Coupling PDEs and SDEs: the illustrative example of the multiscale simulation of viscoelastic flows

Benjamin Jourdain, Claude Le Bris, Tony Lelièvre[1]

CERMICS, Ecole Nationale des Ponts et Chaussées, 6 & 8 Av. Pascal, 77455 Champs-sur-Marne, France {jourdain,lebris,lelievre}@ cermics.enpc.fr

1 A prototypical system

We would like to address here various mathematical and foremost numerical issues raised by the simulation of systems featuring a Partial Differential Equation (PDE) together with a Stochastic Differential Equation (SDE). For such a class of systems, that we henceforth called *hybrid* systems, we choose as a prototypical system the following one:

$$\begin{cases} \dfrac{\partial u}{\partial t}(t,y) - \dfrac{\partial^2 u}{\partial y^2}(t,y) = \dfrac{\partial f}{\partial y}(t,y) \\ \\ \forall\, y, \quad \begin{cases} f(t,y) = \mathbb{E}\big(\varphi(X_t(y))\big) \\ \\ dX_t(y) = g(u(t,y), X_t(y), t)\, dt \,+\, \sigma(X_t(y), t)\, dW_t \end{cases} \end{cases} \tag{1}$$

Here, the PDE of the first line is supposed to hold, say, for the space-variable y varying in a one-dimensional interval $[0, L]$, while time t varies from 0 to T. With respect to the unknown scalar field u, it is of the form of the heat equation, with a right-hand side somehow unusual, though. For any $y \in [0, L]$, we then have the last two lines of (1). The second line rules the coupling between the PDE and the SDE: the solution $X_t(y)$ (varying in $\mathbb{R}$) of the SDE is used to evaluate an expectation value which provides the PDE with a right-hand side (that is a force term). The last line consists in a SDE, that is parameterized in y, and by the solution $u(t, y)$ of the PDE. The data are the functions φ, g, σ. System (1) is at this stage formulated somewhat vaguely, but the mathematical sense of the PDE and the SDE can be made precise, as well as the regularity of the data involved, and the initial conditions (1) is supplied with. The reason why such a system is not only a toy-system convenient for an expository survey, but meaningful and relevant from the application viewpoint will be made clear below.

The main feature we wish to already emphasize and discuss is the nature of system (1). For this purpose, let us at once mention that such a system stands at the intersection of various families

- that of systems coupling a *continuous description* with a *discrete description*, as is the case for instance when coupling a PDE and an Ordinary Differential Equation (ODE): a case of interest is e.g. that where the method of characteristics is used in addition to, or in replacement of, the solution of an advection equation; the same could apply to the use of particle methods; from the physical standpoint, the same could also apply to systems coupling different physical modellings, as is the case when an atomistic description of matter is coupled to a continuum description in material sciences;
- that of systems coupling *deterministic techniques* with *Monte-Carlo type techniques* for solving one, or many, PDE(s); here we could have chosen to replace the third line of (1) by the associated Fokker-Planck equation, since what is only needed is the law of X_t to compute $f(t, y)$, and nothing else, but for computational purposes in the high dimensional case, we have preferred the simulation of the SDE;
- that of systems *coupling different scales*, where the effective coefficients involved in one equation are computed from another one, like is the case when homogenization techniques, or more generally averaging techniques, are resorted to: here the r.h.s. f can be thought of as the averaged response of a finer scale (described by the internal variable X_t) subject to the sollicitation $u(t, y)$.

The above problem is in some sense a superposition of all the previous contexts: it is an hybrid system in the continuous/discrete sense, in the deterministic/stochastic sense, in the multiscale sense. In a somewhat provocative way, we could tentatively say that system (1) is a *multiphysics, multimathematics, multiscale* system !

As we have just underlined the similarity with various classes of systems, let us now mention what system (1) is *not*:

- there are situations when a PDE and a SDE are simulated separately on different domains, and the coupling only holds in terms of boundary or compatibility conditions at the common interface (see [BLTQ] e.g.); such a coupling often holds for computational purposes (solving a PDE rather than a SDE can be cheaper on one zone, while the converse might be true on another zone); this is not the case here as one SDE holds at each point where the PDE is set;
- the deterministic equation and the stochastic equation can be coupled through the time variable, as is the case for mixed ODE/SDE systems in chemical kinetics, e.g.; here we assume that the time variable is alike in the two equations, and that the difference of scales lies in the space variable;
- in some context, the stochastic nature comes as a perturbation of a deterministic equation, as is the case for a PDE with stochastic coefficients (see

e.g. the Stochastic Navier Stokes equation [M98]); here *two* equations are at play.

Each of the above family of systems could equally justify a work in the spirit of the present one, but this is not our aim here.

In the following, we shall as announced concentrate on system (1). Our interest in such a system originates from a particular context, that of the simulation of polymeric fluid flows, which we shall introduce in the next section. We will review there the main results on the mathematical analysis and numerical analysis that are available in the literature to date, and mention some implementation issues. In doing this, as this is the main purpose of the present article, we will as much as possible try to emphasize the general facts and trends that seem to us to be valid outside the necessarily limited scope of the context under examination. Next, in Section 3, we shall see other situations, still in the general context of fluid flow simulations, where systems of the spirit of (1) are relevant. Section 4 will aim at showing one example, in a context far from fluid mechanics, also involving systems of the same type as (1).

Let us conclude this introductory section by emphasizing that simulating a hybrid system such as (1) of course requires up-to-date techniques for either of the two equations, for the PDE on the one hand, and for the SDE on the other hand. Our goal is not to present a state-of-the-art survey of either class of techniques separately, but rather to see how some representative techniques of either category interact with the other camp. Nevertheless, while our main focus is the *back and forth* interaction between the two equations, we shall allow us to review also some works when the SDE can be considered as parameterized by the solution of the PDE, the latter being considered as known (see Sections 2.2 and 3.3).

