Coupling Brownian Motion and Heat Equation: Toward a New Description of Multi-Nature Phenomena∗

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Abstract

In this paper we are concerned with a nonstandard application of the multiscale model presented in [Cristiani et al., Multiscale Model. Simul., 9 (2011), 155–182]. That approach was originally proposed to couple a microscopic and a macroscopic model which describe the same advection-based phenomenon. Here we extend this approach in the direction of coupling the Langevin equation for a particle with the associated Fokker-Plank equation, in order to describe, in a multiscale fashion, multi-nature phenomena like the wave-particle duality in quantum mechanics. As a preliminary attempt, we consider here the simple case of the Brownian motion coupled with the heat equation.

1 Introduction

In this paper we are concerned with a nonstandard application of the multiscale model originally presented in §1. That model allows one to simulate the evolution of a large number of moving and possibly interacting particles both at the microscopic scale (where single particles’ positions are observed) and at the macroscopic scale (where only particles’ average density is observed). The main feature of the model is that the two scales coexist and interact everywhere in the domain and at any time, and they evolve by means of a common multiscale dynamics which can be seen as a linear combination of the microscopic and the macroscopic dynamics. As a result, the overall dynamics is able to catch correctly at both scales some phenomena which are characteristic of one scale only.

A natural application of that model is the description of multi-nature phenomena, like, e.g., the wave-particle duality of elementary particles in quantum mechanics. Moving in this direction, we should couple the Langevin equation for a particle, which describes a single realization of its trajectory, with the associated Fokker-Plank equation, which instead describes the evolution of the particle’s probability density function.

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In this paper we present some preliminary results, more precisely we consider the simple case of the Brownian motion coupled with the heat equation.

2 The multiscale model

In this section we briefly recall the main ideas underlying the multiscale model introduced in [1] avoiding heavy technicalities. A more rigorous, scale-free description of the model can be found in [1], within a modeling framework based on abstract measures.

The multiscale model apply whenever one has two models which describe the same physical phenomenon at different scales. To fix the ideas, we can assume that we are interested in tracking the evolution of \( N \) particles in the space \( \mathbb{R}^d \) and that we can describe the dynamics by means of a microscopic (i.e., agent-based) and a macroscopic (i.e., continuous) first-order model.

We denote by \( X^k(t) \in \mathbb{R}^d \) the position of the \( k \)-th particle, by \( X := (X^1, \ldots, X^N) \) the vector of the positions, and by \( X^{-k} = (X^1, \ldots, X^{k-1}, X^{k+1}, \ldots, X^N) \) the vector of the positions but the \( k \)-th. We also denote by \( \rho(t,x) \) the average density of the particles at \( x \in \mathbb{R}^d \) and time \( t > 0 \). As usual, we assume that the microscopic model is constituted by a system of ordinary differential equations of the form

\[
\dot{X}^k(t) = v_m[X^{-k}(t)](X^k(t)), \quad k = 1, \ldots, N, \tag{1}
\]

where \( v_m[X^{-k}](x) \) is the given microscopic velocity field at \( x \), which possibly depends on the positions of all the other particles. The macroscopic model is instead assumed to be constituted by a conservation law of the form

\[
\frac{\partial}{\partial t} \rho(t,x) + \nabla \cdot (\rho(t,x) v_M[\rho(t,\cdot)](x)) = 0, \quad t > 0, \quad x \in \mathbb{R}^d, \tag{2}
\]

where \( v_M[\rho](x) \) is the macroscopic velocity field at \( x \), which, similarly to the microscopic case, possibly depends on the density \( \rho \) in all the space.

The multiscale model is based on a suitable combination of the microscopic and macroscopic velocity fields. To get it, \( v_m \) and \( v_M \) have to be defined on the same domain. The macroscopic velocity \( v_M \) is already defined at any \( x \in \mathbb{R}^d \), then it can be simply computed at the points \( X^k \) in order to use it in (1) in place of \( v_m \). The case of the microscopic velocity is instead more complicated. Indeed, \( v_m \) is only defined at the particles’ positions, and not everywhere in the space. This can be fixed in several ways depending on the specific application, see [1]. Once the two velocity fields are made directly comparable, they are coupled by defining a multiscale velocity field as a linear combination of the two, i.e.

\[
v[X,\rho] := \theta v_m[X] + (1 - \theta) v_M[\rho], \quad \theta \in [0,1]. \tag{3}
\]

Finally, the new velocity field \( v \) takes the place of both \( v_m \) and \( v_M \) in (1)-(2), so that both the particles and their density evolve by means of the same velocity. As a consequence, the particles and their density should be considered as a whole, since they are driven by the same velocity field, which, in turn, is computed with the contribution of both of them.
The key parameter of the multiscale model is the number $\theta \in [0, 1]$, which controls the contribution of the discrete and continuous components in the computation of the velocity field. Note that both scales evolve regardless the value of $\theta$, and even if $\theta = 0$ or 1.

