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## Stochastic modelling of turbulent flows for numerical simulations

Carlo Cintolesi · Etienne Mémin

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<sup>1</sup> Abstract The stochastic model proposed by Mémin [24] for turbulent flow

<sup>2</sup> simulations is analysed, both theoretically and numerically. It is shown to be a

<sup>3</sup> generalisation of the classical large-eddy simulation approach, and to describe

a richer physics. The model does not lead to the eddy-viscosity assumption
 and can be reduced to Smagorisky model under restrictive hypotheses; hence,

and can be reduced to Smagorisky model under restrictive hypotheses; hence,
 it can be considered as a generalisation of classical models. Simulations of a

<sup>7</sup> turbulent channel flow at  $Re_{\tau} = 590$  shows the presence of physical phenom-

<sup>8</sup> ena usually not reproduced; namely a weak turbophoresis and of a turbulent

<sup>9</sup> compressibility linked to streaks structures. The turbulent kinetic energy bud-

<sup>10</sup> get suggests that the model is more effective in dissipating energy near the

<sup>11</sup> wall. For the sake of completeness, alternative and detailed derivation of the

<sup>12</sup> stochastic model is reported in detail in the appendix.

Keywords Stochastic models · Turbulence modelling · Numerical simula tions · OpenFOAM.

#### 15 1 Introduction

16 The reliable numerical simulation of turbulent flows is still nowadays a chal-

<sup>17</sup> lenging issue, both in terms of mathematical modelling and of computational

<sup>18</sup> cost required. In the last decades, different techniques were developed to tackle

<sup>19</sup> this problem, the most fruitful for practical applications being the Reynolds-

<sup>20</sup> averaged simulation and the Large-Eddy Simulation (LES) methodologies. De-

<sup>21</sup> spite the continuous improvements with increasingF accuracy of the models,

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such methodologies are developed within a deterministic framework. Hence, they cannot completely represent the random nature exhibited by turbulent flows, that eventually requires the use of stochastic calculus. In the field of geophysical flows, probabilistic models are used to correct the effects of the coarse spatial discretisation. Similarly, the stochastic variables can be employed to account for the unresolved processes in the numerical reproduction of engineering and environmental flows.

The literature proposes different approaches on this topic. The stochastic 29 Langevin equation is derived assuming that a fluid-particle velocity is per-30 turbed by a Brownian motion, which is found to well described the dynamics 31 of turbulent flows; see Pope [35]. This equation was used in the framework 32 of Probability Density Function (POF) methods to reproduce homogeneous 33 isotropic turbulence, but also inhomogeneous and anisotropic turbulence by 34 Pope [36] and by Durbin & Speziale [8], respectively. Orszag [33] and Leslie [22] 35 introduced the Eddy-Damped Quasi-Normal Markovian (EDQNM) models; 36 see the overview by Lesieur [21]. The large-scale equations were closed in 37 spectral space through a Gaussian closure. They were particularly suitable 38 to study strong non-linearity in the small-scale turbulence. In the same frame-39 work, Chasnov [5] develops a forced-dissipative model, where the large-eddy 40 Navier-Stokes equations were corrected by a stochastic force terms. This was 41 a Gaussian forcing uncorrelated in time, homogeneous and isotropic in space. 42 Kraichnan [16] exploits a different approach: the momentum equations are 43 replaced by a set of equations with same mathematical properties, which are 44 closed using a Gaussian stochastic model. This theory leads to valuable results 45 in terms of mathematical properties (existence, singularities) and physical ef-46 fects (turbulent diffusion, backscatter) analyses. Frederiksen [11] shows that 47 the same strategy can be used for a stochastic modelling of barotropic flows 48 or in quasi-geostrophic approximation, that includes the interaction between 49 topography and small-scale eddies. The randomness effects can be also explic-50 itly introduced by means of *ad hoc* stochastic terms. Investigating the plane 51 shear mixing layer, Leith [20] improves the accuracy of LES with Smagorinsky 52 model by introducing an explicit stochastic terms. On the theoretical side, 53 Flandoli [9] studied fluid dynamic systems corrected with a random white 54 noise force to reproduce the complex phenomena related to turbulence. 55 These attempts have some limitations: the POF and EDQNM models re-56 quired to work in the spectral space instead of the physical one; there is a 57

certain degree of arbitrariness when explicit random terms are introduced
(e.g. the random forcing should be multiplicative or additive); and overall the
models can be hardly generalised for practical applications.

The methodology here presented aims to overcome these shortcomings. It develops from a different starting point: the fluid-particle trajectory in the Lagrangian framework is assumed to be a random process. It is expressed by a semimartingale, where the finite-variation part represents the smooth macroscopic velocity, while the martingale models the perturbations due to the turbulent motion. Consistently, an expression of the velocity is found and stochastic calculus is used to derived the stochastic equations of motions. In

such a procedure, the use of the Itō-Wentzell formula is crucial to compute the 68 time derivative, see Kunita [18]. A first work in this direction was that one of 69 Brzeźniak [2], subsequently extended by Mikulevicius and Rozovskii [27] and 70 Flandoli [10]. Globally, these works focused on the mathematical properties of 71 the stochastic equations. The work of Mémin [24] follows a similar approach 72 and developed the so called model under Location Uncertainty (LU), which 73 is oriented to practical application in computational fluid dynamics. Recently, 74 Holm [13] derived a similar set of equations using Lagrangian mechanics, which 75 leads to additional terms, while Neves et al. [29] studied theoretically a simi-76 lar system of equations. The LU model was applied to different applications: 77 Resseguier et al. [37, 38, 39] used it for geophysical flows simulations, where 78 it exhibits a high accuracy in reproducing extreme events and provided new 79 analysis tools. Chapron et al. [4] investigated the Lorentz-63 case and found 80 that LU is able to explore the region of the deterministic attractor faster than 81 the classical models. Resseguier *et al.* [40] employed it in conjunction with the 82 proper orthogonal decomposition technique for the numerical simulation of a 83 flow past a circular cylinder at Re = 3900. 84 Although this is a promising methodology, the inherent mathematical com-85

plexity of stochastic partial differential equations poses some difficulties: the 86 resolution of stochastic partial equations is not straightforward and can con-87 siderably increase the simulation time. For these reasons, Mémin [24] also 88 introduces a simplified model, where the resolution of stochastic equations is 89 avoided by modelling the effects of the random velocity term by physical as-90 sumption. This give rise to the so called *pseudo-stochastic simulation* (PSS) 91 methodology: the flow dynamics is described by classical partial differential 92 equations, which includes additional terms provided by the stochastic mod-93 eling. The PSS was adopted by Harouna and Mémin [12] to investigate the 94 Green-Taylor vortex flow applying several models for the stochastic contribu-95 tion. Chandramouli et al. [3] employed it to simulate the transitional wake 96 flow with coarse mesh resolution, proving that it generates a more accurate 97 outcomes with respect to classical LES. 98

Notwithstanding the above mentioned studies, a pointwise analysis of the 99 pseudo-stochastic model is lacking. The aims of the present work is to study 100 in details the characteristics of the LU and the PSS model, both theoretically 101 and numerically, establishing a parallelism with the classical LES methodol-102 ogy. First, a theoretical analysis of the PSS equations is reported; second, a 103 simplified closure model is adopted to perform numerical simulations on the 104 plane channel flow at  $Re_{\tau} = 590$ . The simulation outcomes are discussed in 105 light of the previous theoretical analysis and the peculiarity of the PSS are 106 highlighted. The main novelty of this work is to propose a detailed and sys-107 tematic comparison between PSS and LES approach, pointing out the physical 108 meaning of the extra term arising from the stochastic derivations (supported 109 by simulations). Moreover, after few years from its first formulation, an alter-110 native mathematically derivation of the LU and PSS model is proposed in the 111 appendix. Efforts have been made to simplify and give a linear structure to 112

<sup>113</sup> the procedure, highlighting the key hypotheses.

The paper is organized as follows: section 2 presents the pseudo-stochastic model and the relative turbulent kinetic budget; section 3 reports a physical interpretation of the model and make a comparison with the LES methodology; section 4 describe the closure model for PSS; section 5 discusses the numerical simulation results; section 6 gives some final remarks. In appendix A an alternative and detailed derivation of the stochastic model for turbulent flows is presented.

#### 121 2 Pseudo-Stochastic Model

In this section, the stochastic formalism and the pseudo-stochastic equationsare reported.