2 Modeling dilute solutions of flexible polymers

The numerical simulation of incompressible viscous non-Newtonian fluids typically requires the simulation of systems of the type

$$\begin{cases} \dfrac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\,\mathbf{u} - \Delta\mathbf{u} + \nabla p - \operatorname{div}\boldsymbol{\tau}_p = \boldsymbol{f}_{ext}, \\ \qquad\qquad\qquad\qquad\qquad\qquad \operatorname{div}\mathbf{u} = 0 \\ \qquad\qquad\qquad\qquad\qquad\qquad \dfrac{D\boldsymbol{\tau}_p}{Dt} = \mathcal{G}(\boldsymbol{\tau}_p, \nabla\mathbf{u}), \end{cases} \tag{2}$$

where the first line is the equation of conservation of momentum, the second one translates the incompressibility constraint and the third one is a differential equation ruling the evolution of the non-Newtonian part $\boldsymbol{\tau}_p$ of the stress tensor. In the above equations, $\mathbf{u}$ of course stands for the velocity of the fluid, p for its pressure, while $\boldsymbol{f}_{ext}$ is some external force. On purpose, we have

omitted in the above system (and we will continue to do so throughout this article) all the physical parameters and constants, setting them to unity. The third line is often called a *constitutive law* or a *closure equation* and aims at providing a closed relation between the stress $\boldsymbol{\tau}_p$ and the velocity field $\mathbf{u}$: there, $\dfrac{D}{Dt}$ stands for a convective derivative, while the right-hand side $\mathcal{G}$ symbolically stands for an intricate function of the fields involved. One of the most famous instance of such a system is that for Oldroyd-B fluids, where the third equation precisely reads

$$\boldsymbol{\tau}_p + \frac{\partial \boldsymbol{\tau}_p}{\partial t} + \mathbf{u} \cdot \nabla \boldsymbol{\tau}_p - \boldsymbol{\tau}_p (\nabla \mathbf{u})^T - \nabla \mathbf{u}\, \boldsymbol{\tau}_p = \nabla \mathbf{u} + \nabla \mathbf{u}^T. \tag{3}$$

Alternately, one can replace the differential form of the third line of (2) by an equation in the integral form. We refer to [K89, OP02] for a general introduction to the mechanical context and the standard numerical tools to simulate systems of the form (2).

The well established commonly used strategy in fluid mechanics consists in derivating on the basis of mechanical arguments adequate differential (or integral) equations, i.e. forms for $\mathcal{G}$, and next solving system (2). Apart from this mainstream, an emerging field in non-Newtonian fluid mechanics, still mostly unexplored from the standpoint of mathematical analysis, was born in the early 1990s. It relies upon the introduction of a kinetic description of the fluid, at a finer scale, with a view to modelling the very phenomena from which the non-Newtonian feature of the fluid stems. A successful instance of this alternative track concerns the modelling of polymeric fluids. For such fluids, the key issue is to adequately simulate the evolution of the microstructures present at each macroscopic point of the fluid flow, that is the evolution of the polymeric chains wiggling in the fluid. A complete theory, initiated by the works of Doi and Edwards has given rise to a numerical approach, the so-called *micromacro* approach: see the reference treatises [DE86], [D92], [BAH87, BCAH87] for the physical background, [Ott96], [OP02] for the simulation techniques, and the recent review article [K03]. The idea is to keep the first two equations of (2), but replace the third line of (2), i.e. the effective description of the evolution of $\boldsymbol{\tau}_p$, by the following two-step procedure: the expression of $\boldsymbol{\tau}_p$ reads

$$\boldsymbol{\tau}_p(t,\mathbf{x}) = \int (\mathbf{r} \otimes \boldsymbol{F}(\mathbf{r}))\, \psi(t,\mathbf{x},\mathbf{r})\, d\mathbf{r} \tag{4}$$

and is an averaged response of all the possible configurations of a representative polymer chain subject to the constraints in the flow, the latter being described by the Fokker-Planck equation

$$\begin{aligned} &\frac{\partial \psi(t,\mathbf{x},\mathbf{r})}{\partial t} + \mathbf{u} \cdot \nabla_{\mathbf{x}} \psi(t,\mathbf{x},\mathbf{r}) \\ &= -\mathrm{div}_{\mathbf{r}} \left((\nabla_{\mathbf{x}} \mathbf{u}\, \mathbf{r} - \boldsymbol{F}(\mathbf{r})) \psi(t,\mathbf{x},\mathbf{r}) \right) + \frac{1}{2} \Delta_{\mathbf{r}} \psi(t,\mathbf{x},\mathbf{r}). \end{aligned} \tag{5}$$

The distribution function $\psi(t, \mathbf{x}, \mathbf{r})$ describes the probability to find at time t (in $[0, T]$), and at the macro point $\mathbf{x}$ (in the computational domain $\mathcal{D}$), the polymer chain in the configuration $\mathbf{r}$, the latter variable typically varying in $\mathbb{R}^N$. Equation (5) will be considered henceforth as a prototypical Fokker-Planck type equation. Indeed analogous equations, more involved technically but of the same type formally, would hold when the configuration of the polymer chain is more in details described in a configuration space $\mathbb{R}^N$ of large dimension. Equation (5) is here written in the dumbbell case (see Section 2.1) for which N is equal to the dimension of the ambient space $\mathcal{D}$, i.e. 2 or 3. As N might be very large, depending on the degree of accuracy employed to describe the configuration of the chain, the simulation of the partial differential equation (5) in ψ might not be tractable numerically. Let us nevertheless mention that some groups are making huge efforts and progress in this direction, see [L03, SJA02], and that this validates the need for mathematical studies of the coupled system with the Fokker-Planck equation: see [R91] or [LZZ04] for a local-in-time existence result of regular solutions. An alternative possibility is to simulate the SDE underlying this PDE, and the approach summarizes as the simulation of the system

$$\begin{cases} \begin{cases} \dfrac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\,\mathbf{u} - \Delta\mathbf{u} + \nabla p - \operatorname{div}\boldsymbol{\tau}_p = \boldsymbol{f}_{ext}, \\ \qquad\qquad\qquad\qquad\qquad \operatorname{div}\mathbf{u} = 0, \end{cases} \\ \begin{cases} \qquad\qquad \boldsymbol{\tau}_p(t,\mathbf{x}) = \mathbb{E}\big(\mathbf{R}_t(\mathbf{x}) \otimes \boldsymbol{F}(\mathbf{R}_t(\mathbf{x}))\big), \\ d\mathbf{R}_t(\mathbf{x}) + \mathbf{u}\cdot\nabla\mathbf{R}_t(\mathbf{x}) = (\nabla\,\mathbf{u}\,\mathbf{R}_t(\mathbf{x}) - \boldsymbol{F}(\mathbf{R}_t(\mathbf{x}))\,dt + d\mathbf{W}_t. \end{cases} \end{cases} \tag{6}$$

At this stage, the reader may understand much of the relevance of our toy system (1).