3 Coupling Brownian motion and heat equation

In this section we show, by means of a specific example in mathematical physics and probability theory, how the coupling idea described in Section 2 can be extended to a large class of equations.

3.1 Derivation of the coupled equations

Let us consider the following system of stochastic differential equations

$$\begin{cases}
    dX^k_t = dW^k_t, \\
    X^k_0 = 0
\end{cases}, \quad k = 1, \ldots, N, \quad (4)$$

where $W^k_t$ is the $d$-dimensional Brownian motion (standard Wiener process). The Fokker-Planck equation associated with the Brownian motion is the heat equation

$$\begin{cases}
    \frac{\partial u}{\partial t} - \frac{1}{2} \Delta u = 0, \quad t > 0, \quad x \in \mathbb{R}^d \\
    u(0, x) = \delta_0, \quad x \in \mathbb{R}^d,
\end{cases}, \quad (5)$$

where $\delta_0$ is the Dirac delta centered in 0. The solution $u$ to (5) describes the time evolution of the probability density function of the Brownian motions generated by (4), i.e. $\mathbb{P}(X^k_t \in A) = \int_A u(t, x) \, dx, \forall A \subset \mathbb{R}^d, \forall k$. Defining the macroscopic velocity field $v_M$ as

$$v_M(t, x) := -\frac{\nabla u(t, x)}{2u(t, x)}, \quad (6)$$

equation (5) can be formally written as

$$\begin{cases}
    \frac{\partial u}{\partial t} + \nabla \cdot (uv_M) = 0, \quad t > 0, \quad x \in \mathbb{R}^d \\
    u(0, x) = \delta_0, \quad x \in \mathbb{R}^d.
\end{cases}, \quad (7)$$

The form (7) makes the velocity field $v_M$, which transports the probability density function, appear explicitly. On the microscopic side, let us write (4) as

$$\begin{cases}
    d\xi^k_t = d\xi^k_t, \\
    X^k_0 = 0
\end{cases}, \quad k = 1, \ldots, N, \quad (8)$$

where $\xi^k$ is the Gaussian white noise process. It is important to note that the velocities $\xi^k_t, k = 1, \ldots, N$ define a vector field only at the particle positions $X^k_t, k = 1, \ldots, N$. 3
In order to make the macroscopic part of the system interact with the microscopic part, the latter should define a microscopic velocity field at every point \( x \) of the space. This can be done by using the following natural definition for the microscopic (stochastic) velocity field \( v_m \)

\[
v_m(t, x) := \begin{cases} \frac{1}{|J(t, x)|} \sum_{\ell \in J(t, x)} \xi_{\ell t}, & \text{if } J(t, x) \neq \emptyset \\ 0, & \text{if } J(t, x) = \emptyset, \end{cases}
\]

(9)

where \( J(t, x) := \{ k \in \{1, \ldots, N\} : X_k^t = x \} \).

Once the velocity field is defined at both scales, it is possible to define

\[
v := \theta v_m + (1 - \theta) v_M, \quad \theta \in [0, 1].
\]

(10)

Since

\[
0 = \frac{\partial u}{\partial t} + \nabla \cdot (uv) = \frac{\partial u}{\partial t} + \nabla \cdot \left( u \frac{1}{|J|} \sum_{\ell \in J} \xi_{\ell t} \right) + \nabla \cdot \left( u(1 - \theta) \frac{-\nabla u}{2u} \right)
\]

\[
= \frac{\partial u}{\partial t} + \theta \nabla \cdot \left( u \frac{1}{|J|} \sum_{\ell \in J} \xi_{\ell t} \right) - \frac{1}{2}(1 - \theta) \Delta u,
\]

the fully-coupled dynamics is

\[
\begin{cases}
\frac{dX_k^t}{dt} = \theta dW_k^t + (1 - \theta) \frac{-\nabla u(t, X_k^t)}{2u(t, X_k^t)} dt, \quad t > 0, \quad k = 1, \ldots, N \\
\frac{\partial u}{\partial t} + \theta \nabla \cdot \left( u \frac{1}{|J|} \sum_{\ell \in J} \xi_{\ell t} \right) - \frac{1}{2}(1 - \theta) \Delta u = 0, \quad t > 0, \quad x \in \mathbb{R}^d
\end{cases}
\]

(11a) (11b)

with initial conditions \( X_0^k = 0, \quad k = 1, \ldots, N \), and \( u(0, x) = \delta_0 \). The system (11a)-(11b) couples a system of ordinary-stochastic differential equations with a deterministic-stochastic advection-diffusion partial differential equation.