#### 124 2.1 Stochastic formalism

The particle trajectory in a turbulent regime is not completely known because it is subject to some random (turbulent) effects. Consequently, the fluidparticle displacement is described by the stochastic differential equations of the type:

$$dX_{t}^{i}(x_{0}) = w_{i}(X_{t}, t)dt + d\eta_{t}^{i}(X_{t}),$$
(1)

where the index i = 1, 2, 3 indicates respectively the x, y, z-component in space 130 (they are placed at top or bottom indifferently);  $X_t^i(x_0)$  is the trajectory fol-131 lowed by a fluid-particle initially located in  $x_0$ ;  $w_i$  is a differentiable function of 132 bounded variation (i.e. equivalent to a deterministic function) that corresponds 133 to the resolved flow velocity;  $\eta_t^i = \int_0^t d\eta_t^i$  is a martingale that accounts for the 134 stochastic contributions to the motion. The Einstein summation convention 135 over repeated indexes is adopted. The stochastic contribution is constructed 136 as a combination of a cylindrical Wiener processes  $B_t^k(x)$  not differentiable in 137 time, and a differentiable diffusion tensor  $\sigma_{ik}$  which acts as an integral kernel: 138 139

$$d\eta_t^i(x) = \int_{\Omega} \sigma_{ik}(x, y, t) dB_t^k(y) \, dy.$$
<sup>(2)</sup>

<sup>141</sup> Notice that the stochastic processes  $\eta_t^i$  are uncorrelated in time and correlated <sup>142</sup> in space by means of the diffusion tensor.

The expression of the velocity field  $U_i$  in Eulerian coordinate x is derived from equation (1); it reads:

$$U_i(x,t) = w_i(x,t) + \dot{\eta}_t^i(x), \qquad (3)$$

where the second term on the right-hand side expresses the stochastic velocity defined by formula (22). From a physical point of view,  $w_i$  is the velocity expected value and  $\dot{\eta}_i^i(x)$  represents a noise: a generalised stochastic process that has to be defined in the space of temperate distribution, see Øksendal [31].

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The quadratic variation of the diffusion tensor is a quantity of particular interest; it represents the time-variation of the spatial variance of the stochastic increments along time. It is named *variance tensor* and is defined as:

 $a_{ij}(x,t) = \int_{\Omega} \sigma_{ik}(x,y,t) \sigma_{jk}(x,y,t) \, dy.$ (4)

As a function, it is assumed to have all the regularity (differentiable and integrable in time and space) required by computation; as a tensor, it is a pointwise symmetric and semi-positive definite matrix.

#### 157 2.2 Pseudo-stochastic equations of motion

The stochastic fluid dynamics equations for a Newtonian incompressible fluid 158 are derived in appendix A. The final system (63) is composed by one set of 159 stochastic equations and one of pure deterministic ones. The former allows 160 to find an expression for the variance tensor  $a_{ij}$ , which is required for the 161 resolution of the latter. Together, they provide a close system of equations 162 that composes the LU model. Let us not that full stochastic model can be 163 obtained by relaxing the assumption of bounded variation for the resolved 164 velocity (see [37]). 165

In order to simplify the model by avoiding the resolution of stochastic partial differential equations, the variance tensor  $a_{ij}$  is not computed but modelled through physical assumptions. This choice gives rise to a hybrid model where the stochastic contribution on the governing equations is modelled by a deterministic function, and, overall, no stochastic equations have to be resolved. Such model leads to pseudo-stochastic simulation approach. The PSS momentum and continuity equations for incompressible flows reads, respectively:

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$$\begin{cases} \frac{\partial w_i}{\partial t} + w_j^* \frac{\partial w_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 w_i}{\partial x_j \partial x_j} + \frac{1}{2} \frac{\partial}{\partial x_j} \left( a_{jk} \frac{\partial w_i}{\partial x_k} \right) \\ \frac{\partial w_i^*}{\partial x_i} = 0. \end{cases}$$
(5)

where  $\nu$  is the molecular viscosity, the modified pressure  $p = p_h + \frac{\nu}{3} \frac{\partial w_\ell}{\partial x_\ell}$  is the sum of the hydrostatic pressure and the divergence of the velocity field (which is not solenoidal), and the effective advection velocity  $w_i^*$  reads:

$$w_i^* = w_i - \frac{1}{2} \frac{\partial}{\partial x_k} a_{ik}.$$
 (6)

The terms depending on  $a_{ij}$  account for the effects of the Stochastic Unresolved Scales (SUS) of motion, since the variance tensor is a measure of the intensity and the anisotropy of turbulent random velocities.

Notice that system (5) reduces to the classical Navier-Stokes equations when the  $a_{ij}$  is the zero matrix, i.e. when the stochastic contributions disappear.

#### 184 2.3 Resolved kinetic energy budget

The turbulent kinetic energy (TKE) budget of the resolved scales of motion is presented. The resolved velocity is decomposed in a mean and a fluctuating

u

187 part, respectively:

$$w_i = W_i + w'_i,\tag{7}$$

where the capitol letter indicates the averaged field,  $W_i = \langle w_i \rangle$ . Variance tensor and pressure are decomposed in a similar way:  $a_{ij} = A_{ij} + a'_{ij}$  and p = P + p'. The (resolved) turbulent kinetic energy  $\kappa = w'_i w'_i/2$  budget reads:

$$\frac{\partial\langle\kappa\rangle}{\partial t} + \underbrace{\left(W_{j} - \frac{\partial}{\partial x_{k}}\frac{A_{jk}}{2}\right)\frac{\partial\langle\kappa\rangle}{\partial x_{j}} + \langle\left(w_{j}' - \frac{\partial}{\partial x_{k}}\frac{a_{jk}'}{2}\right)\frac{\partial\kappa}{\partial x_{j}}\rangle}_{advection} = \underbrace{\frac{\partial}{\partial x_{j}}\left[-\langle p'w_{j}'\rangle + \left(\nu\delta_{jk} + \frac{A_{jk}}{2}\right)\frac{\partial\langle\kappa\rangle}{\partial x_{j}} + \langle\frac{a_{jk}'}{2}\frac{\partial\kappa}{\partial x_{j}}\rangle + \langle\frac{a_{jk}'w_{i}'}{2}\rangle\frac{\partial W_{i}}{\partial x_{k}}\right]}_{transport} + \underbrace{\langle\frac{p'}{2}\frac{\partial^{2}a_{jk}'}{\partial x_{j}\partial x_{k}}\rangle}_{turb.\ compress.} - \underbrace{\left(\nu\delta_{jk} + \frac{A_{jk}}{2}\right)\langle\frac{\partial w_{i}'}{\partial x_{j}}\frac{\partial w_{i}'}{\partial x_{k}}\rangle - \langle\frac{a_{jk}'}{2}\frac{\partial w_{i}'}{\partial x_{j}}\frac{\partial w_{i}'}{\partial x_{k}}\rangle}_{dissipation} - \underbrace{\langle\left(w_{j}' - \frac{\partial}{\partial x_{k}}\frac{a_{jk}'}{2}\right)w_{i}'\rangle\frac{\partial W_{i}}{\partial x_{j}}}_{production} - \underbrace{\langle\frac{a_{jk}'}{2}\frac{\partial w_{i}'}{\partial x_{k}}\frac{\partial W_{i}}{\partial x_{j}}}_{loss\ to\ SUS} \tag{8}$$

The TKE terms are interpreted in light of the classical budget analysis, e.g.
see Kundu and Cohen [17]. On the left-hand side, the second and third terms
represent the TKE advection by mean and SUS effective advection velocity.
On the right-hand side:

- first four terms: transport by pressure, molecular viscosity and turbulent
 stresses;

<sup>195</sup> – fifth term: turbulent compression/expansion due to SUS;

<sup>196</sup> - sixth and seventh terms: dissipation by molecular viscosity (it can be <sup>197</sup> proven that  $A_{ij}$  is positive defined), resolved turbulence and SUS motions;

- eight term: shear production, this term appears in the mean kinetic budget
 (not shown here) with opposite sign;

- last term: loss due to SUS also present in the mean kinetic energy budget.

The pseudo-stochastic TKE budget reduces to the classical one if the stochastic contribution is negligible  $a_{ij} \simeq 0$ . It is worth to notice that the production term includes the contribution of the fluctuations of turbulent advection velocity, while the variance tensor plays a role of a turbulent viscosity dissipation tensor.

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#### <sup>205</sup> 3 Analysis of pseudo-stochastic model

The expression of fluid-particle displacement (1) states that a particle trajectory is driven by two actors: a differentiable drift velocity and a Brownian process highly fluctuating in time. In the framework of PSS, the drift velocity  $w_i$  that can be interpreted as the resolved velocity field, while the random field assembles the residual motion that are fast oscillating stochastic components, possibly anisotropic and non-homogeneous in space.