To giving a synthetic view of the micromacro approach and comparing it to the more conventional purely macroscopic approach, a concise statement is to say that system (2), of the form

$$\begin{cases} \dfrac{D\mathbf{u}}{Dt} &= \mathcal{F}(\boldsymbol{\tau}_p, \mathbf{u}), \\ \dfrac{D\boldsymbol{\tau}_p}{Dt} &= \mathcal{G}(\boldsymbol{\tau}_p, \mathbf{u}), \end{cases} \tag{7}$$

is replaced by (6) of the form

$$\begin{cases} \dfrac{D\mathbf{u}}{Dt} &= \mathcal{F}(\boldsymbol{\tau}_p, \mathbf{u}), \\ \boldsymbol{\tau}_p &= \boldsymbol{\tau}_p(\Sigma) \\ \dfrac{D\Sigma}{Dt} &= \mathcal{G}_\mu(\Sigma, \mathbf{u}), \end{cases} \tag{8}$$

where Σ stands for an internal variable describing the state of the microstructure. The micromacro approach (8) essentially consists in increasing the number of scalar unknowns, and therefore is intrinsically more costly (in term of CPU time and memory requirements) than the macroscopic approach (7). In the present state-of-the-art, the micromacro approach (8) is still in its infancy and cannot compete in terms of computational efficiency with the standard and much more mature purely macroscopic approach (7). Nevertheless, it provides with a systematic track for improving closure relations, or at least fitting parameters of those, and already reveals as an efficient backroom strategy for such a purpose. This, and the hope it generates, suffices to justify a mathematical investment in such systems. In addition to this, it must be emphasized that, when simulating system (8), the numerical treatment of the Fokker-Planck equation by deterministic techniques is definitely more efficient than that of the associated SDE. Nevertheless, due to the dimension of the space where Σ varies, the latter techniques are not always tractable. *Unless a deterministic technique can be applied*, the stochastic simulation at the SDE level remains the method of choice, and this calls for a numerical analysis of the approach. In the present state-of-the-art, the latter will be performed in a low dimensional space, but with a view to applying to the large dimension case.

2.1 The simplest possible model

The simplest occurence of a system such as (6) is obtained a) when coarse-graining the description of the polymer chain into a single *dumbbell*, that is *one* spring between two beads, b) when the (purely entropic) force between the two beads simply reads as the *Hookean* force $\boldsymbol{F}(\mathbf{r}) = \frac{1}{2}\mathbf{r}$, and c) when the ambient flow considered is a Couette flow. Then system (6) simplifies into

$$\left\{\begin{array}{l} \dfrac{\partial u}{\partial t}(t,y) - \dfrac{\partial^2 u}{\partial y^2}(t,y) = \dfrac{\partial \tau}{\partial y}(t,y) + f_{ext}(t,y), \\ \forall\, y, \quad \left\{\begin{array}{l} \tau = \mathbb{E}\left(X_t^y Y_t\right), \\ \left\{\begin{array}{l} dX_t^y = (-\dfrac{1}{2}X_t^y + \dfrac{\partial u}{\partial y}(t,y)\, Y_t)\, dt + dV_t, \\ dY_t = -\dfrac{1}{2}Y_t\, dt + dW_t. \end{array}\right. \end{array}\right. \end{array}\right. \tag{9}$$

where u denotes the component along the x axis of the velocity $\mathbf{u}$ depending only on y, while τ denotes the off-diagonal term of the extra stress tensor $\boldsymbol{\tau}_p$, the only relevant component in view of the simple geometry. On the other hand, (X_t, Y_t) denotes the two components of $\mathbf{R}_t$, and (V_t, W_t) is a two dimensional Brownian motion.

The model is typically relevant for a polymeric flow in a rheometer. The radius of the inner cylinder is almost the same as that of the outer cylinder, both are large, and the streamlines are expected to be cylinders as well: this justifies geometrically the approximation by a one dimensional flow. Therefore

the model is not only mathematically convenient, but also rather close to an experimental device indeed utilized in practice in Mechanics.

In comparison to the "general" system (6), system (9) is simplified in two respects. First, because we consider a *shear flow*, the SDE is not a stochastic *partial* differential equation: the transport term $\mathbf{u}\cdot\nabla\mathbf{R}_t$ vanishes for geometrical reasons. Therefore the coupling between two processes $\mathbf{R}_t(\mathbf{x}) = (X_t^y, Y_t^y)$ at different $\mathbf{x}$ boils down into the simple coupling term $\dfrac{\partial u}{\partial y}\, Y_t^y$, i.e. *via* the macroscopic flow. This significantly simplifies both the analysis (see [LL04] for a more general mathematical work) and the implementation. Second, because we consider *Hookean dumbbells* in a shear flow, the nonlinear term $\nabla\,\mathbf{u}\,\mathbf{R}_t(\mathbf{x})$ reduces here to the term $\dfrac{\partial u}{\partial y}\, Y_t$, which is linear since Y_t can be computed independently from $\mathbf{u}$ and X_t^y (and therefore does not depend on y, thus the notation Y_t). It is thus rather easy to prove the existence and uniqueness of a global-in-time weak solution (see [JLL02]). In fact, it is to be noted that the Hookean dumbell model as written in (9) in the Couette case, is indeed equivalent to the Oldroyd-B model, for the stress tensor calculated from (9) indeed satisfies the simplest one-dimensional form of the Oldroyd-B equation (3). In this respect, the Hookean dumbbell appears as a test situation for mathematical analysis, numerical analysis, and also algorithmic techniques, and no more than that.

System (9) is typically discretized as follows: the equation of conservation of momentum is discretized by finite difference in the time variable, and by finite elements for the space variable. $P1$ finite elements for the velocity, and $P0$ finite elements for the stress tensor are both easy to manipulate and convenient. The Galerkin formulation of the macroscopic equation therefore reads:

$$\frac{1}{\Delta t}\int_{\mathcal{D}} (\overline{u}_h^{n+1} - \overline{u}_h^n)v + \int_{\mathcal{D}} \frac{\partial \overline{u}_h^{n+1}}{\partial y}\frac{\partial v}{\partial y} = -\int_{\mathcal{D}} \overline{S}_{h,n}\frac{\partial v}{\partial y} + \int f_{ext}(t_n, y)v, \quad (10)$$

for $P1$ test functions v, where the superscript n stands for the time discretization, while the subscript h stands for the space discretization. Regarding the SDEs, they are discretized by an Euler explicit scheme in time, and of course by a Monte-Carlo sampling (M realizations of each random process)[1]:

$$\begin{cases} \overline{X}^j_{h,n+1} - \overline{X}^j_{h,n} = \left(-\dfrac{1}{2}\overline{X}^j_{h,n} + \dfrac{\partial \overline{u}_h^{n+1}}{\partial y}\overline{Y}^j{}_n\right)\Delta t + \left(V^j_{t_{n+1}} - V^j_{t_n}\right), \\ \overline{Y}^j{}_{n+1} - \overline{Y}^j{}_n \quad = -\frac{1}{2}\overline{Y}^j{}_n\,\Delta t + (W^j_{t_{n+1}} - W^j_{t_n}). \end{cases} \quad (11)$$

