potential lack of physical relevance, such a strategy is very often 526adopted in data-assimilation applications [17]. 527

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

529 where  $\boldsymbol{\sigma}^{\text{ev}} \in \mathbb{R}^{n \times n}$  is the Cholesky decomposition of the ROM's noise covariance  $\boldsymbol{\Sigma}^{\text{ev}} =$ 530  $\boldsymbol{\sigma}^{\text{ev}} (\boldsymbol{\sigma}^{\text{ev}})^T$  and  $t \mapsto \boldsymbol{W}_t \in \mathbb{R}^n$  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 (6.3) 
$$\widehat{\Sigma_{ij}^{\text{ev}}} = \Delta t \ \overline{\left(\frac{\Delta b_i^{\text{obs}}}{\Delta t}\right)''_{\text{ev}}\left(\frac{\Delta b_j^{\text{obs}}}{\Delta t}\right)''_{\text{ev}}}, \ 1 \leqslant i, j \leqslant n,$$

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

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

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

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 valid. Thus, similarly to section 4.5, an optimal down-sampling time step is estimated with  $\sum_{k=1}^{n} \left(\frac{\Delta b_k^{\text{obs}}}{\Delta t}\right)''_{\text{ev}}(t_i) \left(\frac{\Delta b_k^{\text{obs}}}{\Delta t}\right)''_{\text{ev}}(t_j)$  instead of  $C_{ij}^{v'}$ , before the noise covariance estimation.

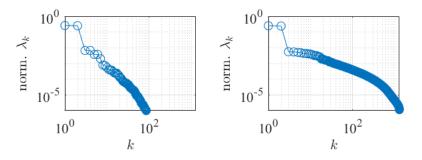


Figure 1: Energies of the reduced solution coefficients normalized by the total solution energy temporal mean  $\|v\|_{L^2}^2$  for the 2D flow at Reynolds 100 (left panel) and the 3D flow at Reynolds 300 (right panel).

**6.2.** 2D wake flow at Reynolds 100. Starting with the simpler of the two test cases, 540800 seconds of DNS simulation data (about 160 pseudo-periods) were generated for a 2D 541wake flow behind a circular cylinder at Re = 100. These data were then split into training 542and test sets, the former (140 pseudo-periods) being utilized for the construction of the 543ROMs, and the latter (20 pseudo-periods), as a reference to which the ROMs will be 544compared. Performance will thus be measured through four different metrics: comparison 545 of temporal coefficients in the time domain, comparison of reconstructed velocity fields in 546the spatial domain, global prediction accuracy as measured by the evolution in time of 547 RMSE, and finally ensemble minimum error. 548

6.2.1. Temporal coefficients forecast. The 2-dimensional LU ROM of the Reynolds-549100 flow is simulated 100 times. In figure 2, the coefficients of the reduced solution  $b_i^{(k)}$ 550 (where k stands for the k-th simulation) are compared to the coefficients of the reference 551 solution  $b_i^{\text{ref}} = (\phi_i, v_{\text{ref}})$  (plotted in black). The ensemble mean (in green) follows almost 552perfectly the reference's phase, and exhibits a slightly damped magnitude. The damping 553 effect can be seen as a consequence of the exchange of energy between the mean and the 554variance (see equation (5.3)). This interplay is also evidenced by the growth of the confi-555dence interval. The realization we have (randomly) singled-out shows a slowly divergent 556behavior. 557

**6.2.2.** Velocity forecasts. Having analyzed the model's forecast capabilities in terms 558 of the ROM's temporal coefficient, we now focus on the analysis of the velocity fields' 559 560 forecast and compare them to the reference – i.e. the projection of full DNS solution onto the POD basis :  $\widetilde{\Pi}_{\phi}[\boldsymbol{v}_{\mathrm{ref}}] \stackrel{\triangle}{=} \Pi_{\phi}[\boldsymbol{v}_{\mathrm{ref}} - \overline{\boldsymbol{v}}] + \overline{\boldsymbol{v}} = \sum_{i=0}^{n} b_{i}^{\mathrm{ref}} \boldsymbol{\phi}_{i}$  (with  $b_{0}^{\mathrm{ref}} = 1$ ). Here, our 561 goal will be to assess qualitatively the potential limitations of the ROM. Through equation 562(3.1), we will compute the velocity fields for the mean, the lowest error realization, and the 563 prediction generated by the eddy viscosity ROM (6.1) of same dimension. At each time 564565 step, we define the lowest-error realization as follows:

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

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

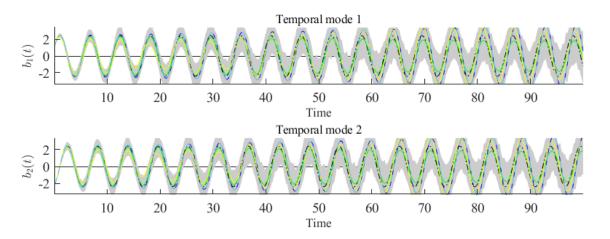


Figure 2: LU POD-ROM forecast for n = 2 coefficients of the reduced solution for a 2D wake flow at Reynolds 100: ensemble mean (green line), one random realization (yellow line), confidence interval (gray shade). Blue lines correspond to deterministic ROMs: baseline eddy-viscosity POD-ROM (6.1) (light-blue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

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

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

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

590 (6.7) RMSE 
$$\stackrel{\triangle}{=} \hat{\mathbb{E}} \left\| \boldsymbol{w}^R - \widetilde{\Pi}_{\phi}[\boldsymbol{v}_{\mathrm{ref}}] \right\|_{\boldsymbol{L}^2}^2 = \left\| \hat{\mathbb{E}} \{ \boldsymbol{w}^R \} - \widetilde{\Pi}_{\phi}[\boldsymbol{v}_{\mathrm{ref}}] \right\|_{\boldsymbol{L}^2}^2 + \int_{\Omega} \widehat{\mathrm{Var}}(\boldsymbol{w}^R).$$

In all the following normalized error plots, the blue line corresponds to the solution 591 computed using a deterministic POD-Galerkin ROMs (with and without eddy viscosity) 592593 and the red one, to the RMSE. The green line represents the ensemble bias, whereas the magenta line is the error incurred by the ensemble's solution closest to the reference (6.6), 594and the gray shade corresponds to  $1.96 \times$  the standard-deviation. These quantities are 595computed for the whole set of generated realizations. The initial condition is common to 596all and the values are normalized by the square root of the solution's energy averaged over 597 the training set :  $\left( \|\overline{\boldsymbol{v}}\|_{\boldsymbol{L}^2}^2 + \sum_{i=1}^n \lambda_i \right)^{1/2}$ . 598

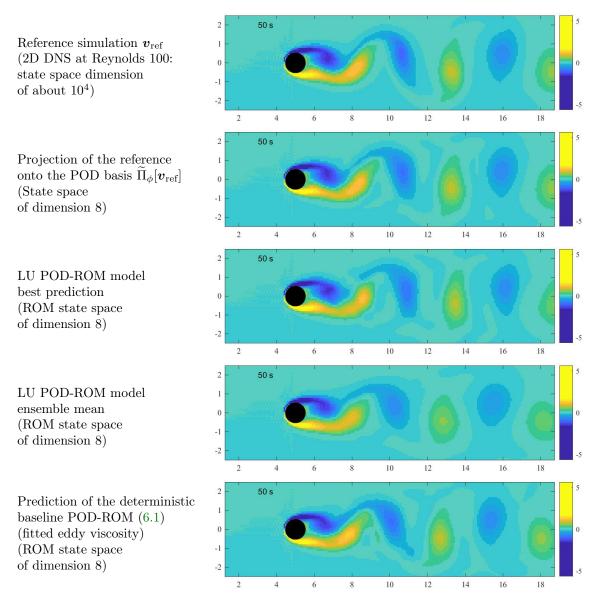


Figure 3: Vorticity fields – 10 vortex shedding cycles after the learning period – from (from top to bottom) the reference simulation  $\boldsymbol{v}_{ref}$  (2D DNS at Reynolds 100: state space dimension of about 10<sup>4</sup>), its projection onto the POD basis  $\Pi_{\phi}[\boldsymbol{v}_{ref}]$ , 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.