### 3.2 Numerical approximation of the single-scale equations

In the following we restrict the discussion to the dimension one \( (d = 1) \). The heat equation \([5]\) can be solved analytically and we have

\[
u(t, x) = \frac{1}{\sqrt{2\pi t}} e^{-x^2/2t}, \quad v_M(t, x) := -\frac{\nabla u(t, x)}{2u(t, x)} = \frac{x}{2t}.
\]

(12)

Let us introduce a structured space-time grid with spatial cell size \( \Delta x \) and a time step \( \Delta t \). We denote space cells by \( E_i = [x_i - \frac{\Delta x}{2}, x_i + \frac{\Delta x}{2}] \), where \( x_i = i \Delta x \), and by \( \phi_{in} \) the approximate value of a generic function \( \phi(t, x) \) at \( x = x_i \) and \( t = t_n = n \Delta t \).
The numerical approximation of (11a)-(11b) is extremely hard. Let us approach it step by step. First of all, let us discretize (5) and (7). Equation (5) can be easily discretized by means of a first-order centered finite difference scheme

\[ u_{n+1}^i = u_n^i + \frac{1}{2} \frac{\Delta t}{\Delta x^2} \left( u_{n+1}^{i+1} - 2u_n^i + u_{n-1}^i \right), \quad n \in \mathbb{N}, \ i \in \mathbb{Z}. \]  

(13)

Equation (7) instead, although it is formally equivalent to (5), must be carefully approximated by a scheme which respects the directionality of the vector field \( v_M \) (assumed to be given) [2]. To this end, let us define the flux \( f[v_M] := uv_M \) and consider the standard upwind scheme for space-dependent changing-sign velocities,

\[ u_{n+1}^i = u_n^i + \frac{\Delta t}{\Delta x} \left( -L_n^i[f] + G_n^{-i}[f] + G_n^{i+}[f] \right), \quad n \in \mathbb{N}, \ i \in \mathbb{Z}, \]  

(14)

where the L(oss) term is given by

\[ L_n^i[f] := |f_n^i|, \]  

(15)

and the G(ain) terms are given by

\[ G_n^{-i}[f[v_M]] := \begin{cases} f_n^{i-1}, & \text{if } (v_M)_n^{i-1} \geq 0 \\ 0, & \text{if } (v_M)_n^{i-1} < 0 \end{cases}, \quad G_n^{i+}[f[v_M]] := \begin{cases} -f_n^{i+1}, & \text{if } (v_M)_n^{i+1} \leq 0 \\ 0, & \text{if } (v_M)_n^{i+1} > 0 \end{cases}. \]  

(16)

To avoid to manage the initial datum \( \delta_0 \) at the discrete level, we set the initial time for the simulation at \( t_0 = \frac{1}{2} \) and, consequently, the new initial datum at \( u(t_0, x_0) = \frac{1}{\sqrt{2\pi t_0}} \exp \frac{-x^2}{2t_0} \). The computational domain is set at \([-10, 10]\).

Figure 1: Left: Initial datum \( u(t_0, x) \). Center: Function \( u_{\text{parab}}(t = 5, x) \). Right: Function \( u_{\text{iperb}}(t = 5, x) \)

Figure 1 shows the initial datum \( u(t_0, x) \), the numerical solution \( u_{\text{parab}} \) of (5) obtained by (13) at time \( t = 5 \), and the numerical solution \( u_{\text{iperb}} \) of (7) obtained by (14) at time \( t = 5 \).

Regarding the microscopic part, the Ito processes satisfying (4) can be approximated by using the weak Euler scheme

\[ X_{n+1}^k = X_n^k + \Delta W_n^k, \quad k = 1, \ldots, N \]  

(17)
where the random increments $\Delta W^k_n$'s are given by

$$\Delta W^k_n = \pm \sqrt{\Delta t}, \quad P(W^k_n = \pm \sqrt{\Delta t}) = \frac{1}{2}. \quad (18)$$

The discrete velocity $\xi^k_n$ of the Brownian motion can be computed \textit{a posteriori} as $\Delta W^k_n \Delta t$, and then it is possible to define the discrete microscopic velocity as (cf. (9))

$$v_m^i := \begin{cases} 
\frac{1}{|J^i_n|} \sum_{\ell \in J^i_n} \Delta W^\ell_n \Delta t, & \text{if } J^i_n \neq \emptyset \\
0, & \text{if } J^i_n = \emptyset,
\end{cases} \quad (19)$$

where $J^i_n := \{ k \in \{1, \ldots, N\} : X^k_n \in E_i \}$.