This then provides

[1] We omit here a cut-off procedure on the process Y_t that is unbounded, and refer to [JLL02] for this technical detail.

$$\overline{S}_{h,n+1} = \frac{1}{M} \sum_{j=1}^{M} \overline{X}^j_{h,n+1} \overline{Y}^j_{n+1}, \tag{12}$$

which is to be inserted in the right hand side of (10) at the next timestep. The crucial point to make, and that applies to all the models we refer to in this section, is that unlike the continuous level where the velocity u is a deterministic quantity, the fully discretized equations involve a velocity $\overline{u}^n_h$ that is indeed a random variable, since the empirical mean (12) is inserted in (10), *in lieu of* the expectation $\tau = \mathbb{E}\left(X^y_t Y_t\right)$. The three-fold discretization (discretization in time, discretization in space, discretization in Monte-Carlo) is a highly unusual feature, that in some sense characterizes the family of problems we are dealing with here. Correspondingly, this translates in the error estimate that has been first established in [JLL02] (see [ELZ02] for an independent work), that is

$$\left|\left|u(t_n) - \overline{u}^n_h\right|\right|_{L^2_y(L^2_\omega)} + \left|\left|\mathbb{E}(X_{t_n} Y_{t_n}) - \frac{1}{M} \sum_{j=1}^{M} \overline{X}^j_{h,n} \overline{Y}^j_n\right|\right|_{L^1_y(L^1_\omega)} \leq C \left(h + \Delta t + \frac{1}{\sqrt{M}}\right),$$

for a constant C independent of h and $\Delta t \leq \frac{1}{2}$, but dependent on the data.

Note the occurence of L^p_ω norms in the left-hand side, in order to account for the random nature of the objects manipulated. The orders of convergence in the right-hand side are as expected: Δt in time because of the Euler scheme (used twice), $\dfrac{1}{\sqrt{M}}$ for the Monte-Carlo sampling, while the rate h stands here because of the $P0$ finite element approximation for the stress (while it can be shown, see [L04], that the error in L^2 norm for the velocity itself scales as h^2, again as expected for $P1$ finite element).

2.2 Non Hookean models

Less simple models than the Hookean model have been introduced, with a view to accounting for various physical phenomena of importance. In this respect, one important step is to account for the finite extensibility of the polymer chains, a fact that was ignored in the simple Hookean dumbell model where X_t and Y_t were unbounded processes.

The FENE model

Still in the context of a Couette flow, the FENE model (this acronym standing for Finite Extensible Nonlinear Elastic) reads

$$\begin{cases} \dfrac{\partial u}{\partial t}(t,y) - \dfrac{\partial^2 u}{\partial y^2}(t,y) = \dfrac{\partial \tau}{\partial y}(t,y) + f_{ext}(t,y), \\ \tau = \mathbb{E}\left(\dfrac{X_t^y Y_t^y}{1 - \frac{(X_t^y)^2 + (Y_t^y)^2}{b}} \right), \\ \begin{cases} dX_t^y = \left(-\dfrac{1}{2} \dfrac{X_t^y}{1 - \frac{(X_t^y)^2 + (Y_t^y)^2}{b}} + \dfrac{\partial u}{\partial y}(t,y)\, Y_t^y \right) dt + dV_t, \\ dY_t^y = \left(-\dfrac{1}{2} \dfrac{Y_t^y}{1 - \frac{(X_t^y)^2 + (Y_t^y)^2}{b}} \right) dt + dW_t. \end{cases} \end{cases} \tag{13}$$

where the parameter b stands for the maximum (squared) length of the polymer chain.

Contrary to (9), due to the fact that Y_t^y here depends on X_t^y, the system (13) is fully nonlinear through the term $\dfrac{\partial u}{\partial y}(t,y)\, Y_t^y$, and its mathematical analysis is one order of magnitude more difficult than that of (9).

Mathematically, only a small-in-time existence and uniqueness result for system (13) has been established to date. It can be established either in Sobolev spaces (see [JLL04a]) or in Hölder spaces (see [ELZ04]), the former aiming at giving a sound ground to the numerical simulations. Regarding the SDE itself, the proof of the existence of a strong global-in-time solution falls in four steps, by a standard sequence of arguments in stochastic analysis: first, proof of existence of strong solution to the SDE without the shear term $\dfrac{\partial u}{\partial y}\, Y_t^y$, second, proof of existence of a weak solution by the use of a Girsanov transform to account for the shear term, third, proof of trajectorial uniqueness, and fourth, application of the Yamada-Watanabe Theorem. An alternative direct proof of existence of strong solutions is also possible by using the notion of multivalued SDEs (see [C94, JL02]). Nevertheless, the introduction of the notion of weak solutions is useful for establishing the regularity of the stress τ with a view to proving the existence for the coupled system. For the latter, only a local-in-time result has been proven. All efforts to improve this local-in-time result into a global one have failed to date[2]. In particular, the mathematical study of the Cauchy problem for such a nonlinear system cannot be expected to be, by any means, simpler than purely nonlinear macroscopic system of the type (2), which requires huge efforts mathematically, see [LM00, FGO02].

This difficulty encountered at the very mathematical level gives us the opportunity to make a few remarks, that we believe to be valid generally. In the absence of a transport term in the SDE (a fact due, we recall it, to the simplicity of the geometry of the Couette flow), and in the absence of any dependence of the diffusion coefficient upon the stochastic processes (X_t^y, Y_t^y)

[2]We have recently become aware that E. Süli (see [BSS04]) and P.L. Lions have independently announced proofs of existence of global weak solutions for the FENE model, under convenient conditions.

(we will see an opposite situation for rod-like models in Section 3.1), the only difficulty in analyzing the SDE lies in the possible singular character of the drift coefficient. Of course, the lack of regularity of the drift term might be circumvented by dealing with weak solutions of the SDE rather than strong solutions[3].