#### 212 3.1 Physical interpretation

Recalling the decomposition of the velocity gradient in symmetric and antisymmetric parts, respectively called the strain-rate tensor and the rotation-rate tensor:

$$\frac{\partial w_i}{\partial x_j} = \frac{1}{2} \left( \frac{\partial w_i}{\partial x_j} + \frac{\partial w_j}{\partial x_i} \right) + \frac{1}{2} \left( \frac{\partial w_i}{\partial x_j} - \frac{\partial w_j}{\partial x_i} \right) = S_{ij} + \Omega_{ij}, \tag{9}$$

the pseudo-stochastic Navier-Stokes equation (5) and continuity equation (6) are rearranged as, respectively:

$$\frac{\partial w_i}{\partial t} + \underbrace{\left(w_j - \frac{1}{2}\frac{\partial a_{jk}}{\partial x_k}\right)}_{effective \ advection} \underbrace{\frac{\partial w_i}{\partial x_j} = -\frac{\partial}{\partial x_i} \underbrace{\left(p_h + \frac{\nu}{3}\frac{\partial^2 a_{sk}}{\partial x_k \partial x_s}\right)}_{modified \ pressure} + \underbrace{\frac{1}{2}\frac{\partial}{\partial x_s}\left(a_{sk}S_{ki}\right) - \frac{1}{2}\frac{\partial}{\partial x_s}\left(a_{sk}\Omega_{ki}\right)}_{diffusion \ due \ to \ SUS} + (10)$$

217 and

$$\frac{\partial w_i}{\partial x_i} = \underbrace{\frac{1}{2} \frac{\partial^2 a_{jk}}{\partial x_j \partial x_k}}_{turb.\ compr.}$$
(11)

The terms that depend on variance tensor account for the influence of the SUS on the resolved scales. A physical interpretation of such terms is proposed:

Effective advection: the advection velocity is corrected by an inhomogeneous turbulence contribution. It corresponds to a velocity induced by the unresolved turbulent motions, that can be linked to the *turbophoresis* phenomenon detectable in geophysical flows; i.e. the tendency of fluid-particle to migrate in the direction of less energetic turbulence (see also [37]).

Modified pressure: the non-solenoidal velocity field leads to the presence of an isotropic turbulent factor, that has the dimension of a pressure:  $p_t = \frac{\nu}{3} \frac{\partial^2 a_{sk}}{\partial x_k \partial x_s}$ . This term does not contribute to the flow and it is included in the pressure gradient in the same manner as the isotropic residual stress in the Smagorinsky model, see [35]. Diffusion due to SUS: they account for the turbulent diffusion; the variance tensor plays the role of a diffusion tensor similar to a generalised
eddy-viscosity matrix. Both the deformation rate and rotation-rate contribute to diffusion, unlike to the classical eddy-viscosity model in which
fluid rotation-rate is assumed to be irrelevant in turbulent modelling (see also following section 3.2).

Turbulent compressibility: the continuity equation (11) suggests that the
 flow is turbulent-compressible; i.e. the unresolved turbulence induces a local
 fluid compression or expansion.

The variance tensor is the key parameter of the pseudo-stochastic model. It 240 has the physical dimension of a dynamic viscosity  $[m^2/s]$  and carries informa-241 tion on the intensity and the anisotropy of the SUS. As already mentioned, 242  $a_{ij}$  can be interpreted as a generalised eddy-viscosity parameter. Implicitly, 243 this leads to the hypothesis that the SUS influences the resolved flow as an 244 alteration of fluid viscosity, that is an empirical consideration largely accepted. 245 The divergence of the variance tensor is hereafter named *turbulent advection* 246 velocity: 247

$$u_{\mathrm{TA},i} = -\frac{1}{2} \frac{\partial a_{ij}}{\partial x_i},\tag{12}$$

while the divergence of the turbulent advection velocity measured the *turbulent compressibility*:

$$\Phi_{\rm TC} = \frac{1}{2} \frac{\partial^2 a_{ij}}{\partial x_i \partial x_j},\tag{13}$$

and it is directly proportional to the isotropic turbulent factor  $p_t$  appearing in the modified pressure. The numerical simulations reported later allow to gain additional insights regarding these two quantities, we refer to section 5.3 for the numerical analysis.

#### <sup>256</sup> 3.2 Comparison with LES eddy-viscosity models

The LES methodology consists in applying a spatial filter to velocity field, and then directly resolve the filtered velocity and model the sub-filter velocities. See Sagaut [42] and Piomelli [34] for an extended introduction on this subject. Practically, the computational grid acts as an implicit spatial filter on the governing equations, which generates an extra term  $\tau_{ij}$  in the classical Navier-Stokes equations:

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$$\begin{cases} \frac{\partial \overline{u}_i}{\partial t} + \overline{u}_j \frac{\partial \overline{u}_i}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_i} + \nu \frac{\partial^2 \overline{u}_i}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j}, \\ \frac{\partial \overline{u}_i}{\partial x_i} = 0, \end{cases}$$
(14)

where the sub-grid scale (SGS) tensor is 
$$\tau_{ij} = \overline{u_i u_j} - \overline{u}_i \overline{u}_j$$
, and the straight  
over-bar denotes the spatial filter associated to the local cell width, com-  
puted as  $\overline{\Delta} = (\Delta x \Delta y \Delta z)^{1/3}$ . Adopting the eddy-viscosity assumption, the

<sup>267</sup> anisotropic part of such tensor reads:

$$\tau_{ij}^R = \tau_{ij} - \frac{\tau_{kk}}{3} \delta_{ij} = -2\nu_{\text{SGS}}\overline{S}_{ij},\tag{15}$$

where  $\nu_{\text{SGS}}$  is the SGS viscosity parameter, which has to be specified by additional models (e.g. Smagorinsky model, Spalart-Allmaras,  $k - \omega$ ,  $k - \epsilon$ ). Equation (15) implies that: (a) the anisotropic Reynolds stress tensor is aligned with the mean strain-rate tensor; (b) the two are directly proportional through a single parameter, equal for all the six independent components of  $\tau_{ij}^R$ .

The pseudo-stochastic model is equivalent to a constant eddy-viscosity model if the variance tensor is expressed by  $a_{ij} = 2\nu_{\text{SUS}}\delta_{ij}$  where the SUS viscosity  $\nu_{\text{SUS}}$  is constant. In this sense, the pseudo-stochastic model can be considered a generalisation of the eddy-viscosity model. The theoretical advantages of the former to the latter are pointed out:

- 1. The PSS does not rely on hypothesis (a). The effects of unresolved scales of motion are given by  $a_{ij}$ , without imposing any constrains on the directions along with the SUS acts on the resolved flow.
- 282 2. The PSS does not rely on hypothesis (b). The tensorial form of  $a_{ij}$  allows to 283 reproduce the anisotropy of unresolved turbulence, i.e. different turbulent 284 contributions along different directions.
- <sup>285</sup> 3. The extra terms in PSS account for turbulent effects usually not consid-
- ered in the classical models, namely turbulent advection and turbulent compressibility.

The eddy-viscosity models are quite reasonable for simple shear flows and 288 it is largely applied in computational fluid dynamics. However, most of their 289 shortcomings derive from the fact that hypotheses (a) and (b) are not generally 290 satisfied; see Pope [35]. Efforts have been made to develop alternative models 291 where the principal axis of  $\tau_{ij}^R$  are not forced to be aligned with those of 292 the mean strain tensor (e.g. the Reynolds-stress models), or where equation 293 (15) is substituted by a non-linear viscosity models, in which the rotation 294 strain-rate comes into play, see for example Bauer *et al.* [1]. In geophysical 295 flow simulations, the strong grid anisotropy between horizontal and vertical 296 directions is successfully handled using a directional eddy-viscosity, see Roman 297 and Armenio [41]. 298

It is worth mentioning that the eddy-viscosity parameter  $a_{ij}$  comes directly from the basic assumption of velocity decomposition in a smooth and a fast oscillating components (3), whereas it is introduced in LES equations through an *ad hoc* physical assumption.

#### <sup>303</sup> 4 Variance tensor model

<sup>304</sup> In the LES framework, a popular model for  $\nu_{\text{SGS}}$  in LES methodology is the <sup>305</sup> the Smagorinsky model, first proposed by Smagorinsky [43] for simulation of

the Smagorinsky model, first proposed by Smagorinsky [43] for simulation of environmental flows (see also Deardorff [7]). It is derived under the hypothesis of local equilibrium between production and dissipation of turbulent kinetic
 energy, and reads:

ν

$$_{\rm SGS} = c_s^2 \overline{\Delta}^2 |\overline{S}|, \tag{16}$$

where  $|\overline{S}|$  is the norm of the strain-rate tensor. The parameter  $c_s^2$  is set constant and can be evaluated from experiments, direct numerical simulations or analytical considerations, e.g. see Lilly [23].

In order to perform a close comparison with the LES methodology, the variance tensor is modelled by a simple model analogous to the Smagorinsky model:

$$a_{ij} = c_m \Delta^2 |\overline{S}| \delta_{ij} \tag{17}$$

where  $\Delta$  is the cell grid width and  $c_m$  is a model parameter. Hence, the variance tensor reduces to a diagonal matrix with equal elements because turbulence is assumed isotropic and homogeneous in all directions.

