**Corrected scheme for the integration of the SDEs in Lagrangian simulations**

As a reminder and to introduce notations, the system of stochastic differential equations (SDEs) for the particle-attached variables making up the particle state-vector $\mathbf{Z} = (\mathbf{x}_p, \mathbf{U}_p, \mathbf{U}_s)$ (with $\mathbf{x}_p$ the particle position, $\mathbf{U}_p$ its velocity and $\mathbf{U}_s$ the velocity of the fluid seen) is written as

$$dx_{p,i} = U_{p,i}\, dt \ , \tag{1a}$$

$$dU_{p,i} = \frac{U_{s,i} - U_{p,i}}{\tau_p}\, dt + A_{p,i}\, dt \ , \tag{1b}$$

$$dU_{s,i} = \Pi_{s,i}\, dt - \frac{U_{s,i} - \langle U_{f,i} \rangle}{T_i}\, dt + \sigma_i\, dW_i \ . \tag{1c}$$

The index $i$ refers to the space direction and in the SDE for $\mathbf{U}_s$, Eq. (1c), there is thus no summation on $i$. The term $\mathbf{A}_p$ contains possible additional forces acting on discrete particles, such as gravity, etc., which do not involve the instantaneous values of $\mathbf{U}_p$. In Eq. (1c), $\mathbf{\Pi}_s$ stands for a mean drift term involving the fluid mean pressure-gradient as well as other contributions. All these terms are described in several publications (cf. [1, 2, 4, 3]) and are not of real concern here since there are already handled by the current numerical scheme detailed in [2]. An important point is to note that the system of equations, Eq. (1), is written in the coordinate system aligned with the mean drift velocity, that is after the necessary rotation of coordinate system so that the system of equations involves only diagonal terms for the return-to-equilibrium and diffusion terms (each component is then treated separately, in other words $i$ by $i$).

In [2], a complete numerical approach based on exponential schemes was developed to obtain first- and even second-order numerical schemes in the weak sense (meaning that statistics derived from particles are approximated to a first or second order of accuracy with respect to the time step $\Delta t$). A rather unique characteristic of these schemes is that they allow to retrieve the correct numerical behaviour when one, or two, of the physical timescales involved in Eq. (1), namely $\tau_p$ and $T$, become much smaller than the time step. From a continuous point of view, this is referred to as 'fast-variable elimination' and the numerical scheme handles such limit behaviour without any switch between different formulas.

However, it was later revealed (I realized it about five years ago) that one such limit behaviour, or asymptotic cases as they are called in [2], was not correct. This corresponds to the situation where $\Delta t \gg \tau_p$ and $\Delta t \gg T$ *and when* $T = T(\mathbf{x})$ is varying in space. Since $T$ is proportional to $k/\langle\epsilon\rangle$, this is the case in non-homogeneous turbulent flows where it can happen that, in some flow areas, the chosen time step is much larger than local values. Thus, for fluid particles ($\tau_p \simeq 0$) and when $T \ll \Delta t$ while still varying in space, the limit behaviour was not correct and, in particular, the numerical scheme was not able to maintain a uniform particle concentration (the well-mixed condition). That shortcoming was analysed and addressed, from a continuous point of view in [3] (see the whole section 9.3 devoted to such issues). Further (unpublished)

numerical developments later revealed that it is possible to retrieve the correct limit behaviour by adding corrective terms to the expression of the numerical schemes already existing for $\mathbf{U}_s$, $\mathbf{U}_p$ and $\mathbf{x}_p$. Basically, this follows from the idea that a first-order expansion of $1/T(\mathbf{x})$ can be made in Eq. (1c), yielding additional terms such as

$$dU_{s,i} \simeq \Pi_{s,i}\,dt - \frac{U_{s,i} - \langle U_{f,i}\rangle}{T_i^{(0)}}\,dt - \left[\frac{1}{(T_i^{(0)})^2}\left(\frac{dT}{dx_i}\right)\delta x_{p,i}\right](U_{s,i} - \langle U_{f,i}\rangle) + \sigma_i\,dW_i$$

which introduce new correlations between $\mathbf{U}_s$ and $\mathbf{x}_p$ that need to be evaluated.