Concerning the existence of solution for the SDE, if $\dfrac{\partial u}{\partial y}$ has a meaning pointwise in y, the natural idea is to also give a sense to the SDE pointwise in y[4]. Then the stress τ has also a meaning pointwise in y, which is, one should notice it, precisely what is done for models with a macroscopic constitutive law (2), see the review article [FGO02]. We then concentrate on the regularity *in time* of the drift coefficient. This coefficient is a combination of two terms which are very different in nature: the entropic force term $\dfrac{(X_t^y, Y_t^y)}{1 - \frac{(X_t^y)^2 + (Y_t^y)^2}{b}}$ and the shear term $\dfrac{\partial u}{\partial y} Y_t^y$. Due to physical reasons, the force term often derivates from a convex potential and is more an advantage than a difficulty for the analysis. On the other hand, the regularity in time of the shear term is typically bootstrapped from the macroscopic equation itself.

The solution of the SDE is used for the computation of the stress τ. Since all what is needed is the expectation value τ that only depends on the law, it seems it is enough to concentrate on the existence of weak solutions. However, this does not seem to be enough to provide the regularity needed for defining the stress. Fortunately, as the singularity of the function in the expression of the stress tensor is *the same as* that in the drift term of the SDE, the analysis turns out to be possible.

As far as the numerical analysis of system (13) is concerned, a bottleneck that has not been circumvented nor overcome so far, is the lack of a numerical analysis concerning the convergence of a singular function of the Euler discretized process associated with an SDE involving a drift coefficient with a related singularity. It is indeed possible to prove the weak convergence of the Euler scheme, even in the presence of a singular drift coefficient of the explosive form of (13) (see [GK96]), but the convergence of the stress τ remains an open problem. In the absence of such an analysis, it has not been possible to date to address that of the coupled system (13).

[3] Recall that for a weak solution, the driving Brownian motion, the probability space and the filtration are altogether part of the solution, while they are considered given for a strong solution.

[4] If u is not regular enough to define its derivative $\dfrac{\partial u}{\partial y}$ pointwise in y, our approach collapses, and one would need to build a "variational" definition of the solution of the SDEs.

The FENE-P model

A slight modification of the above FENE model proceeds from the wish to obtain an equivalent purely macroscopic model (a property that the FENE model does not enjoy, to the best of the common knowledge) while keeping track in the modelling of the finite extensibility of the polymer chain. This modification consists in replacing the squared length of the chain in the denominators of (13) by its expectation value. The model obtained this way is called FENE-P (the P standing for Peterlin):

$$\begin{cases} \dfrac{\partial u}{\partial t} - \dfrac{\partial^2 u}{\partial y^2} = \dfrac{\partial \tau}{\partial y} + f_{ext}, \\ \tau = \mathbb{E}\left(\dfrac{X_t^y Y_t^y}{1 - \frac{\mathbf{E}\left((X_t^y)^2 + (Y_t^y)^2\right)}{b}} \right), \\ \begin{cases} dX_t^y = \left(-\dfrac{1}{2} \dfrac{X_t^y}{1 - \frac{\mathbf{E}\left((X_t^y)^2 + (Y_t^y)^2\right)}{b}} + \dfrac{\partial u}{\partial y} Y_t^y \right) dt + dV_t, \\ dY_t^y = \left(-\dfrac{1}{2} \dfrac{Y_t^y}{1 - \frac{\mathbf{E}\left((X_t^y)^2 + (Y_t^y)^2\right)}{b}} \right) dt + dW_t. \end{cases} \end{cases} \tag{14}$$

It should be remarked that the SDE is now nonlinear in the sense of MacKean, precisely because of the presence of the expectation value in the drift coefficient.

In [JL04], the well-posedness of the SDE, together with the convergence of the stress tensor, when the expectation values in the SDEs and in the expression of the stress are replaced by empirical means, toward the exact stress tensor are proven. Both proofs are performed for a more general geometry than that of a Couette flow, however in the context where the flow u is supposed to be known and regular enough.

2.3 Variance reduction issues

Needless to say, noise reduction issues are crucial in the numerical simulation of systems such as (1). Again, we do concentrate on the peculiarity of this question *in the presence of a coupling* and not on the general question of noise reduction. As a pedagogic case study, let us come back to the simulation of the simplest system (9) and mention the following practical observation. Two numerical experiments can be performed: the simulation of (9) as such and the simulation of (9) when the Brownian motion V_t is assumed to also depend on the space variable y (or more precisely on its discrete counterpart):

$$dX_t^y = \left(-\frac{1}{2} X_t^y + \frac{\partial u}{\partial y}(t, y)\, Y_t \right) dt + dV_t^y.$$

It is intuitive that in the latter case, as the noise inserted in the system is more important, the variance on the result is higher. It is indeed the case, and this observation is valid beyond the simple one-dimensional simulation considered here, that the variance on the velocity u increases. However, and this is a highly counterintuitive fact, the variance on the stress tensor τ_p diminishes. In [JLL04b], the phenomenon was analyzed in details, which is possible precisely because of the simplicity of the situation at hand. It was demonstrated how a coupling between the SDEs and the PDE makes possible such an observation. Notably, it was shown that in the absence of the coupling, that is when the term $\dfrac{\partial u}{\partial y}$ is given extrinsically, the counterintuitive diminution of the variance of the stress is replaced by a growth in the variance, as is the case for the velocity !

Related to this observation on the crucial impact that the coupling may have on the variance of the results is the following one. As we pointed out, the velocity field u and the stress τ are both, once fully discretized, random variables. Therefore, the relevant output of a simulation is the averaged result over many simulations, carried out independently. Apart from the discretization parameters h, Δt and M mentioned above, a fourth relevant parameter is thus N_e, the number of numerical experiments carried out. In the absence of a coupling, the result is insensitive to each of M and N_e, only the product of the two being meaningfull. But, because of the coupling between various realizations of the SDE *via* the macroscopic term $\dfrac{\partial u}{\partial y}$, there is an intricate non trivial interplay between M and N_e. On system (9), it can be again explained which is the most efficient choice for M and N_e (see [JLL04b]).

3 Modeling various fluids

3.1 Liquid crystals

In Section 2, we have considered dilute solutions of flexible polymers. Some other polymers behave more like rigid rods, and this introduces some anisotropy in the system. Solutions of such rigid polymers are called polymeric liquid crystals. One of the main aspect to take into account in the modelling of solutions of rodlike polymers is that the interaction of the polymers becomes important at much a lower concentration than with flexible polymers.