The relation with the classical Smagorinsky model is now highlighted. In LES, having applied the Smagorinsky model, the anisotropic Reynolds stress tensor reads:

$$-\frac{\partial \tau_{ij}^R}{\partial x_i} = \frac{\partial}{\partial x_i} \left( 2c_s^2 \Delta^2 |\overline{S}| S_{ij} \right) = S_{ij} \frac{\partial C_s |\overline{S}|}{\partial x_i} + \frac{C_s}{2} |\overline{S}| \frac{\partial^2 w_j}{\partial x_i \partial x_i}, \tag{18}$$

where  $C_s = 2c_s^2 \Delta^2$  denotes an auxiliary variable,  $c_s^2$  is the Smagorinsky parameter and the velocity is divergence-free. In the PSS, the total turbulent model can be expressed by a single term, that gathers the dissipative and turbulent advective contributions. Applying formula (17) with  $c_m = 2c_s^2$  and defining  $C_m = c_m \Delta^2$ , such a term becomes:

$$\frac{1}{2}\frac{\partial^2 a_{sk}w_i}{\partial x_s\partial x_k} = \underbrace{\left(S_{ij}\frac{\partial C_m|\overline{S}|}{\partial x_i} + \frac{C_m}{2}|\overline{S}|\frac{\partial^2 w_j}{\partial x_i\partial x_i}\right)}_{eddy-viscosity\ terms} + \underbrace{\Omega_{ij}\frac{\partial C_m|\overline{S}|}{\partial x_j}}_{rotational\ term} + \underbrace{\frac{w_i}{2}\frac{\partial^2 C_m|\overline{S}|}{\partial x_j\partial x_j}}_{strain-rate\ diff.}$$
(19)

where the first two terms on the right-hand side have (formally) the same expression as (18), while the third and fourth term are additional contributions. The PSS with isotropic constant model reduces to the LES Smagorinsky

<sup>323</sup> model under two approximations:

1. the rotation-rate does not contribute to turbulence effects on the mean flow, thus it is neglected;

2. the norm of strain-rate tensor is almost harmonic (Laplacian is close to zero), which makes the fourth term negligible.

Notice that the latter hypothesis implies that the continuity equation (6) turns into the classical solenoidal constrain. Therefore, the LES Smagorinsky model can be interpreted as a particular case of the PSS constant isotropic model.

Approximation (1) is valid if the turbulent energy is mainly concentrated in the region where the irrotational strain dominates vorticity. Exceptions on this behaviour have been found and have motivated the development of alternative

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Approximation (2) implies that the flow deformation rate can be represented

337 by a linear function in each spatial point; thus it is a particularly regular

<sup>338</sup> function. This is equivalent to neglect the turbulent correction on advective

<sup>339</sup> velocity and continuity equation, hence the associated physical phenomena of

<sup>340</sup> turbophoresis and turbulent compressibility are not reproduced.

#### 341 5 Numerical simulations

PSS and LES are compared on turbulence channel flow at  $Re_{\tau} = 590$ . The former adopts a constant isotropic model for variance tensor, the latter adopts a constant Smagorinsky model for sub-grid scale viscosity. The Direct Numerical

<sup>345</sup> Simulation (DNS) of Moser *et al.* [28] is taken as reference.

#### <sup>346</sup> 5.1 Case geometry and settings

The channel is composed by two horizontal and parallel walls between which a shear flow develops. The dimensions in stream-wise (x), vertical (y) and span-wise (z) directions are  $2\pi\delta \times \delta \times \pi\delta$ , respectively. The flow is driven by a constant pressure gradient  $\frac{\partial p}{\partial x} = -\rho u_{\tau}/\delta$ . The Reynolds number based on the friction velocity  $u_{\tau}$  is defined as  $Re_{\tau} = u_{\tau}\delta/\nu$ . The spatial variables are made non-dimensional as  $y^+ = yu_{\tau}/\nu$ , the velocity as  $u^+ = u/u_{\tau}$ , time as  $t^+ = tu_{\tau}/\nu$ . The characteristic flow time is estimated as  $t_0 = U_0/2\pi\delta$ , where  $U_0$  is the bulk velocity in stream-wise direction.

The computational domain is discretised by  $96 \times 96 \times 96$  points. They are 355 uniformly distributed in stream-wise and span-wise directions, leading to a 356 cell width  $\Delta x^+ < 40$  and  $\Delta z^+ < 20$ , respectively. In vertical direction, the 357 grid is stretched in a way such that the first cell is within  $y^+ = 1$  and with 9 358 cells in  $y^+ \leq 11$ ; thus ensuring an accurate resolution of the boundary layer. 359 The stretching is symmetric with respect to the channel centre plane  $y = \delta$ , 360 and it is obtained with a double-side stretching function based on hyperbolic 361 tangent: 362

363

$$y(\xi) = \frac{1}{2} \left( 1 + \frac{\tanh(\lambda(\xi - 1/2))}{\tanh(\lambda/2)} \right),\tag{20}$$

where  $\xi$  is the vertical coordinate of uniform point distribution and the stretching factor is set to  $\lambda = 5.25$ .

<sup>366</sup> Cyclic boundary conditions are set at the vertical boundaries, while velocity
 <sup>367</sup> no-slip condition and pressure zero-gradient are imposed at the horizontal
 <sup>368</sup> walls. All the cases are initialised with the instantaneous fields provided by a
 <sup>369</sup> preliminary LES with constant Smagorinsky SGS model, that has reached the
 <sup>370</sup> statistical steady state.

371 5.2 Algorithm and implementation

Simulations are performed taking advantage of the open-source software OpenFOAM v. 2.3.0. This is a C++ library for computational fluid dynamics and
adopts the finite volume methods.

The LESs are carried out using the solver pisoFoam included in the standard software distribution. The implementation details on this basic solver can be found in the official OpenFOAM documentation and in the work of Jasak *et al.* [15]. The constant Smagorinsky SGS model is provided by OpenFOAM, and its correct implementation was checked.

Two PSSs are performed using the code pseudoStochasticPisoFoam, a home-made solver developed by the authors within the Fluminance research group at INRIA Rennes (France). The non-conservative form of pseudo-stochastic governing equations (5) are solved employing the Pressure-Implicit with Splitting of Operators (PISO) algorithm proposed by Issa *et al.* [14] and Oliveira & Issa [32].

Variables are discretised in space with a second-order central difference 386 scheme, while time integration is performed using an implicit Euler backward 387 scheme. Such a scheme employs the variables at the previous two time steps, 388 leading to a second order accuracy. Globally, the numerical solvers are second-389 order accurate in time and space. The time advancement fulfils the Courant-390 Friedrichs-Lewy condition Co < 0.5. The Courant number is computed as 391  $Co = \Delta t |v| / \delta x$ , where:  $\Delta t$  is the time step, |v| is the velocity magnitude 392 through the cell,  $\delta x$  is the cell length. The model constants are chosen to be 393  $c_s^2 = c_m/2 = 0.004225$ , and for PSS  $v = w^*$  while for LES  $w^* = u$ . 394

#### <sup>395</sup> 5.3 Results discussion

The simulations are run till the statistical steady state is reached, then they are re-run for an additional period of  $12t_0$  where the statistics are collected. The quantities are averaged in time and in space along span-wise and streamwise directions, and exploiting the domain symmetry in vertical direction. The angular brackets  $\langle \psi \rangle$  denote the average in time and wall-parallel directions for a generic variable  $\psi$ .

#### 402 First and second order statistics

<sup>403</sup> The first and second order statistics of the velocity filed are analysed.

Figure 1 top-panel reports the mean non-dimensional stream-wise velocity along the wall coordinate. PSS and LES lead to similar profiles in the near-wall region  $(y^+ < 30)$ , while the former exhibits slightly lower values in the log-law region  $(y^+ > 30)$ . They underestimate the velocity magnitude at the centre channel and, as expected, both are not accurate in reproducing the boundary layer profile. This is a well known shortcoming of Smagorinsky model when  $c_s^2$ to constant, and it is inherited by the constant isotropic model.



Fig. 1 First and second order statistics of velocity field versus non-dimensional vertical coordinate (wall coordinate). Top panel: non-dimensional mean stream-wise velocity. Bottom panel: non-dimension velocity root-mean square. Reference DNS by [28].

Figure 1 bottom-panel displays the velocity RMS components. If  $\psi$  is a generic variable, we denote  $[\psi]_{rms} = \sqrt{\langle \psi'^2 \rangle}$  the root-mean square, where  $\psi' = \psi - \langle \psi \rangle$  is the instantaneous fluctuation. Both PSS and LES collapse on the same profiles.