At time $t = t_0 = \frac{1}{2}$, we assume the microscopic particles $\{X^k_{t_0}\}_{k=1}^N$ to be randomly distributed in $\{x \in \mathbb{R} : |x| < r\}$ with $r = \frac{3}{2}$.

### 3.3 Numerical approximation of the coupled equations

A preliminary coupling of the microscopic and macroscopic scale can be obtained by assuming that the solution $u$ to the heat equation (5) is known (see (12)), and then solving the equation for $X^k_n$ in (11a), discretized as follows:

$$X^k_{n+1} = X^k_n + \theta \Delta W^k_n + (1 - \theta) \frac{X^k_n}{2t_n} \Delta t, \quad k = 1, \ldots, N. \quad (20)$$

Figure 2 shows the solution of (20) for $\theta = 0, 0.3, 1$ (with $N = 1$ and $N = 100$). We notice that, as expected, trajectories are smoother for $\theta < 1$, while the overall statistical properties of the collective dynamics are kept.

The numerical scheme for the fully-coupled system (11a)-(11b) can be obtained by means of the ingredients introduced above, ending up with the following discrete explicit system

\[
\begin{align*}
X^k_{n+1} &= X^k_n + \theta \Delta W^k_n + (1 - \theta) \Delta t \left( \frac{-1}{2u^i_n} \left( \frac{u^{i+1}_n - u^{i-1}_n}{2\Delta x} \right) \right) \\
u^i_{n+1} &= u^i_n + \theta \frac{\Delta t}{\Delta x} \left( -L^i_n[f] + G^i_n[f] + G^i_n[f] \right) + (1 - \theta) \frac{1}{2} \frac{\Delta t}{\Delta x^2} \left( u^{i+1}_n - 2u^i_n + u^{i-1}_n \right)
\end{align*}
\]

where $L$ and $G$'s are defined in (15) and (16), respectively, $j$ is defined, for any $n$ and $k$, as the unique index such that $X^k_n \in E_j$ (we assume a zeroth order interpolation for the values of $u$ not sitting on grid nodes), and $f = f[v_m]$ is defined, at grid nodes, as $f^i_n = u^i_n(v_m)_n$, $n \in \mathbb{N}$, $i \in \mathbb{Z}$, with $v_m$ as in (19).

The scheme (21a)-(21b) raises severe numerical issues. Three of them are in order:

- The function $u$ is very close to 0 (close to or below the machine precision) in some portion of the domain, see Figure 1. This makes the division by $u$ in (21a) be a source
of errors; • The microscopic dynamics is very irregular and, consequently, the function $u$ becomes in short time quite irregular. This makes it almost impossible to compute the approximate $\nabla u$ in (21a) with a certain precision; • Limiting our attention to the advection part of (21b), the hyperbolic CFL condition [2] takes the nonstandard implicit form

$$\Delta t \max_{n,i} |(v_m(\Delta t))^i_n| \leq \Delta x.$$ 

Indeed, the discrete microscopic velocity field $(v_m)_n$ depends on the choice of $\Delta t$, cf. (19).

Figure 3(left) shows the approximate solution $u$ of the coupled dynamics (11a)-(11b) at $t = 5$ with $\theta = 1$ and $N = 100$. Here the Brownian motion leads the dynamics, making the macroscopic solution $u$ strongly irregular. It is interesting to note that the microscopic dynamics is able to “stretch” the Gaussian in the correct way. This is perfectly visible comparing Figure 1(center,right) and Figure 3(left): The support of the solutions is approximately the same, i.e. $[-7,7]$.

Figure 3(center,right) shows the approximate solutions $u$ and $X^k$’s of the coupled dynamics (11a)-(11b) with $\theta = 0.3$ and $N = 100$. Here both scales contribute to the overall dynamics, making the result quite unpredictable. We observe a clustering effect
Figure 3: Approximate solutions of the system (11a)-(11b). Left: Function $u(t=5, x)$, with $\theta = 1$ and $N = 100$. Center: Function $u(t=5, x)$, with $\theta = 0.3$ and $N = 100$. Right: Trajectories $X_k^t$’s, with $\theta = 0.3$ and $N = 100$, in the plane $x$-$t$ for $x \in [-10, 10]$ and $t \in [t_0, 5]$

Figure 4: Trajectories of $N = 100$ particles in the plane $x$-$y$. Red circles are the initial positions of the particles. Left: $\theta = 0$ (macroscopic velocity is leading). Center: $\theta = 0.1$ (coupled velocity). Right: $\theta = 1$ (pure Brownian motion)

in the microscopic particles, likely due to numerical issues rather than actual effects of scale interactions.

Similar results can be obtained analogously in two dimensions. Figure 4 shows the two-dimensional version of the simulation described in Figure 2 (second row).

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