One model is the Doi model (see [DE86, Ott96]), which describes the evolution for a configuration vector $\mathbf{R}_t$ by a stochastic differential equation:

$$\begin{aligned} & d\mathbf{R}_t + \mathbf{u}.\nabla \mathbf{R}_t \, dt \\ & = \left(\mathrm{Id} - \frac{\mathbf{R}_t \otimes \mathbf{R}_t}{||\mathbf{R}_t||^2} \right) \left(\left(\nabla \mathbf{u} \, \mathbf{R}_t - \frac{1}{2} B^2 \nabla V(\mathbf{R}_t) \right) dt + B d\mathbf{W}_t \right) \\ & \quad - \frac{d-1}{2} B^2 \frac{\mathbf{R}_t}{||\mathbf{R}_t||^2} \, dt, \end{aligned} \tag{15}$$

where B is a positive constant and $d = 2$ or 3 is the dimension of the ambient space. Notice that B may also be a function $B(\mathbf{R}_t)$ in some models (with then an additional term involving $\nabla(B^2)$ in the drift term). Notice also that we assume that all the initial conditions $\mathbf{R}_0(\boldsymbol{x})$ have a fixed length L so that $\forall(t, \boldsymbol{x})$, $||\mathbf{R}_t(\boldsymbol{x})|| = ||\mathbf{R}_0(\boldsymbol{x})|| = L$. The potentiel V accounts for the mean-field interaction between the polymers. For example, the Maier-Saupe potential is:

$$V(\mathbf{R}) = -\frac{1}{L^4}\mathbb{E}(\mathbf{R}_t \otimes \mathbf{R}_t) : \mathbf{R} \otimes \mathbf{R}. \tag{16}$$

The stress tensor is then given by:

$$\boldsymbol{\tau}_p(t) = \mathbb{E}(\mathbf{U}_t \otimes \mathbf{U}_t) + \mathbb{E}\Big(\mathbf{U}_t \otimes \big((\mathrm{Id} - \mathbf{U}_t \otimes \mathbf{U}_t)\, \nabla V(\mathbf{U}_t)\big)\Big) - \mathrm{Id} \tag{17}$$

where $\mathbf{U}_t = \dfrac{\mathbf{R}_t}{L}$ is the rod orientation. We have neglected the viscous contribution in (17). The fully coupled system then consists in the first two equations of (6) with (15)–(17), thus again giving a system of type (1). Notice that the main differences with system (6) are the nonlinearity in the sense of MacKean due to the presence of the expectation value in the potential V and the fact that the diffusion term depends on the process $\mathbf{R}_t$.

For an analysis of the coupled system with the Fokker-Planck version of (15)–(17) in the special case of shear flow, we refer to [ZZ04]. The long-time behaviour of the Fokker-Planck equation has been studied in [CKT04]. Some numerical methods to solve the stochastic differential equation (15) are proposed in [Ott96]. On the other hand, we are not aware of any rigorous numerical analysis of numerical methods to solve this system without closure approximation.

3.2 Concentrated suspensions

Let us now slightly change the context. For concentrated suspensions (such as muds or clays), one model available in the literature is the Hebraud-Lequeux model [HL98]. This model describes the rheology of the fluid in terms of a Fokker-Planck equation ruling the evolution in time of the probability of finding, at each point, the fluid in a given state of stress. In a one-dimensional setting such as, again, the Couette flow, the stress at the point y and at time t is determined by one scalar variable σ:

$$\begin{cases} \dfrac{\partial p}{\partial t}(t, y, \sigma) = -\dfrac{\partial u}{\partial y}(t, y)\dfrac{\partial p}{\partial \sigma}(t, y, \sigma) + D(p)\,\dfrac{\partial^2 p}{\partial \sigma^2}(t, y, \sigma) \\ \qquad\qquad -H(|\sigma| - 1)p(t, y, \sigma) + D(p)\delta_0, \\ D(p) = \displaystyle\int_{|\sigma|\geq 1} p(t, y, \sigma)\, d\sigma. \end{cases} \tag{18}$$

In the above system, where we have again on purpose omitted all physical constants, the function H denotes the Heaviside function. It aims at modelling

the presence of a threshold constraint (here set to one): when the constraint is above the threshold, the stress relaxes to zero, which translates into the two last terms of the Fokker-Planck equation. The diffusion in the stress space is also influenced nonlinearly by the complete state of stress, as indicated by the definition of $D(p)$. On the other hand, the function $\dfrac{\partial u}{\partial y}(t,y)$ accounts for a shear rate term, here provided by the macroscopic flow. The contribution to the stress at the point y under consideration is then given by the average

$$\tau(t,y) = \int_{\mathbf{R}} \sigma\, p(t,y,\sigma)\, d\sigma. \tag{19}$$

The fully coupled system consisting of the Fokker-Planck equation (18), the expression (19) of the stress tensor, and the macroscopic equation for the Couette flow (first line of (9)) has been studied mathematically in a series of work [CCG03, CCGL04, CL04].

Alternately to a direct attack of the Fokker-Planck equation (18), one might wish to simulate the associated SDE *with jumps* that reads

$$d\sigma_t = \frac{\partial u}{\partial y}\, dt \,+\, \sqrt{2\mathbb{P}(|\sigma_t| \geq 1)} \quad dW_t \,-\, 1_{\{|\sigma_{t^-}|\geq 1\}}\sigma_{t^-}\, dN_t, \tag{20}$$

where W_t is a Brownian motion and N_t is an independent Poisson process with unit intensity. Note that, in addition to the jumps, equation (20) is nonlinear in the sense of MacKean, as the diffusion coefficient depends on the marginal law of the solution at time t.

The coupled system to simulate then reads in the form of a system of type (1) (note the SDE has jumps, though)

$$\left\{ \begin{array}{l} \dfrac{\partial u}{\partial t}(t,u) - \dfrac{\partial^2 u}{\partial y^2}(t,y) = \dfrac{\partial \tau}{\partial y}(t,y) \\ \forall y, \left\{ \begin{array}{l} \tau(t,y) = \mathbb{E}(\sigma_t(y)) \\ d\sigma_t(y) = \dfrac{\partial u}{\partial y}\, dt \,+\, \sqrt{2\mathbb{P}(|\sigma_t(y)| \geq 1)} \quad dW_t \,-\, 1_{\{|\sigma_{t^-}(y)|\geq 1\}}\sigma_{t^-}(y)\, dN_t. \end{array} \right. \end{array} \right. \tag{21}$$

Numerical simulations of this system have been carried out successfully (see [G]), but in the absence of any numerical analysis to date.