In this document, I will skip the numerical approximations made in the course of evaluating these (numerous) extra terms. However, should anyone be willing to check the formulas, I still have all the calculations on paper and that person would be quite welcome (Any candidate? Please, do not hesitate to send your application). Thus, in what follows, I directly state the results for the various extra terms that must be implemented in the code: this corresponds, respectively, to Eq. (3) for the numerical integration of $\mathbf{U}_s$, Eq. (5) for $\mathbf{U}_p$, and Eq. (7) for $\mathbf{x}_p$. As indicated in each of the three paragraphs below, these terms are to be added to the current expression of the corresponding numerical scheme. Note that they are presented in Eqs. (3), (5) and (7) without any attempt to factorize them even though some expressions appear several times. They need, of course, to be reorganized to avoid redundant calculations.

Remark: The specific work to be carried out corresponds to the implementation of the terms listed in Eqs. (3), (5) and (7) in Code_Saturne. Nevertheless, I have tried to provide further details and explanations with the introduction above and, especially, by developing afterwards the case of fluid particles under the heading 'Application to the tracer-particle limit'. I believe this to be of interest for applications in environmental studies when we mostly consider fluid elements or small aerosols that behave nearly as fluid particles.

In the following formulas, $\beta$ stands for

$$\beta = \left(\frac{dT}{dx}\right)\frac{\sigma^2}{T - \tau_p}$$

with, as already indicated, $T$ the timescale of the velocity of the fluid seen $\mathbf{U}_s$. In the various articles published (see [1, 2, 3, 4]), it is usually noted as $T_L^*$ but, for the sake of simplified notation (actually by sheer laziness), I have written it here as $T = T_L^*$ since there can be no confusion as to its meaning. Furthermore, we are basically dealing with an Euler exponential kind of scheme and, in that sense, all values are to be taken at the beginning of the time step $t = t^n$. Thus, $T = T^n = T(\mathbf{x}_p^n)$, $\tau_p = \tau_p^n$, $\beta = \beta^n$. I am also leaving out the indexes $i$ for $T_i$ and $\sigma_i$, which are often written as $T$ and $\sigma$, since we are treating each direction separately.

(i) **Added term to the numerical scheme for the integration of $\mathbf{U}_s$**

$$U_{s,i}^{n+1} = U_{s,i}^{n} + \text{ current scheme } + \delta\left(U_{s,i}\right) \tag{2}$$

where

$$\delta\left(U_{s,i}\right) = \beta\, T\left(T-\tau_p\right)\left[1-\left(1+\frac{\Delta t}{T}\right)e^{-\Delta t/T}\right] \tag{3a}$$

$$-\,\beta\,\frac{T^2}{2}\left[1-2e^{-\Delta t/T}+e^{2\Delta t/T}\right] \tag{3b}$$

$$+\,\beta\frac{\tau_p^2}{T+\tau_p}\left[T\left(1-e^{-\Delta t/T}\right)-\tau_p e^{-\Delta t/T}\left(1-e^{-\Delta t/\tau_p}\right)\right] \tag{3c}$$

(ii) **Added term to the numerical scheme for the integration of $\mathbf{U}_p$**

$$U_{p,i}^{n+1} = U_{p,i}^{n} + \text{ current scheme } + \delta\left(U_{p,i}\right) \tag{4}$$

where

$$\delta\left(U_{p,i}\right) = \beta\,\frac{T\,\tau_p^2}{T+\tau_p}\left(1-e^{-\Delta t/\tau_p}e^{-\Delta t/T}\right)-\beta\,T\Delta t\,e^{-\Delta t/T} \tag{5a}$$

$$+\,\frac{1}{2}\beta\,T\left(T-2\tau_p\right)\left(1-e^{-\Delta t/\tau_p}\right) \tag{5b}$$

$$+\,\beta\frac{T\,\tau_p}{T-\tau_p}\left(2T-\tau_p\right)\left(e^{-\Delta t/T}-e^{-\Delta t/\tau_p}\right) \tag{5c}$$

$$-\,\frac{1}{2}\frac{T^3}{\left(T-2\tau_p\right)}\left(e^{-2\Delta t/T}-e^{-\Delta t/\tau_p}\right) \tag{5d}$$