Because the isotropic model is very similar to the Smagorinsky model, an improvement of accuracy by the PSS is not expected. The interest of this validation is to prove that the pseudo-stochastic model is as accurate as the state-of-the-art LES methodologies, despite its derivation relies to a substantially different framework and its governing equations include several extra terms, which are analysed in the following sections.



Fig. 2 Mean value of non-dimensional terms appearing in the pseudo-stochastic model with constant isotropic model, equation (19): component x along the wall-normal coordinate. EV, eddy-viscosity terms; RT, rotational term; SD, strain-rate diffusion.

#### 421 Effects of the extra terms in PSS

The LES constant Smagorinsky model and the PSS constant isotropic model lead to similar governing equations, but the latter has some additional terms not present in the former: the eddy-viscosity terms (EV), the rotational term (RT) and the strain-rate diffusion (SD) defined in equation (19). The influence of such terms is checked.

Figure 2 shows the x-component of the above-mentioned terms (averaged) 427 versus the wall coordinate. They are made non-dimensional by  $u_{\tau}^3/\nu$ . In LES, 428 the term EV accounts for all sub-grid scale effects and represents a negative 429 turbulent diffusion near the wall. In the PSS constant isotropic model, two 430 other terms come into play: SD is negative in the region  $y^+ < 10$ , while it 431 shows positive value at  $y^+ > 10$ ; RT exhibits a positive contribution against 432 the negative one of EV. The three terms become negligible in the log-law 433 region; hence, the SUS model acts mainly at the near-wall region. The point 434  $y^+ = 10$ , located in the buffer layer, is of particular interest: approximately 435 at this height, EV and RT reach the minimum and maximum (respectively), 436 while SD changes sign. Globally, the RT and SD terms reduce the negative 437 contribution of EV to the velocity equations in the buffer region, eventually 438 producing a positive turbulent diffusion. 439

#### 440 Turbulent advection and compressibility

Figure 3 presents the non-dimensional turbulent advection velocity  $u_{TA}^+ = u_{TA}/u_{\tau}$  and the turbulent compressibility  $\Phi_{TC}^+ = \Phi_{TC}u_{\tau}^2/\nu$  are scrutinised. The stream-wise component of  $u_{TA}$  is practically zero, as well as the span-wise component; thus they are not displayed. The vertical component profile reveals low



Fig. 3 Mean value of non-dimensional turbulent advenction (12) and compressibility (13) appearing in the pseudo-stochastic model with constant isotropic model: x-component along the wall coordinate.

negative values, with a climax at  $y^+ \cong 10$ . Quantitatively, the turbulent ad-445 vection is not strong enough to produce remarkable results on the mean flow; 446 however, it generates a weak vertical velocity  $w_y$  directed from the center to 447 the wall of the channel (not reported). Hence,  $u_{\text{TA}}$  is qualified as a weak tur-448 bophoresis velocity: it advects the flow from the buffer region to the log-law 449 region, i.e. in the direction of decreasing turbulence level (estimated by the 450 velocity RMS intensity). The turbulent compressibility  $\Phi_{\rm TC}$  assumes negative 451 values in the viscous sub-layer and positive values in the buffer layer. Else-452 where, it is practically zero. In light of equation (11), this behaviour is related 453 to the presence of a turbulent fluid compression and expansion, respectively. 454 Additional insight on this phenomenon is gained visualising the  $\Phi_{\rm TC}$  instanta-455 neous values. 456

Figure 4 displays the  $\Phi_{\rm TC}$  negative (blue) and positive (orange) isosurfaces 457 near the bottom wall, at an instantaneous flow configuration. They are organ-458 ised in spots, confined in the near-wall region and elongated in the stream-459 wise direction. In accordance with the  $\varPhi_{\rm \scriptscriptstyle TC}$  mean profile, the negative spots 460 are closer to the wall  $(y^+ < 10)$ , while the positive one are immediately above 461  $(10 < y^+ < 20)$ . The shape and the location of the isosurfaces suggest a corre-462 lation with the streaks structures that characterises turbulent wall flows. The 463 streaks are generated in a region of low velocity, very close to the wall, ap-464 proximately at  $y^+ \simeq 5$ . They are elongated in the stream-wise direction, with 465 a characteristic length of  $\Delta x^+ \cong 1000$  and a span-wise period of  $\Delta z^+ \cong 100$ . 466 This estimation can vary with respect to the wall distance, see Smith & Met-467 zler [44]. Despite their widespread presence, there is no clear consensus on 468 the streak formation mechanism and multiple theories have been proposed in 469 literature, see Chernyshenko & Baig [6]. The  $\Phi_{\rm TC}$  isosurfaces have, overall, the 470



Fig. 4 Positive and negative isosurfaces of  $\Phi_{\rm TC}$  near the bottom wall at an instantaneous flow configuration. Orange: isosurface at  $\Phi_{\rm TC}^+ = 3.5/times10^-4$ . Blue: isosurface at  $\Phi_{\rm TC}^+ = -3.5/times10^-4$ .



Fig. 5 Selected contributions to the pseudo-stochastic TKE budget versus wall-normal coordinate. The TKE terms are labelled as in equation (8). Results of three simulations are displayed: PSS with constant isotropic model, black lines with solid symbols; LES with constant Smagorinsky model, red lines with empty symbols.

471 same stream-wise extension and span-wise period. Also, the negative spots are
472 located at the same height at which steaks are triggered. Therefore, these two

 $_{\rm 473}$   $\,$  structures appears to be related.

### 474 Resolved turbulent kinetic budget

The pseudo-stochastic TKE budget (8) is finally scrutinised for PSS and LES simulations

Figure 5 shows selected terms of the TKE budget. Production and dissipation profiles are similar for PSS and LES, but the former appears to be more effective in energy dissipation in near-wall region and has a higher production of TKE in the range  $5 < y^+ < 20$ . In the PSS, the turbulent compression term is almost zero and does not contribute to the budget; while the loss due to SUS presents slightly negative values mainly localised in the viscous layer. Hence, it contributes to global energy dissipation.

#### 484 6 Conclusions

The pseudo-stochastic simulation (PSS) methodology introduced by Mémin [24] 485 is analysed theoretically and numerically, through a direct comparison with 486 the classical large-eddy simulations (LES) approach. The PSS model is based 487 on an innovative decomposition of the fluid-particle trajectory in a drift dis-488 placement and a stochastic perturbation. The former reproduces the mean 489 flow, the later accounts for the turbulent perturbations which are modeled 490 as a Brownian motion. Imposing such a decomposition, together with a reg-491 ularity assumption on the drift velocity, a set of deterministic and stochastic 492 equations of motion are derived using stochastic calculus; then, the pseudo-493 stochastic equations are obtained by neglecting the solution of stochastic equa-494 tions and closing the system by physical assumptions. The result is a new set 495 of governing equations which includes extra terms deriving from the stochas-496 tic modeling of turbulence. The PSS model is found to be a generalisation of 497 the classical Navier-Stokes equations, and reproduces phenomena usually not 498 considered: turbophoresis and turbulent compressibility. 499

The PSS of turbulent channel flow at  $Re_{\tau} = 590$  is performed, together 500 with the LES with constant Smagorinsky sub-grid scale model. For a better 501 comparison, a closure model analogous to the Smagorinsky one is used for the 502 PSS. However, it is shown that this last does not rely on the eddy-viscosity hy-503 potheses, hence it is not affected by its shortcomings. The PSS does not show 504 improvement in first and second order statistics, possibly because of the sim-505 ple expression of  $a_{ii}$ , but reproduces additional features: a weak turbophoresis 506 is detected in the buffer region, while a turbulent compression and expansion 507 is identified in the viscous and buffer layer (respectively). This quantity ap-508 pears to be related to the streaks, turbulent structures appearing near the wall 509 region. 510

Finally, the pseudo-stochastic model is a generalisation of the LES eddyviscosity model and describes a richer physics. Overall, it represents a promising approach for simulation of turbulent flows: the mathematical analysis here reported gives a clear physical interpretation of the model, supported by numerical results.

#### A . Formal derivation of stochastic model 516

The mathematical conditions under which this derivation is consistent are reported in [9, 26, 26]517 27]. An introduction to the mathematical framework in which the present model is developed 518

can be found in Øksendal [31] and Kunita [18]. 519

#### A.1 Trajectory and stochastic velocity definitions 520

As already mentioned, expression (1) has to be understood in an integral sense: 521

$$X_t^i = X_0^i + \int_0^t w_i(X_s, s) ds + \int_0^t d\eta_s^i(X_s),$$
(21)

523 where the Itō stochastic integral is used to integrate the random process. The process  $X_t^i(x_0)$ is a semimartingale defined for each spatial point  $x_0 \in \Omega$  and time  $t \in T \subseteq \mathbb{R}^+$  in an 524 525 appropriate probability space.