3.3 Coupling PDEs and SDEs for the simulation of dispersed two-phase flows

Dispersed two-phase flows are characterized by the presence of one phase (either solid, liquid or vapour) as separate inclusions called particles in the other phase called fluid. In both the following examples, the evolution of particles is modelled by a SDE (or the associated Fokker-Planck equation) while fluid equations are written for the other phase. In the example of dispersed turbulent two-phase flows, there is only a one-way coupling : the particles motion is

influenced by the drag force of the fluid. In the example of sprays, the reverse coupling also holds : the drag force appears as a driving force in the equation for the conservation of the momentum of the fluid.

Dispersed turbulent two-phase flows

In the approach proposed by [M01], the fluid phase is described by a classical turbulence model such as the $k-\epsilon$ model. It gives at each time t and each point x the mean velocity of the fluid $\langle U_f\rangle$, the covariance matrix of the velocity, the mean pressure $\langle P\rangle$ and the mean dissipation rate of energy $\langle\epsilon\rangle$. On the other hand, the particles are described by a Lagrangian approach. An extension of Kolmogorov theory suggests that the acceleration of the fluid velocity U_s seen by particles is a fast variable which can be modeled by a SDE driven by a d-dimensional Brownian motion W. This leads to the following evolution for the position X, the velocity U_p and the fluid velocity seen U_s

$$dX(t) = U_p(t)dt \tag{22}$$

$$dU_p(t) = \frac{1}{\tau_p}(U_s(t) - U_p(t))dt + gdt \tag{23}$$

$$dU_s^i(t) = \left(\sum_{j=1}^{d}(\langle U_p^j\rangle - \langle U_s^j\rangle)\frac{\partial\langle U_f^i\rangle}{\partial x_j} - \frac{1}{\rho_f}\frac{\partial\langle P\rangle}{\partial x_i} - \frac{U_s^i(t) - \langle U_s^i\rangle}{T_{L,i}^*}\right)(t, X(t))dt + \sqrt{C_0^*\langle\epsilon\rangle(t, X(t))}\, dW_t^i,\ i \le d, \tag{24}$$

where g denotes the gravity and ρ_f the fluid density. On the other hand, the quantities τ_p, $T_{L,i}^*$ and C_0^* depend on U_p, U_s and on the mean fields representing the fluid in a very intricate manner that is made precise in [M01]. Function $\langle U_p\rangle(t,x)$ (resp. $\langle U_s\rangle(t,x)$) stands for the conditional expectation $\mathbb{E}(U_p(t)|X(t) = x)$ (resp. $\mathbb{E}(U_s(t)|X(t) = x)$). The full coupled system then reads:

$$\begin{cases} k-\epsilon \text{ model giving } < U_f >, < P >, < \epsilon > \\ \qquad \text{and (together with } U_p \text{ and } U_s)\ \tau_p,\ T_{L,i}^* \text{ and } C_0^*, \\ (22)\text{–}(23)\text{–}(24). \end{cases}$$

When $(X(t), U_p(t), U_s(t))$ admits a density $p(t,x,u,v)$ with respect to the Lebesgue measure, one has

$$\langle U_p\rangle(t,x) = \frac{\displaystyle\int_{\mathbb{R}^{2d}} up(t,x,u,v)dudv}{\displaystyle\int_{\mathbb{R}^{2d}} p(t,x,u,v)dudv} \quad \text{and} \quad \langle U_s\rangle(t,x) = \frac{\displaystyle\int_{\mathbb{R}^{2d}} vp(t,x,u,v)dudv}{\displaystyle\int_{\mathbb{R}^{2d}} p(t,x,u,v)dudv}.$$

Because of the presence of these functions in the r.h.s. of (24), the SDE (22)–(24) is nonlinear in the sense of MacKean with an ill-behaved nonlinearity. As

a consequence, a rigorous study of existence and uniqueness is an open issue probably of outstanding difficulty.
The numerical approach proposed in [MPC03] is a particle-mesh method. The mean quantities are evaluated at the grid points either from the $k-\epsilon$ fluid model ($\langle U_f \rangle$, $\langle P \rangle$ and $\langle \epsilon \rangle$) or from the particle data ($\langle U_p \rangle$ and $\langle U_s \rangle$). These values are projected on the particles positions to integrate forward in time (22)–(24). Last, $\langle U_p \rangle$ and $\langle U_s \rangle$ are averaged at the grid points from the new positions and velocities of the particles.

Modelling of sprays in a fluid phase

According to [D00], a spray can be modelled by a kinetic equation, usually a variant of the Boltzmann equation in which a force acting on the particles is due to the surrounding fluid. It describes the evolution of the particle density function $f(t,x,v,r)$ which gives the density of particles in the spray with position x, velocity v and radius r at time t. In a simple form, it writes

$$\partial_t f + v.\nabla_x f + \nabla_v.(Ff) = Q(f), \tag{25}$$

where Q is a kernel modelling the effects of collisions, coalescences and breakups of the particles and the drag force F of the fluid on the particles is given by

$$F(t,x,v,r) = -\frac{4}{3}\pi r^3 \nabla_x p(t,x) - D(v-u(t,x)), \tag{26}$$

p and u being the pressure and the velocity fields of the fluid and D a drag coefficient. This equation can be considered as the Fokker-Planck equation associated with a stochastic process with jumps, at least in the absence of the coalescence and breakup phenomena which may modify the total amount of particles $\int f dx dv dr$. The ambient fluid is described by a set of Euler equations, relative to the density ρ and the velocity u multiplied by the volume fraction $\alpha = 1 - \int \frac{4}{3}\pi r^3 f dv dr$:

$$\begin{cases} \dfrac{\partial(\alpha\rho)}{\partial t} + \nabla_x.(\alpha\rho u) = 0, \\ \dfrac{\partial(\alpha\rho u)}{\partial t} + \nabla_x.(\alpha\rho u \otimes u) + \nabla_x p = \displaystyle\int -Ff\, dv dr, \\ p = p(\rho). \end{cases} \tag{27}$$

The full coupled system of type (1) is then (27)–(25).

From a numerical point of view, the fluid equations (27) are usually solved by standard deterministic methods (finite volume techniques for instance). As the phase space dimension is 7, equation (25) is discretized by a particle method involving a stochastic treatment of the r.h.s. like for the standard Boltzmann equation [BD03]. Only few mathematical studies concerning the derivation of the above equations or the existence and behaviour of solutions seem to exist (see the references in [D00]).