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

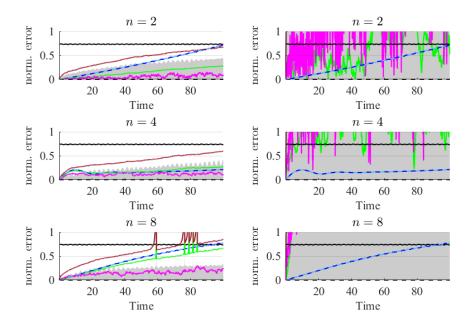


Figure 4: Normalized error for n = 2, 4 and 8 coefficients of the reduced solution of a 2D wake flow at Reynolds 100 – with the projection of the DNS onto the POD basis  $\tilde{\Pi}_{\phi}[\boldsymbol{v}_{ref}]$  as reference : RMSE (brown line), bias (green line), ensemble minimum error (magenta line) and 1.96 × 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.

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

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

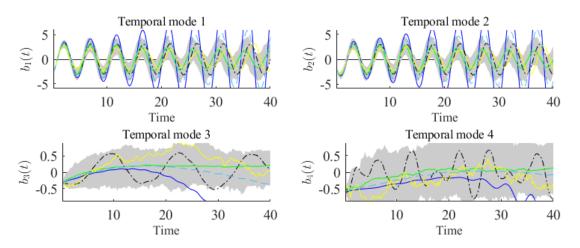


Figure 5: LU POD-ROM forecast for n = 4 coefficients of the reduced solution of a 3D wake flow at Reynolds 300: ensemble mean (green line), one random realization (yellow line), confidence interval (gray shade). Blue lines correspond to deterministic ROMs: baseline eddy-viscosity POD-ROM (6.1) (light-blue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

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

Interestingly enough, in the n = 8 dimension ROM, even when the ensemble variance increases with the temporal coefficient order, coefficients 5, 6, 7 and 8 of the random realization (yellow line) also attempt to follow the right reference amplitude and variability, 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.

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

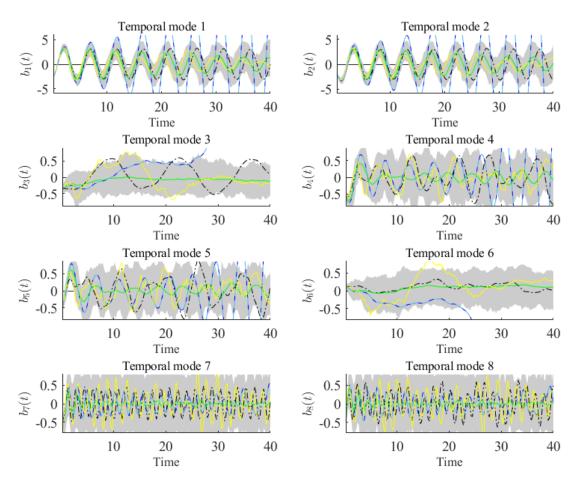


Figure 6: LU POD-ROM forecast for n = 8 coefficients of the reduced solution of a 3D wake flow at Reynolds 300: ensemble mean (green line), one random realization (yellow line), confidence interval (gray shade). Blue lines correspond to deterministic ROMs: baseline eddy-viscosity POD-ROM (6.1) (light-blue 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 curves are plotted and compared to the results obtained with the stochastic eddy viscosity 654model (6.2). The curves in figure 8 evidence the predictive power of our proposed model: it 655 is capable of great stability and accuracy even after 40 seconds while the deterministic and 656 eddy viscosity models prove to be quite unstable by rapidly diverging. These properties are 657 showcased by the bias and mean curves that converge to the zero-temporal-coefficient error 658 curve instead of growing in an unbounded manner, while still having at least one realization 659 with relatively low error that could eventually be identified through data assimilation 660 661 techniques.