The stochastic velocity in equation (3) is a symbolic expression that is defined as a weak 526 derivative of the random displacement: 527

528 
$$\int h(t)\dot{\eta}_t^i(x)dt = \int h'(t)\eta_t^i(x)dt,$$
 (22)

for each h test function; see also [31]. 529

#### A.2 The stochastic Reynolds transport theorem 530

Being the velocity field a stochastic process, the governing equations of fluid dynamics 531 532 cannot be recovered using deterministic calculus, ref. [24, 27]. In this concern, the key point is to give an expression of the Reynolds transport theorem (RTT) for stochastic quantities. 533 Subsequently, the stochastic Navier-Stokes equations are found imposing conservation of 534 mass and momentum. 535

**Theorem 1 (Stochastic RTT)** Let us consider a physical quantity q(x,t) within a ma-536 terial volume  $V(t) \subset \mathbb{R}^3$ , transported by a stochastic flow of the form (1) and such that it 537 538 can be written as a semimartingale of the type:

539 
$$q(x,t) = q(x,0) + \int_0^t g(x,s)ds + \int_0^t \int_{\Omega} f_k(x,y,s)dB_s^k(y)dyds,$$
 (23)

where g, f are processes of bounded-variation and the Itō integral are employed. If the fol-540 lowing properties holds: 541

- 542
- 1. symmetric diffusion tensor:  $\sigma_{ij} = \sigma_{ji}$ , 2. solenoidal diffusion tensor:  $\frac{\partial}{\partial x_i} \sigma_{ij}(x, y, t) = 0$  for all j, 543
- 3. conserved quantity:  $dq(X_t, t) = 0$ , 544

then the stochastic RTT has an explicit differential form that reads:

$$d\int_{V(t)}q(x,t)dx = \int_{V(t)} \left[\partial_t q + \frac{\partial(qw_i)}{\partial x_i}dt - \frac{1}{2}\frac{\partial^2(qa_{ij})}{\partial x_i\partial x_j}dt + \frac{\partial q}{\partial x_i}d\eta_t^i\right]dx,\tag{24}$$

- where  $\partial_t$  is the differential with respect to the second variable, and d denotes the total time 545
- increment at a fixed spatial point. 546

Assumption (1) greatly simplifies the computation and can be justified a *posteriori*: it implies 547 that the variance tensor  $a_{ii}$  is symmetric, a desirable properties in light of its physical 548

interpretation (see section 3.1). Therefore, this assumption is considered reasonable in the 549

fluid dynamics context; however it is not mandatory, see [37]. Hypothesis (2) can be removed, 550

but the stochastic RTT expression assumes a more complex formulation. It is found that this 551

552 constrain is naturally satisfied by fluids where density is constant in space (see section A.3).

thus formula (24) is directly applied when the flow is incompressible or when the Boussinesq 553 approximation is applied. On the contrary, an explicit formula has not been derived for a 554

generic non-conserved quantity; hence hypothesis (3) is essential. 555

Notice that equation (24) reduces to the classical RTT when the stochastic contribu-556 tion in equation (1) is suppressed. This happens e.g. when  $\sigma_{ij} = 0$  and, consequently, the 557 558 martingale  $\eta_t^i$  as well as the variance tensor are identically zero.

559

A concise derivation of the stochastic RTT is now presented. A generic random process 560  $\phi(x,t)$  is expressed hereafter as a semimartingale of the form: 561

$$\phi(x,t) = \phi(x,0) + \int_0^t g(x,s)ds + \int_0^t \int_{\Omega} f_k(x,y,s)dB_s^k(y)dyds,$$
(25)

where q, f are processes of bounded-variation and the Ito integral are used. 563

**Proposition 1** (Differential of transported process) Let us consider  $\phi$  a semimartingale of the type (25), sufficiently regular in space (bounded spatial gradient, two times derivable). If it is transported by a flow of the form (21); then, the time total-differential of  $\phi$  is expressed by:

$$d\phi(X_t,t) = \partial_t \phi + \frac{\partial \phi}{\partial x_i} dX_t^i + \frac{1}{2} a_{ij}(X_t,t) \frac{\partial^2 \phi}{\partial x_i \partial x_j} dt + \int_{\Omega} \sigma_{ij}(X_t,y,t) \frac{\partial}{\partial x_i} f_j(X_t,y,t) dy dt,$$
(26)

where  $\partial_t$  is the time partial-differential (i.e. with respect to second variable), and  $a_{ij}$  is the variance tensor defined by equation (4). 565

Proof: The Ito -Wentzell formula is used to differentiate (in time) the transported process  $\phi(X_t, t)$ , corresponding to a composition of two processes. It reads:

$$d\phi(X_t, t) = \partial_t \phi + \frac{\partial \phi}{\partial x_i} dX_t^i + \frac{1}{2} d\left\langle X^i, X^j \right\rangle_t \frac{\partial^2 \phi}{\partial x_i \partial x_j} + d\left\langle \frac{\partial \phi}{\partial x_i}, X^i \right\rangle_t, \tag{27}$$

where the angular brackets denote the quadratic variation operation; e.g. see Le Gall [19] for 566

567 an extended presentation. The following properties of the quadratic variation are recalled: 1. is symmetric and bilinear; 568

- 569
- 2. if g is a process of bounded-variation:  $\langle g, B^k \rangle_t = 0$ 3. if f is deterministic function:  $\langle fB^i, B^j \rangle_t = f \langle B^i, B^j \rangle_t$ 570

4. singularity:  $d\langle B^i(y), B^j(z) \rangle_t = \delta(y-z) \delta_{ij} dt$ 571

where  $B_t$  is a cylindrical Wiener process,  $\delta(x)$  is the Dirac function and  $\delta_{ij}$  is the Kronecker symbol. Using these properties, the third and fourth terms in equation (27) are written explicitly. The third term is directly computed:

$$d\langle X^{i}, X^{j} \rangle_{t} = \int_{\Omega} \sigma_{ik}(X_{t}, y, t) \sigma_{jk}(X_{t}, y, t) dy dt = a_{ij}(X_{t}, t) dt.$$
<sup>(28)</sup>

In the fourth term, the gradient of  $\phi$  is obtained differentiating equation (25):

$$\frac{\partial}{\partial x_i}\phi(X_t,t) = \frac{\partial\phi_0}{\partial x_i} + \int_0^t \frac{\partial}{\partial x_i}g(X_s,s)ds + \int_0^t \int_\Omega \frac{\partial}{\partial x_i}f_k(X_s,y,s) \ dB_s^k(y)dyds, \tag{29}$$

then, the last term in (27) is rewritten as:

$$d\left\langle \frac{\partial \phi}{\partial x_i}, X^i \right\rangle_t = \int_{\Omega} \sigma_{ij}(X_t, y, t) \frac{\partial}{\partial x_i} f_j(X_t, y, t) dy dt.$$
(30)

Substituting formula (28) and (29) in equation (27), expression (26) is recovered. 572

**Proposition 2 (Differential of transported and conserved process)** Let us consider a stochastic process  $\phi$  of the type (25). If such a process is transported by a stochastic flow (21) and is conserved, i.e.  $d\phi(X_t, t) = 0$ , then:

$$\partial_t \phi(X_t, t) = -\frac{\partial \phi}{\partial x_i} w_i dt + \frac{1}{2} a_{ij} \frac{\partial^2 \phi}{\partial x_i \partial x_j} dt + \int_{\Omega} \frac{\partial \phi}{\partial x_k} \frac{\partial \sigma_{kj}}{\partial x_i} \sigma_{ij} dy dt - \int_{\Omega} \frac{\partial \phi}{\partial x_i} \sigma_{ik} dB_t^k dy.$$
(31)

573 This formula expresses the time variation along a fluid-particle trajectory.

*Proof:* If  $\phi(X_t, t)$  is conserved, then equation (26) can be re-arranged as follows:

$$\partial_t \phi(X_t, t) = -\frac{\partial \phi}{\partial x_i} w_i dt - \int_{\Omega} \frac{\partial \phi}{\partial x_i} \sigma_{ik}(X_t, y, t) dB_t^k(y) dy - \frac{1}{2} a_{ij} \frac{\partial^2 \phi}{\partial x_i \partial x_j} dt - \int_{\Omega} \sigma_{ij}(X_t, y, t) \frac{\partial}{\partial x_i} f_j(X_t, y, t) dy dt.$$
(32)

An expression of  $\partial_t \phi$  is obtained also from (25), and is compared with formula (32). Exploiting the unique decomposition of the semimartingales, one obtains:

$$g(X_t,t) = -\frac{\partial\phi}{\partial x_i} w_i - \frac{1}{2} a_{ij} \frac{\partial^2 \phi}{\partial x_i \partial x_j} - \int_{\Omega} \sigma_{ij}(X_t, y, t) \frac{\partial}{\partial x_i} f_j(X_t, y, t) dy,$$
(33)

and the following implicit formula for f:

$$\int_{\Omega} \left[ f_k(X_t, y, t) + \frac{\partial \phi(X_t, t)}{\partial x_i} \sigma_{ik}(X_t, y, t) \right] dB_t^k(y) dy = 0.$$
(34)

576 This latter holds for every Brownian motion  $dB_t^k$ , thus:

$$f_k(X_t, y, t) = -\frac{\partial \phi(X_t, t)}{\partial x_i} \sigma_{ik}(X_t, y, t).$$
(35)

Substituting formula (35) in equation (32) the final expression (31) is obtained.  $\Box$ 

Notice that a general form of a conserved semimartingale can be found by substituting equation (33) and (35) in formula (25).