(iii) **Added term to the numerical scheme for the integration of $\mathbf{x}_p$**

$$x_{p,i}^{n+1} = x_{p,i}^{n} + \text{ current scheme } + \delta\left(x_{p,i}\right) \tag{6}$$

where

$$\delta\left(x_{p,i}\right) = \beta\,\frac{T\,\tau_p^2}{T+\tau_p}\Delta t+\beta\,T^2\Delta t\,e^{-\Delta t/T}-\beta\,T^3\left(1-e^{-\Delta t/T}\right) \tag{7a}$$

$$+\,\frac{1}{2}\beta\,T\left(T-\tau_p\right)\left[\Delta t-\tau_p\left(1-e^{-\Delta t/\tau_p}\right)\right] \tag{7b}$$

$$+\,\beta\,\frac{T\,\tau_p}{T-\tau_p}\left(2T-\tau_p\right)\left[T\left(1-e^{-\Delta t/T}\right)-\tau_p\left(1-e^{-\Delta t/\tau_p}\right)\right] \tag{7c}$$

$$-\,\frac{1}{2}\,\beta\,\frac{T^3}{\left(T-2\tau_p\right)}\left[\frac{T}{2}\left(1-e^{-2\Delta t/T}\right)-\tau_p\left(1-e^{-\Delta t/\tau_p}\right)\right] \tag{7d}$$

$$-\,\beta\,\frac{T^2\,\tau_p^4}{\left(T+\tau_p\right)^2}\left[1-e^{-\Delta t/\tau_p}e^{-\Delta t/T}\right] \tag{7e}$$

Application to the tracer-particle limit

The best way to appreciate the meaning of these additions is to consider the fluid-limit case, that is when we are dealing with fluid particles (this corresponds to the PDF method to turbulent single-phase flows). This is also probably the most relevant situation, as shown below. In both the continuous (*i.e.*, the SDEs) and numerical models, this is obtained by setting directly $\tau_p = 0$, which, in the numerical formulations, is properly handled thanks to the exponential scheme.

In this limit case of tracer or fluid particles, we get from Eqs. (3) and (5) that

$$\delta\left(U_{p,i}\right) = \delta\left(U_{s,i}\right) = \frac{1}{2}\,\tilde{\beta}\,T^2\left[1 - e^{-2\Delta t/T} - \frac{2\Delta t}{T}\,e^{-\Delta t/T}\right] \tag{8}$$

with

$$\tilde{\beta} = \beta(\tau_p = 0) = \left(\frac{dT}{dx}\right)\frac{\sigma^2}{T}\ . \tag{9}$$

The fact that $\delta\left(U_{p,i}\right) = \delta\left(U_{s,i}\right)$ is normal and is, in fact, a first consistency check since when $\lim \tau_p \to 0$, we have that $\mathbf{U}_p \to \mathbf{U}_s$.

In the usual situation, the time step is smaller than the characteristic timescale $T$ (in the fluid-limit case, there is of course only one physical timescale left, which is the correlation timescale of the velocity of fluid particles). Thus, when considering a Taylor expansion of Eq. (8) with $\Delta t \ll T$, we get

$$\delta\left(U_{s,i}\right) = \mathcal{O}(\Delta t^3) \tag{10}$$

which is, therefore, negligible even for a second-order scheme. In other words, in all 'normal situations' (corresponding to a time step which is much smaller than *local* values of $T(\mathbf{x})$), these added terms play no role. However, in the opposite situation when $\Delta t \gg T$ (usually in a local sub-domain of a complex flow), we obtain

$$\delta\left(U_{s,i}\right) = \frac{1}{2}\left(\frac{dT}{dx}\right)\sigma^2\,T\ . \tag{11}$$