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

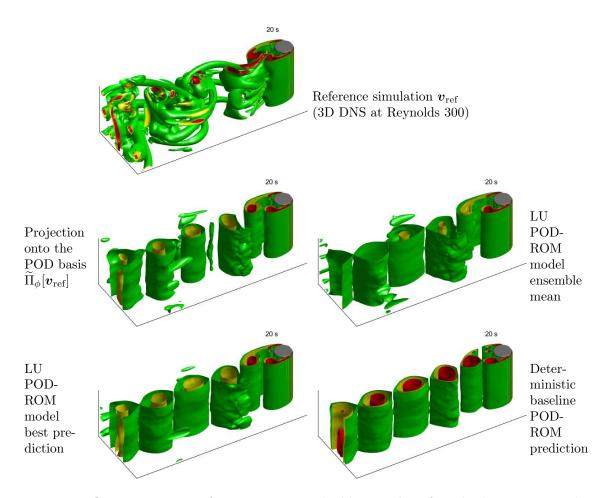


Figure 7: Q-criterion iso-surfaces – 4 vortex shedding cycles after the learning period – from (from left to right and from top to bottom) the reference simulation  $\boldsymbol{v}_{ref}$  (3D DNS at Reynolds 300: state space dimension of about 10<sup>7</sup>), its projection onto the POD basis  $\tilde{\Pi}_{\phi}[\boldsymbol{v}_{ref}]$ , 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.

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

The implementation necessitates additional off-line computations on top of the classical 671 672 POD-Galerkin procedure: estimations of a variance tensor and of the reduced multiplicative noise's covariance matrix. The former, proportional to the point-wise  $d \times d$  covariance 673 674 matrix of POD's residual, is readily computed. The latter can constitute a formidable computational challenge. Moreover, with a fully data-driven method, the risk of over-675 fitting is very high. To circumvent these issues, an intermediate solution is proposed 676 677 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 assumption of the POD residual – measures are taken to enforce them on the model, as 679 part of its constitutive steps. Namely, to force the decorrelation – and in doing so, improve 680 the accuracy of the estimators and the ROM as a whole -a down-sampling of the dataset 681

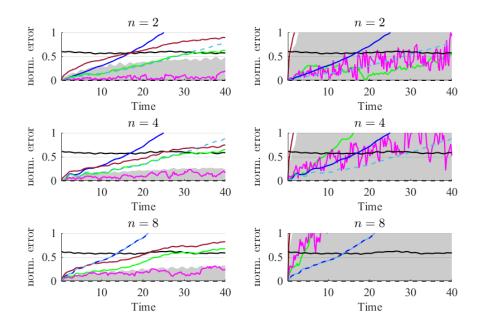


Figure 8: Normalized error for n = 2, 4 and 8 coefficients of the reduced solution of a 3D wake flow at Reynolds 300 – with the projection of the DNS onto the POD basis  $\Pi_{\phi}[\boldsymbol{v}_{ref}]$  as reference : RMSE (red line), bias (green line), ensemble minimum error (magenta line) and 1.96 × 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.  $b_i = 0, \forall i > 0$ .

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

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

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

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

705

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

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

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

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

Finally, relying purely on data can offer the advantage of directly tackling very high Reynolds number configurations. It would require us to filter noisy measurements, and most likely, to rely on simplified (often 2D) data-driven models [1, 13, 29, 78]. From this latter point of view, modeling under location location offers a great flexibility which might be of great interest. As a matter of fact, the LU formalism enables us to derive random dynamics close to the data but still based on stochastic transport principles [3]. The noise parameters can be updated online from incoming data and simulations. A full characterization of the noise dynamics through statistical learning procedures would then probably enable us to devise advanced data-driven models that are able to handle even more complex situations.