Translating equation (31) from Lagrangian to Eulerian coordinates and rearranging the second and third terms in the left-hand side, one obtains the expression of the material derivative (in differential form) within the stochastic framework.

**Proposition 3 (Stochastic transport operator)** If  $\phi$  is a stochastic process of the type (25), transported by a stochastic flow (21) and conserved, then the stochastic material derivative in differential form is:

$$D\phi(x,t) = \partial_t \phi + (w_i dt + d\eta_t^i) \frac{\partial \phi}{\partial x_i} - \frac{1}{2} \frac{\partial}{\partial x_i} \left( a_{ij} \frac{\partial \phi}{\partial x_j} \right) dt - \left( \frac{1}{2} \frac{\partial a_{ij}}{\partial x_i} - \int_{\Omega} \sigma_{kj} \frac{\partial \sigma_{ij}}{\partial x_i} dy \right) \frac{\partial \phi}{\partial x_j} dt,$$
(36)

which is reported in [37] as the stochastic transport operator for a conserved quantity.

The derivation of Stochastic RTT is now summarised. Let us consider a generic physical

quantity, mathematically expressed by a stochastic scalar process q(x,t) that satisfies the hypotheses of Stochastic RTT. The solution of transport equation is found in the space of weak solutions.

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Proof (Stochastic RTT): Consider a control volume V(t) and a test function  $\varphi(x, t)$  in the space domain  $\Omega$  such that: it has compact support on V(t), it is conserved and satisfies (25). Then, the weak transport equation for q reads:

$$d\int_{V(t)} q(x,t)\varphi(x,t)dx = \int_{\Omega} \left[\varphi \partial_t q + q \partial_t \varphi + d \langle q, \varphi \rangle_t\right] dx, \tag{37}$$

applying the Itō integration by part and passing to the integral on  $\Omega$  because  $\varphi$  has compact support on V. The last term on the right-hand side needs to be explicited. An expression of q and  $\varphi$  is given by the semimartingale decomposition (25):

$$\varphi = \varphi(x,0) + \int_0^t g(x,s)ds + \int_0^t \int_\Omega f_j(x,y,s)dB_s^j dy, \tag{38}$$

$$q = q(x,0) + \int_0^t h(x,s)ds + \int_0^t \int_{\Omega} \kappa_j(x,y,s)dB_s^j dy,$$
(39)

where explicit formulae for  $g, h, f, \kappa$  are given, see proof of Proposition 2. Using these expressions to compute the quadratic variation, we get:

$$d\langle q,\varphi\rangle_t = d\int_0^t \left\langle \int_\Omega \kappa_i dB^i dy, \int_\Omega f_j dB^j dz \right\rangle_t = \frac{\partial q}{\partial x_k} \frac{\partial \varphi}{\partial x_\ell} a_{k\ell} dt, \tag{40}$$

The same expressions are differentiated to express  $\partial_t q(x,t)$  and  $\partial_t \varphi(x,t)$ , that are substituted in the transport equation (37) together with formula (40). Subsequently,  $\varphi$  is used to compute the weak derivative and gathered; the final equation reads:

$$d\int_{\Omega} q(x,t)\varphi(x,t)dx = \int_{\Omega} \varphi \left[ \partial_t q + \frac{\partial q w_i}{\partial x_i} dt + \frac{1}{2} \frac{\partial^2}{\partial x_i \partial x_j} \left( q a_{ij} \right) dt - \frac{\partial}{\partial x_k} \int_{\Omega} q \frac{\partial \sigma_{kj}}{\partial x_i} \sigma_{ij} dy dt + \frac{\partial}{\partial x_i} \left( q d\eta_t^i \right) - \frac{\partial}{\partial x_\ell} \left( \frac{\partial q}{\partial x_k} a_{k\ell} \right) dt \right] dx.$$
(41)

Equation (41) is valid for every test function  $\varphi$  with compact support in V(t), thus:

$$d\int_{V} q(x,t)dx = \int_{V} \left[ \partial_{t}q + \frac{\partial qw_{i}}{\partial x_{i}}dt + \frac{\partial}{\partial x_{i}}\left(qd\eta_{t}^{i}\right) + \frac{1}{2}q \left\| \frac{\partial\sigma}{\partial x} \right\|^{2} dt - \frac{1}{2}\int_{\Omega} \left(q\frac{\partial\sigma_{ik}}{\partial x_{j}}\frac{\partial\sigma_{kj}}{\partial x_{i}} + \frac{\partial^{2}q}{\partial x_{i}\partial x_{j}}\sigma_{ik}\sigma_{kj} + 2\sigma_{ij}\frac{\partial q}{\partial x_{k}}\frac{\partial\sigma_{kj}}{\partial x_{i}}\right)dydt \right] dx,$$
(42)

where the terms are rearranged and the definition of variance tensor is used to simplify some terms. Equation (42) is the general form of Stochastic RTT, that is quite complex and eventually difficult to handle. One can notice that under the additional hypothesis that the

<sup>594</sup> random term is solenoidal in space, i.e.

$$\frac{\partial}{\partial x_i} d\eta_t^i(x) = 0 \quad \Leftrightarrow \quad \frac{\partial}{\partial x_i} \sigma_{ik}(x, y, t) \equiv 0, \tag{43}$$

where the if and only if statement holds because the Brownian motion is arbitrarily chosen, the equation (42) simplifies to:

$$d\int_{V} q(x,t) \, dx = \int_{V} \left[ \partial_t q + \frac{\partial \left(qw_i\right)}{\partial x_i} dt - \frac{1}{2} \frac{\partial^2 \left(qa_{ij}\right)}{\partial x_i \partial x_j} dt + \frac{\partial \left(qd\eta_t^i\right)}{\partial x_i} \right] dx,\tag{44}$$

596 that is the final form of Stochastic RTT.

597

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In the following section, it is shown that the assumption of a solenoidal random turbulence field is satisfied by incompressible fluids, thus the simpler equation (44) can be used to derived the equation of motion.

It is worth noticing that the Stochastic RTT can be applied to all functions of the form (25); specifically, to all process of bounded-variations that are a particular case of semimartingale where the martingale term is zero.

## 604 A.3 Derivation of Stochastic Navier-Stokes equations

The derivation of governing equations for fluid flows is performed with a similar strategy as in the classical framework, e.g. see [17].

### 607 Conservation of mass

If  $\rho(x,t)$  is the mass density, then the conservation of mass is:

$$d\int_{V(t)}\rho dx = \int_{V(t)} \left[\partial_t \rho + \frac{\partial\rho w_i}{\partial x_i}dt + \frac{\partial}{\partial x_i}\left(\rho d\eta_t^i\right) + \frac{1}{2}\rho \left\|\frac{\partial\sigma}{\partial x}\right\|^2 dt$$
(45)

$$-\frac{1}{2}\int_{\Omega}\left(\rho\frac{\partial\sigma_{ik}}{\partial x_j}\frac{\partial\sigma_{kj}}{\partial x_i} + \frac{\partial^2\rho}{\partial x_i\partial x_j}\sigma_{ik}\sigma_{kj} + 2\sigma_{ij}\frac{\partial\rho}{\partial x_k}\frac{\partial\sigma_{kj}}{\partial x_i}\right)dydt\Big]dx = 0,$$
(46)

where the general form of Stochastic RTT (42) is used here. For an incompressible fluid, density is constant  $\rho(x,t) = \rho$  and the mass conservation equation simplifies accordingly.