The interesting limit concerns fluid particle positions. Taking $\tau_p = 0$ in Eq. (7), we have

$$\delta\left(x_{p,i}\right) = \frac{1}{2}\left(\frac{dT}{dx}\right)\sigma^2\,T\left[\Delta t + 2\Delta t\,e^{-\Delta t/T} - 2\,T\left(1 - e^{-\Delta t/T}\right) - \frac{T}{2}\left(1 - e^{-2\Delta t/T}\right)\right]\ . \tag{12}$$

In the usual situation when $\Delta t \ll T$, a Taylor expansion yields that

$$\delta\left(x_{p,i}\right) = \mathcal{O}(\Delta t^4) \tag{13}$$

which is therefore quite negligible. However, in the opposite case when $\Delta t \gg T$, the particle position correction term in Eq. (12) becomes

$$\delta\left(x_{p,i}\right) = \left[\frac{1}{2}\left(\frac{dT}{dx}\right)\sigma^2\,T\right] \times \Delta t \tag{14}$$

which is now a first-order corrective term. Note that, in this non-homogeneous diffusive limit (when $dT/dx \neq 0$), we get from Eqs. (11) and (14) that $\delta\left(x_{p,i}\right) = \delta\left(U_{s,i}\right) \times \Delta t$, which can be seen as an additional consistency check.

Let us see how the complete scheme for fluid particle positions is transformed when $T$ is much smaller than the timescale while still accounting for its variations. Using the expression of the current scheme given in [2] (when $\Delta t \gg T$), we get the following expression for particle positions in which I have reintroduced the superscripts $n$ and $n+1$ for previous and updated values

$$x_{p,i}^{n+1} = \underbrace{x_{p,i}^{n} + \langle U_f^n \rangle\, \Delta t + \left(\Pi_i^n\, T^n\right)\, \Delta t + \left(\sigma^n\, T^n\right)\, \sqrt{\Delta t}\, \xi_i^n}_{\text{current scheme}} + \underbrace{\left[\frac{1}{2}\left(\frac{dT^n}{dx}\right)(\sigma^n)^2\, T^n\right] \times \Delta t}_{\text{new term}} \tag{15}$$

where $\boldsymbol{\xi}$ are random numbers sampled in a normalized Gaussian distribution. In this equation, $\boldsymbol{\Pi}$ stands for the fluid mean-pressure gradient, which is the limit value of $\boldsymbol{\Pi}_s$ in the particle-tracer limit (*i.e.*, $\boldsymbol{\Pi}_s(\tau_p = 0) = \boldsymbol{\Pi}$) assuming also that particles are well-mixed.

For reasons explained in [3, section 9.3.4, pp. 86-92], the proper limit for the mean-pressure gradient $\boldsymbol{\Pi}$ in the present situation is the one obtained when velocities relax infinitely fast, and is given by (again there is an implicit dependence on space direction $i$ but I have left it out)

$$\Pi^n = \frac{d}{dx}\left[\frac{1}{2}(\sigma^n)^2\, T^n\right] \ . \tag{16}$$

This is equivalent to saying that, in this limit case, there is an equilibrium between the mean pressure gradient and the derivatives of Reynolds stresses, that is (using here proper indexes for the sake of clarity)

$$\Pi_i = -\frac{1}{\rho_f}\frac{\partial \langle P \rangle}{\partial x_i} \simeq \frac{\partial \langle u_{f,i}\, u_{f,j} \rangle}{\partial x_j} \ . \tag{17}$$