4 An example outside fluid mechanics: photon transport

Hot enough matter (such as plasma) spontaneously emits photons. The photons travel in the spatial domain $\mathcal{D}$ and can be emitted, scattered by the electrons or absorbed by the matter. A simple model reads as follows:

$$\lambda(\theta)\frac{\partial\theta}{\partial t}(t,x) + q(x)\theta(t,x) = \frac{q(x)}{4\pi}\int_{\mathcal{S}_2} f(t,x,w)dw, \tag{28}$$

$$\frac{\partial f}{\partial t}(t,x,v) + v.\nabla_x f(t,x,v) + \sigma(x)\left(f(t,x,v) - \frac{1}{4\pi}\int_{\mathcal{S}_2} f(t,x,w)dw\right) + q(x)f(t,x,v) = q(x)\theta(t,x), \tag{29}$$

where the unknows are the photon density (or radiative intensity) $f(t,x,v)$ (here supposed not to depend on the frequency of the photons) and the fourth power $\theta(t,x)$ of the temperature. The space variable is $x \in \mathcal{D}$ and v denotes the velocity which belongs here to the unit sphere $\mathcal{S}_2$. Equation (28) is the energy balance equation, while (29) rules the motion of the photons. In equations (28)–(29), $\lambda(\theta)$ denotes the heat capacity of the matter multiplied by $\theta^{3/4}$, and q and σ are respectively the opacity of the matter and the Thomson scattering coefficient. We assume that the nonnegative function σ is bounded from above be the constant $\bar{\sigma}$.

As in previous cases (see e.g. Section 3.2), one can use a stochastic process to represent solutions to (29). More precisely, when $q \equiv 0$, (29) is the Fokker-Planck equation associated with the following SDE with jumps (see [LPS98]):

$$\begin{cases} dX_r^{x,v} = V_r^{x,v}\,dr, \\ dV_r^{x,v} = 1_{\{\bar{\sigma}\mathcal{U}_{N_r} \le \sigma(X_{r^-}^{x,v})\}}\left(\mathcal{V}_{N_r} - V_{r^-}^{x,v}\right)dN_r, \\ (X_0^{x,v}, V_0^{x,v}) = (x,v), \end{cases} \tag{30}$$

where $(N_r)_{r\ge 0}$ is a Poisson process with intensity $\bar{\sigma}$ independent from the sequence $(\mathcal{U}_k, \mathcal{V}_k)_{k\ge 1}$ of independent vectors uniformly distributed $[0,1]\times\mathcal{S}_2$. Using the process $(X_r^{x,v}, V_r^{x,v})$, the solution of (29) can be expressed for a general opacity q as the solution of the following variational formulation: for any test function φ on $\mathcal{D}\times\mathcal{S}_2$, $\forall t \ge s$,

$$\begin{aligned} &\int_{\mathcal{D}\times\mathcal{S}_2} \varphi(x,v)f(t,x,v)dxdv \\ &= \int_{\mathcal{D}\times\mathcal{S}_2} \mathbb{E}\left(\varphi(X_{t-s}^{x,v}, V_{t-s}^{x,v})e^{-\int_0^{t-s} q(X_\tau^{x,v})d\tau}\right) f(s,x,v)\,dxdv \\ &+ \int_s^t \int_{\mathcal{D}\times\mathcal{S}_2} \mathbb{E}\left(\varphi(X_{t-r}^{x,v}, V_{t-r}^{x,v})e^{-\int_0^{t-r} q(X_\tau^{x,v})d\tau}\right) q(x)\theta(r,x)\,dxdvdr. \end{aligned} \tag{31}$$

From a numerical point of view, the difficulty in the discretization of (28)–(29) comes from the r.h.s. of (28). It is needed to build a discretization scheme

which allows for an implicit treatment of the dependence of $\int_{\mathcal{S}_2} f(t,x,w)dw$ upon θ, in order to get the most stable scheme. The so-called Symbolic Monte Carlo method (see [S01]) consists in computing f as a function of θ from (29) in order to get a closed implicit equation (see (32) below) for θ (see also [FC71] for another approach).

Let us introduce a spatial mesh $\{M_i,\ i \in I\}$ and a time-step $\Delta t > 0$. The numerical procedure consists in approximating θ by space-time functions, piecewise constant on the cells $[n\Delta t,(n+1)\Delta t] \times M_i$:

$$\theta^n = \sum_{i\in I} \theta_i^n 1_{M_i}(x)$$

and f by a sum of (weighted) Dirac masses:

$$f^n = \sum_{k=1}^{\nu_n} w_k^n \delta_{(X_k^n,V_k^n)},$$

where ν_n denotes the number of Dirac masses, w_k^n the weights and (X_k^n,V_k^n) some random variables associated with a discretization of (30). Equation (28) is then discretized by a classical implicit Euler and finite element scheme, while one uses (31) with $\varphi(x,v) = 1_{M_i}(x)$ to implicitely compute the r.h.s. of (28).

We thus obtain the following algorithm: knowing (θ^n, f^n), θ^{n+1} is obtained as the solution (obtained by a Newton method) of:

$$\lambda(\theta_i^{n+1})\frac{\theta_i^{n+1}-\theta_i^n}{\Delta t} + q_i\theta_i^{n+1} = \frac{q_i}{4\pi|M_i|\Delta t}\left(A_i^n + \sum_{j\in J} W_{i,j}\theta_j^{n+1}\right),\ i \in I \quad (32)$$

where A_i^n and $W_{i,j}$ are defined by:

$$A_i^n = \int_{\mathcal{D}\times\mathcal{S}_2} \mathbb{E}\left(\int_0^{\Delta t} 1_{M_i}(X_s^{x,v}) e^{-\int_0^s q(X_\tau^{x,v})d\tau} ds\right) f^n(dx,dv),$$

$$W_{i,j} = \int_{M_j\times\mathcal{S}_2} \mathbb{E}\left(\int_0^{\Delta t} (\Delta t - s) 1_{M_i}(X_s^{x,v}) e^{-\int_0^s q(X_\tau^{x,v})d\tau}\, ds\right) q(x)\, dxdv.$$

Notice that the matrix W does not depend on time and can be precomputed off-line by a Monte Carlo method. The vector A^n is also computed by a Monte-Carlo method, using an ensemble of processes obtained by a time-discretization of (30). These processes are then used to compute f^{n+1}, together with an appropriate updating of the weights and of the number of particles, to account for the opacity q in (29).

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