Appendix A. Estimation formulas. In this appendix, we consider a full probability space  $(A, \mathcal{F}, P)$ , and a filtration of  $\sigma$ -algebra  $\{\mathcal{F}_t\}_{t\geq 0}$ . For the Hilbert space  $H^2(\Omega)$ , we 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 processes  $\boldsymbol{u} : \mathbb{R}^d \times [0, T] \to \mathbb{R}^d$  such that  $(\boldsymbol{x} \mapsto \boldsymbol{u}(\boldsymbol{x}, t))$  belong to  $H^2(\Omega)$  for every  $t \in [0, T]$ and

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

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

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

766 (A.2) 
$$\left\langle \int_{0}^{t} \mathbf{X} d\mathbf{M}, \mathbf{N} \right\rangle = \int_{0}^{t} \mathbf{X} d\langle \mathbf{M}, \mathbf{N} \rangle$$

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

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

where  $\| \bullet \|$  stands for the Euclidean norm on  $\mathbb{R}^{d \times d}$  and  $|\Omega^2|$  the Lebesgue measure of  $\Omega^2$ . As such,  $((\boldsymbol{x}, t) \mapsto \boldsymbol{\sigma}(\boldsymbol{x})\boldsymbol{B}_t)$  belong to  $\mathcal{H}^2$ . In particular,  $(\boldsymbol{x} \mapsto \boldsymbol{\sigma}(\boldsymbol{x})\boldsymbol{B}_t)$  belong to  $H^2(\Omega)$ 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  $1 \leq i, j \leq d$ . Additionally, we assume that the POD modes  $\boldsymbol{\phi}_i$  belong to  $H^2(\Omega)$  and have bounded gradients.

After defining boundary conditions,  $\mathcal{P}$  and  $\mathbf{K}$  are well defined on  $H^1(\Omega)$  and  $H^2(\Omega)$ 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 then, for every  $\boldsymbol{\xi} \in H^2(\Omega)$ , by Cauchy-Schwarz and triangular inequalities:

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

779 where  $\|\nabla \phi_i^T\|_{\infty} = \sup_{\Omega} \|\nabla \phi_i^T\| < \infty$ . The bound above gives the continuity of K on 780  $H^2(\Omega)$ . We also assume that the observed coefficients of the reduced solution  $b_i^{\text{obs}} =$ 781  $(\phi_i, v_{\text{obs}})$  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 (A.5) 
$$\int_{0}^{T} b_{p} \mathrm{d} \langle b_{i}, \int_{0}^{t} \left( \tilde{\boldsymbol{\alpha}}_{qj \bullet} \mathrm{d} \boldsymbol{B}_{s} \right) \rangle = \int_{0}^{T} \sum_{k=0}^{n} b_{p} \mathrm{d} \langle \int_{0}^{t} \left( \tilde{\boldsymbol{\alpha}}_{ki \bullet} \mathrm{d} \boldsymbol{B}_{s} \right) b_{k}, \int_{0}^{t} \tilde{\boldsymbol{\alpha}}_{qj \bullet} \mathrm{d} \boldsymbol{B}_{s} \rangle,$$
$$-\frac{n}{2} \left( \int_{0}^{T} \left( \int_{0}^$$

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

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

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

788 (A.8) 
$$\tilde{\boldsymbol{\alpha}}_{qj\bullet} \mathrm{d}\boldsymbol{B}_s = \left(\boldsymbol{\phi}_j, -\boldsymbol{\mathcal{P}}\left[\left(\boldsymbol{\sigma}\mathrm{d}\boldsymbol{B}_s \cdot \boldsymbol{\nabla}\right)\boldsymbol{\phi}_q\right] + \delta_{q0} \ \nu \Delta \boldsymbol{\sigma}\mathrm{d}\boldsymbol{B}_s\right) = \mathrm{d}\left(K_{jq}\left[\boldsymbol{\sigma}\boldsymbol{B}\right]\right).$$

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

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

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

794 (A.11) 
$$= \frac{1}{\lambda_p T} \mathbb{P}_{\Delta t \to 0} \sum_{t_k=0}^{T} b_p(t_k) (\Delta b_i)(t_k) K_{jq} \left[ \boldsymbol{\sigma} \Delta \boldsymbol{B}_{t_k} \right],$$

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

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

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

800 where

801 (A.14) 
$$\Delta b'_{i} = \Delta b_{i} - \left( \boldsymbol{b}^{T} (\boldsymbol{l} + \boldsymbol{\breve{f}})_{\bullet i} + \boldsymbol{b}^{T} \boldsymbol{c}_{\bullet \bullet i} \, \boldsymbol{b} \right) \Delta t.$$