By working out the limit value of the Reynolds stresses resulting from the Simplified Langevin Model (SLM) used in the particle-tracer limit of Eq. (1c), we obtain the expression given in Eq. (16) (see further details and the use of an ersatz of Reynolds stresses due to the implicit parametrization of the SDEs to apply fast-variable elimination in [3, section 9.3.4]). Then, gathering the third and last terms on the rhs of Eq. (15) leads to

$$x_{p,i}^{n+1} = x_{p,i}^{n} + \langle U_f^n \rangle\, \Delta t + \frac{d}{dx}\left[\frac{1}{2}(\sigma^n\, T^n)^2\right]\, \Delta t + \left(\sigma^n\, T^n\right)\, \sqrt{\Delta t}\, \xi_i^n \ . \tag{18}$$

Noting

$$\Gamma_t = 1/2(\sigma\, T)^2 \ , \tag{19}$$

the complete scheme for fluid particle positions can thus be written as

$$x_{p,i}^{n+1} = x_{p,i}^{n} + \langle U_f^n \rangle\, \Delta t + \left(\frac{d\,\Gamma_t^n}{dx}\right)\, \Delta t + \sqrt{2\,\Gamma_t^n\, \Delta t}\, \xi_i^n \ . \tag{20}$$

This is indeed the correct complete expression for what is referred to as the 'composition PDF model'. As explained in Pope's book (see [5, section 12.7.4 and, especially, exercise 12.56 on page 548]), this is the right expression with $\Gamma_t$ the turbulent diffusivity. It is further taken up and developed in [3, section 9.3.4 on page 92].

From the previous developments, it can be seen that the satisfactory limit of the numerical scheme relies upon using the expression of the mean pressure-gradient consistent with the underlying behaviour of the Langevin model for the velocity of fluid particles in the limit when they become infinite fast variables, cf. Eq. (16). In a Moment/PDF hybrid formulation (the wrongly named Euler-Lagrange one), this is not necessarily verified by the mean pressure gradient provided by the fluid solver (here Code_Saturne). This means that we should introduce an additional closure for this term, for instance a simple interpolation between the provided value, say $\mathbf{\Pi}^E$, and the one, say $\mathbf{\Pi}^L$, given by Eq. (16), for instance something like

$$\mathbf{\Pi} = \left(1 - e^{-\Delta t/T}\right) \mathbf{\Pi}^L + e^{-\Delta t/T}\, \mathbf{\Pi}^E \ . \tag{21}$$

But, at the moment, this is just a basic proposition and this point will need to be addressed in more detail later on.

conclusion: This means that we have now a numerical scheme matching theoretical developments in the sense that *the diffusive limit of a velocity PDF retrieves a composition PDF*. To my knowledge, this has never been achieved before, perhaps even never addressed (see how things are presented in Pope's book in the section mentioned above where there is no hint to a possible link). In more practical terms, this means that we should be able to run simulations for particles (here fluid particles but that remains valid for discrete ones) even when locally $\Delta t \gg T$ with $T(\mathbf{x})$ being non-constant, since we would get the correct diffusive limit in such sub-domains without loosing the underlying physics and, in particular, the respect of the well-mixed condition.

Should this be easier to grasp for you, I can re-express what is stated above in terms of more classical formulations based on Moments (as you know, I strongly dislike and refute the terminology of so-called Eulerian methods). To get the key points, it is useful to consider that we are also adding a scalar (or a set of scalars) to the model in Eqs. (1) which becomes

$$dx_{p,i} = U_{p,i}\, dt \ , \tag{22a}$$

$$dU_{p,i} = \frac{U_{s,i} - U_{p,i}}{\tau_p}\, dt + A_{p,i}\, dt \ , \tag{22b}$$

$$dU_{s,i} = \Pi_{s,i}\, dt - \frac{U_{s,i} - \langle U_{f,i}\rangle}{T_i}\, dt + \sigma_i\, dW_i \ , \tag{22c}$$

$$d\phi = -\frac{\phi - \langle\phi\rangle}{\tau_\phi}\, dt + S(\phi)\, dt \ . \tag{22d}$$

The first term of the rhs of Eq. (22d) is the IEM (Interaction by Exchange with the Mean) model which accounts for micro-mixing effects (due to molecular diffusivity) while the second

one represents a possible chemical source term (usually a non-linear but known function in terms of $\phi$). The fact that both particle polydispersity (through $\tau_p$) and chemical source terms (through $S(\phi)$) are treated without approximation is probably the key interest of PDF, or particle stochastic, methods for polydisperse turbulent reactive flows. Yet, what is emphasized below is not linked to either the specific choice of a micro-mixing model or a chemical source term and we could limit ourselves to a passive scalar, whereby $d\phi = 0$ along each particle trajectory. The relevant point is what happens to corresponding closures of the scalar flux terms.