 $r_{\rm form}$  The integral is then removed exploiting the arbitrariness of control volume:

$$\frac{\partial w_i}{\partial x_i}dt + \frac{\partial}{\partial x_i}d\eta_t^i + \frac{1}{2} \left\|\frac{\partial\sigma}{\partial x}\right\|^2 dt - \frac{1}{2}\int_{\Omega}\frac{\partial\sigma_{ik}}{\partial x_j}\frac{\partial\sigma_{kj}}{\partial x_i}\,dydt = 0.$$
(47)

Separating the processes of bounded-variation and the martingales, the following system is recovered:

$$\left(\frac{\partial w_i}{\partial x_i} + \frac{1}{2} \left\|\frac{\partial \sigma}{\partial x}\right\|^2 - \frac{1}{2} \int_{\Omega} \frac{\partial \sigma_{ik}}{\partial x_j} \frac{\partial \sigma_{kj}}{\partial x_i} dy\right) dt = 0, \quad \frac{\partial}{\partial x_i} d\eta_t^i = 0.$$
(48)

Equation (48) shows that for an incompressible fluid the Brownian term is solenoidal; thus, the use of the simplified expression Stochastic RTT (44) is a *posteriori* justified for incom-

pressible fluids. Using the solenoidal constraint, equations (48) leads to the system:

$$\frac{\partial}{\partial x_i} \left( w_i - \frac{1}{2} \frac{\partial}{\partial x_j} a_{ij} \right) = 0, \quad \frac{\partial}{\partial x_i} \sigma_{ik} = 0, \tag{49}$$

616 which expresses the conservation of mass.

#### 617 Conservation of momentum

Two derivations are proposed, they are named Lagrangian and Eulerian for convenience of notation. The former is based on the work of [27], the latter on that one of [24].

621 • LAGRANGIAN: The second Newton's law is:

$$\frac{d}{dt}\rho U_i(X_t, t) = F_i(X_t, t), \tag{50}$$

where  $F_i$  are the forces acting on a fluid-particle. If  $I_i$  if the time integral of the forces (the *impulse*), equation (50) is re-written in a differential form as  $d\rho U_i = dI_i$ . It is expressed in a weak form as:

$$\rho \int h \ dU_i(X_t, t) = \int h \ dI_i(X_t, t), \tag{51}$$

where h are test functions and  $\rho$  is constant. The left-hand side is:

$$\rho \int h \ dU_i(X_t, t) = \rho \int h \ dw_i(X_t, t) - \rho \int h' d\eta_t^i, \tag{52}$$

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then, the right-hand side of equation (51) must have the same structure, see [27]. Hence,
the impulse divides into two contributions and equation (51) becomes:

$$\rho \int h \, dw_i(X_t, t) - \rho \int h' d\eta_t^i = \int h \, d\mathcal{J}_i - \int h' d\lambda_t^t.$$
(53)

Matching similar terms, we arrived at the following relations:

$$\rho dw_i = d\mathcal{J}_i, \quad d\eta_t^i = d\lambda_t^i. \tag{54}$$

- Equations (54)-first is exploited to obtain the governing equation of motion, while (54)-
- second states that the forces balance the contribution of random velocities. In Eulerial
- 634 framework, this latter reads:

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$$\rho Dw_i(x,t) = d\mathcal{J}_i(x,t),\tag{55}$$

Applying the stochastic transport operator (36) with the solenoidal constrain (49), one gets:

$$Dw_i = \partial_t w_i + (w_j - \frac{1}{2} \frac{\partial a_{kj}}{\partial x_k}) \frac{\partial w_i}{\partial x_j} dt - \frac{1}{2} \frac{\partial}{\partial x_k} \left( a_{jk} \frac{\partial w_i}{\partial x_j} \right) dt + d\eta_t^j \frac{\partial w_i}{\partial x_j}, \tag{56}$$

while the impulse is determined by a physical analysis of the forces acting on the system, as in the classical derivation:

$$d\mathcal{J}_i = -\frac{\partial}{\partial x_i} \left( p dt - d\xi_t \right) + \mu \frac{\partial^2}{\partial x_j \partial x_j} \left( dX_t^i \right) + \frac{\mu}{3} \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_\ell} \left( dX_t^\ell \right)$$
(57)

$$= \left[ -\frac{\partial p}{\partial x_i} + \mu \frac{\partial^2 w_i}{\partial x_j \partial x_j} + \frac{\mu}{3} \frac{\partial^2 w_\ell}{\partial x_i \partial x_\ell} \right] dt - \frac{\partial (d\xi_t)}{\partial x_i} + \mu \frac{\partial^2 \left( d\eta_t^i \right)}{\partial x_j \partial x_j} + \frac{\mu}{3} \frac{\partial^2 \left( d\eta_t^\ell \right)}{\partial x_i \partial x_\ell}, \quad (58)$$

<sup>639</sup> with  $\mu$  is the fluid viscosity, and pressure is written in a semimartingale form (25) where <sup>640</sup>  $d\xi_t(x) = \int_{\Omega} \vartheta_i(x, y, t) dB_t^i(y) dy$  denotes the martingale contribution to pressure. Imposing <sup>641</sup> the equality (55) and using the unique decomposition of semimartingale, the governing equa-<sup>642</sup> tions (63) are recovered. <sup>643</sup>

• EULERIAN: Once again, the momentum conservation is formulated in differential form. If  $\mathcal{J}_i(x,t)$  is the impulse of total forces per volume, the second law of mechanics reads:

$$d\int_{V(t)}\rho U_i(x,t)dx = \int_{V(t)} d\mathcal{J}_i(x,t)dx.$$
(59)

The Stochastic RTT is applied to the left-hand side in order to get:

$$d\int_{V(t)} \rho U_i \, dx = \int_{V(t)} \rho \left[ \partial_t w_i + \frac{\partial}{\partial x_j} (w_i w_j) dt - \frac{1}{2} \frac{\partial^2}{\partial x_s \partial x_k} (w_i a_{sk}) \, dt + \frac{\partial}{\partial x_j} \left( w_i d\eta_t^j \right) \right] dx + d \int_{V(t)} \rho \, \dot{\eta}_t^i dx, \tag{60}$$

where the velocity decomposition (3) is employed. The impulse acting on V(t) is expressed by (58). Then, imposing equality (59) and separating the processes of bounded-variation to the martingales, one obtains:

$$\partial_t w_i + \frac{\partial w_i w_j}{\partial x_j} dt - \frac{1}{2} \frac{\partial^2 (w_i a_{sk})}{\partial x_s \partial x_k} dt = -\frac{\partial p}{\partial x_i} dt + \nu \frac{\partial^2 w_i}{\partial x_j \partial x_j} dt + \frac{\nu}{3} \frac{\partial}{\partial x_i} \frac{\partial w_\ell}{\partial x_\ell} dt \qquad (61)$$

with  $\nu = \mu/\rho$  is the dynamic viscosity, and

$$d\int_{V(t)}\dot{\eta}_t^i dx = \int_{V(t)} \left[ -\frac{\partial}{\partial x_i} d\xi_t + \nu \frac{\partial^2}{\partial x_j \partial x_j} d\eta_t^i - d\eta_t^j \frac{\partial w_i}{\partial x_j} \right] dx \tag{62}$$

where the conservation of mass constrain (49) is applied to simplify the formula. Notice that the expected value of noise is zero because the random displacement is uncorrelated in time.

Then, the integral at the right-hand side can be interpreted as a spatial empirical mean of

zero-mean random process, and have to be null. With this simplification, the system (63) of

651 fluid dynamics equations is obtained.

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<sup>653</sup> Finally, the stochastic model for an incompressible (Newtonian) fluid reads:

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$$\begin{cases}
\frac{\partial w_i}{\partial t} + \frac{\partial (w_j w_i)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 w_i}{\partial x_j \partial x_j} + \frac{\nu}{3} \frac{\partial}{\partial x_i} \frac{\partial w_\ell}{\partial x_\ell} + \frac{1}{2} \frac{\partial^2 (a_{sk} w_i)}{\partial x_s \partial x_k} \\
\frac{\partial}{\partial x_i} \left( w_i - \frac{1}{2} \frac{\partial}{\partial x_j} a_{ij} \right) = 0 \\
\left( \frac{1}{\rho} \frac{\partial}{\partial x_i} d\xi_t = \nu \frac{\partial^2}{\partial x_j \partial x_j} d\eta_t^i - d\eta_t^j \frac{\partial w_i}{\partial x_j} \\
\frac{\partial}{\partial x_i} d\eta_t^i = 0
\end{cases}$$
(63)

The system is composed by two coupled sets of deterministic and stochastic non-linear partial differential equations, in the unknowns  $w_i$  and  $\sigma_{ij}$ . The pseudo-stochastic model is obtained by avoiding the resolution of the last two stochastic equations, and closing the system by providing an expression  $a_{ij}$  through physical assumptions.

Let us also outline that the system (63) has been obtained under the assumption that the drift velocity is of bounded variation. Removing this assumption, the separation of the regular and the stochastic terms cannot be performed anymore. Hence, one obtains a fully stochastic Nevier-Stokes composed by stochastic partial differential equations. For geophysical flows (for isochoric flows in general), the continuity equations is also stochastic; see [37].

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