802

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

807

#### Appendix B. Energy dissipation.

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

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

817 (B.1) 
$$d_t \boldsymbol{w}^R = \sum_{\substack{i=1\\n}}^n \left( \boldsymbol{\phi}_i, \boldsymbol{\mathcal{P}}(d\mathbb{M})(\boldsymbol{w}^R) \right) \boldsymbol{\phi}_i = \sum_{\substack{i=1\\n}}^n \left( \boldsymbol{\mathcal{P}} \boldsymbol{\phi}_i, (d\mathbb{M})(\boldsymbol{w}^R) \right) \boldsymbol{\phi}_i,$$

818 (B.2) 
$$= \sum_{i=1}^{n} \left( \phi_i, (\mathrm{d}\mathbb{M})(\boldsymbol{w}^R) \right) \ \phi_i = \Pi_{\phi} \left[ \left( \boldsymbol{C}(\boldsymbol{w}^R, \boldsymbol{w}^R) + \boldsymbol{F}(\boldsymbol{w}^R) \right) \mathrm{d}t + (\boldsymbol{G}\mathrm{d}\boldsymbol{B}_t)(\boldsymbol{w}^R) \right].$$

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

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

To remove the (orthogonal) projection operator  $\Pi_{\phi}$  from the first term, we exploit its symmetry, and afterwards, the fact that  $\boldsymbol{w}^{R}$  is already in the reduced subspace:

823 (B.4) 
$$\int_{\Omega} d_{t}(\boldsymbol{w}^{R})^{T} \boldsymbol{w}^{R} = \left( \Pi_{\phi} \left[ (d\mathbb{M})(\boldsymbol{w}^{R}) \right], \boldsymbol{w}^{R} \right),$$
  
824 (B.5) 
$$= \left( (d\mathbb{M})(\boldsymbol{w}^{R}), \Pi_{\phi} \left[ \boldsymbol{w}^{R} \right] \right),$$
  
825 (B.6) 
$$= \left( (d\mathbb{M})(\boldsymbol{w}^{R}), \boldsymbol{w}^{R} \right),$$
  
826 (B.7) 
$$= \left( ((\boldsymbol{F}_{\text{dif}} + \boldsymbol{F}_{\text{adv}})(\boldsymbol{w}^{R}) + \boldsymbol{C}(\boldsymbol{w}^{R}, \boldsymbol{w}^{R})) dt + (\boldsymbol{G} d\boldsymbol{B}_{t})(\boldsymbol{w}^{R}), \boldsymbol{w}^{R} \right)$$
  
827 
$$= \underbrace{\left( -\frac{1}{2}\boldsymbol{G}^{*} \left( \circledast \boldsymbol{G}(\boldsymbol{w}^{R}) \right), \boldsymbol{w}^{R} \right) dt}_{\text{from} \left( \boldsymbol{F}_{\text{dif}}(\boldsymbol{w}^{R}), \boldsymbol{w}^{R} \right) \text{ using } (2.12)} \underbrace{\left( \underbrace{1}_{2}((\boldsymbol{\nabla} \cdot \boldsymbol{a})\boldsymbol{\nabla})\boldsymbol{w}^{R}, \boldsymbol{w}^{R} \right)}_{\text{from} \left( \boldsymbol{F}_{\text{adv}}(\boldsymbol{w}^{R}), \boldsymbol{w}^{R} \right)}$$

828 (B.8) 
$$+ \underbrace{\left(\boldsymbol{C}(\boldsymbol{w}^{R}, \boldsymbol{w}^{R}) \mathrm{d}t + (\boldsymbol{G} \mathrm{d}\boldsymbol{B}_{t})(\boldsymbol{w}^{R}), \boldsymbol{w}^{R}\right)}_{=0 \text{ by skew-symmetry of } \boldsymbol{\xi} \mapsto \boldsymbol{C}(\boldsymbol{w}^{R}, \boldsymbol{\xi}) \text{ and } \boldsymbol{G} \mathrm{d}\boldsymbol{B}_{t}},$$