The model in Eqs. (22) yields a fluid one by putting $\tau_p = 0$ (note therefore that fluid turbulence models including scalars are then simply a sub-category of the complete one in Eqs. (22))

$$dx_{p,i} = U_{s,i}\, dt \ , \tag{23a}$$

$$dU_{s,i} = \Pi_{s,i}\, dt - \frac{U_{s,i} - \langle U_{f,i} \rangle}{T_i}\, dt + \sigma_i\, dW_i \ , \tag{23b}$$

$$d\phi = -\frac{\phi - \langle \phi \rangle}{\tau_\phi}\, dt + S(\phi)\, dt \ , \tag{23c}$$

or, alternatively, $d\phi = 0$ as mentioned above. This is referred to as a velocity-scalar PDF model (since these models are formulated as Lagrangian ones, the particle position variable always exists). As demonstrated in several publications (see, for instance, [6, 7]) and specifically detailed in Pope's book (see [5, chapter 12]), the system of Eqs. (23) corresponds to a full second-order moment, that is a Reynolds-stress model (here a Rotta model) for $\langle u_i\, u_j \rangle$ as well as a full second-order model (*i.e.*, transport equations) for the scalar fluxes $\langle u_i\, \phi \rangle$. In that case, both the Reynolds stresses and scalar fluxes are non-local functions in space since they are solutions of transport equations. Now, when considering that $T \to 0$ while $\sigma \to +\infty$ but such that $(\sigma\, T) \to \Gamma_t$ (from a continuous point of view), we get the continuous limit system

$$dx_{p,i} = \langle U_{f,i} \rangle\, dt + \left( \frac{d\, \Gamma_t}{dx} \right)\, dt + \sqrt{2\, \Gamma_t}\, dW_i \ , \tag{24a}$$

$$d\phi = -\frac{\phi - \langle \phi \rangle}{\tau_\phi}\, dt + S(\phi)\, dt \ . \tag{24b}$$

The resulting moment equation for the mean scalar $\langle \phi \rangle$ shows that this corresponds to a first-order model and to an eddy-diffusivity type of closure (see details in [5, section 12.7.4] and [3, section 9.3.4]). Note that such closures are now local in space. From a numerical point of view, these manipulations are reflected by the limit $\Delta t \gg T$ (with implicitly the same assumptions on $\sigma$), which led us to Eq. (20) which is, precisely, the numerical scheme corresponding to the continuous limit equation in Eq. (24a)!

*Let me reformulate*: with the present extended numerical scheme, we are able to simulate the transition between second-order models (transport equations for scalar fluxes) to first-order ones (local expressions of scalar fluxes through a gradient hypothesis and an eddy-diffusivity concept).

This transition is simulated in a 'continuous' manner, *i.e.* there are no artificial switches: the numerical scheme simply obeys to the underlying physical behaviour (as it should be).

As a remark, you can note that, with present parametrization, fluid particle velocities become infinitely fast-variables and are eliminated from the continuous system, cf. Eqs. (24). From a numerical point of view, particle velocities do not cease to exist but become independent variables at each time step. Actually, it is quite possible to analyse in a similar manner the transition between Reynolds-stress models to turbulent-viscosity ones such as the (dubious) $k-\epsilon$ model. This is a bit trickier than the presentation above for scalars (which is why I chose the one with scalars, for the sake of simplicity), since it involves handling two different types of parametrization at the same time. However, this can be done, showing that we would have the same numerical transition from second- to first-order models both for scalars and for the Reynolds stress. But, this will be shown in another episode of our saga...

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