829 (B.9) 
$$= \frac{1}{2} \left\| \boldsymbol{G}(\boldsymbol{w}^R) \right\|_{\mathrm{HS}}^2 - \frac{1}{2} \left( \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} \cdot \boldsymbol{a})^T, \| \boldsymbol{w}^R \|^2 \right)$$

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

832 (B.10) 
$$\int_{\Omega} \frac{1}{2} \mathrm{d}_t \langle (\boldsymbol{w}^R)^T, \boldsymbol{w}^R \rangle = \frac{1}{2} \left\| \Pi_{\phi} \left[ (\boldsymbol{G}) (\boldsymbol{w}^R) \right] \right\|_{\mathrm{HS}}^2 \mathrm{d}t,$$
  
833 (B.11) 
$$= \sum_{p,q=0}^n \left( \frac{1}{2} \int_{\Omega} \Pi_{\phi} \left[ \boldsymbol{G}(\boldsymbol{\phi}_p) \right] \circledast \Pi_{\phi} \left[ \boldsymbol{G}(\boldsymbol{\phi}_q) \right] \right) b_p b_q \mathrm{d}t.$$

From the definition of the projection operator  $\Pi_{\phi}$  and using the extended notation  $(\boldsymbol{\eta} \circledast \boldsymbol{\theta}) \stackrel{\triangle}{=} \int_{\Omega} \boldsymbol{\breve{\eta}}(\boldsymbol{z}) \boldsymbol{\breve{\theta}}^{T}(\boldsymbol{z}) d\boldsymbol{z}$ , we can express the above quadratic operator with the noise statistics as follows:

837 (B.12) 
$$\int_{\Omega} \Pi_{\phi} \left[ \boldsymbol{G}(\boldsymbol{\phi}_{p}) \right] \circledast \Pi_{\phi} \left[ \boldsymbol{G}(\boldsymbol{\phi}_{q}) \right] = \sum_{i=1}^{n} \left( \boldsymbol{\phi}_{i}, \boldsymbol{G}(\boldsymbol{\phi}_{p}) \right) \circledast \left( \boldsymbol{\phi}_{i}, \boldsymbol{G}(\boldsymbol{\phi}_{q}) \right) = \sum_{i=1}^{n} \Sigma_{pi,qi}^{\boldsymbol{\alpha}}.$$

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

839 (B.13) 
$$\frac{d}{dt} \left( \frac{1}{2} \| \boldsymbol{w}^R \|_{\boldsymbol{L}^2}^2 \right) = \frac{1}{2} \left\| \boldsymbol{G}(\boldsymbol{w}^R) \right\|_{\mathrm{HS}}^2 - \frac{1}{2} \left( \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} \cdot \boldsymbol{a})^T, \| \boldsymbol{w}^R \|^2 \right) - \frac{1}{2} \left\| \Pi_{\phi} \left[ \boldsymbol{G}(\boldsymbol{w}^R) \right] \right\|_{\mathrm{HS}}^2$$
  
840 (B.14)  $= -\frac{1}{2} \left\| \Pi^{\perp} \left[ \boldsymbol{G}(\boldsymbol{w}^R) \right] \right\|_{\mathrm{HS}}^2 - \frac{1}{2} \left( \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} \cdot \boldsymbol{a})^T, \| \boldsymbol{w}^R \|^2 \right)$ 

840 (B.14) 
$$= -\frac{1}{2} \left\| \Pi_{\phi}^{\perp} \left[ \mathbf{G}(\mathbf{w}^{*}) \right] \right\|_{\mathrm{HS}} - \frac{1}{2} \left[ \mathbf{\nabla} \cdot \left( \mathbf{\nabla} \cdot \mathbf{a} \right)^{2}, \|\mathbf{w}^{*}\|^{2} \right],$$
841 where  $\Pi^{\perp} = \Pi_{\mathbf{v}} - \Pi_{\mathbf{v}}$  is the projector into the orthogonal complement of the r

841 where  $\Pi_{\phi}^{\perp} = \mathbb{I}_d - \Pi_{\phi}$  is the projector into the orthogonal complement of the reduced 842 subspace.

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