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Modelling of Langevin Equations by the Method of Multiple Scales

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Abstract: We are motivated to model particle Coulomb collisions to simulate the physical interaction of charged particles with electromagentic fields. Such collision operators can be modelled by a Langevin equation, which is a multiscale stochastic differential equation. Due to its multiple scales, we have to apply a multiscale method simultaneously on widely different scales. We extend standard splitting approaches to such multiscale equations. In the numerical experiments, we discuss our results for the different scales.

Keywords: Langevin equation, Method of Multiple Scales, Multiscale analysis, Coulomb collision, Operator Splitting, Predictor-Corrector AB-Splitting.

1. INTRODUCTION

We are motivated to apply a multiscale model to solve Langevin equations, which are used to simulate the relaxation of a Fokker–Planck equation with Coulomb collisions in sufficiently dense plasma applications (e.g., magnetic fusion, inertial fusion), see Nanbu (1997) and Cohen et al. (2010).

The particle transport and Coulomb collision (long-range collision) in a dense plasma can be modelled by the following multiscale equation:

$$\frac{\partial f_\alpha}{\partial t} + \mathbf{v} \cdot \frac{\partial f_\alpha}{\partial \mathbf{x}} + \frac{q_\alpha}{m_\alpha}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \frac{\partial f}{\partial \mathbf{v}} = \tag{1}$$
$$= \frac{\partial f_\alpha}{\partial t}|_{coll},$$

where $f_\alpha(\mathbf{x}, \mathbf{v})$ is the phase-space distribution function (density) of a charged plasma species α submitted to electromagnetic field $(\mathbf{E}, \mathbf{B})$. Further the collision operator of the Fokker-Planck (forward Kolmogorov) equation is given by the Landau's collision term, see Landau (1937) and Risken (1996),

$$\frac{\partial f_\alpha}{\partial t}|_{coll} = \tag{2}$$
$$= \frac{\partial}{\partial \mathbf{v}} \cdot \left(\pi\, q_\alpha^2\, \lambda \sum_\beta q_\beta^2 \int (f_\alpha \frac{\partial f'_\beta}{\partial \mathbf{v}'} - f'_\beta \frac{\partial f_\alpha}{\partial \mathbf{v}'})\, \frac{u^2 I - \mathbf{u}\mathbf{u}}{u^3} \right)$$

where the sum is over the index β of the plasma charged-particle species, q_β is the charge of species β, $f_\beta(\mathbf{x}, \mathbf{v}')$ is the phase-space distribution function (density) of a charged plasma species β, the relative velocity is given as $\mathbf{u} = \mathbf{v} - \mathbf{v}'$, $u = |\mathbf{u}|$ and λ is the Coulomb logarithm. The collision parameters (in the vector notation), we have the drag and diffusion coefficients, are derived from a classical theory of the screened Coulomb collision in the Fokker-Planck limit, see Nanbu (1997).

To solve such a delicate equation (2), it is important to develop accurate numerical algorithms, which take into account the nonlinear and singular perturbed collision operator.

For a simpler test problem, we consider a scalar particle transport and collision in an electric field, which has different scales, e.g., blow-up scales (impact oscillators) and also oscillating scales (harmonic oscillators), see Dimits et al. (2010) and Manheimer et al. (1997).

We consider for the simpler model the distribution function f of a particle in a dense plasma problem and we apply the appropriate description with a one-dimensional Fokker–Planck (FP) equations in the phase space (x, v):

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} + E(x,\epsilon)\frac{\partial f}{\partial v} = \frac{\partial}{\partial v}(-\gamma v f + \beta^{-1}\gamma \frac{\partial f}{\partial v}), \tag{3}$$

where we assume to have a nonlinear and singular perturbed electric-field $E(x, \epsilon) = \epsilon \frac{2}{x^2} - 2x,\ \epsilon \in (0, 1]$ and ϵ is the perturbation parameter. The Coulomb collision parameters are γ (thermostat parameter) and β (inverse temperature), see Bou-Rabee et al. (2012). We concentrate on the nonlinear molecular collisions (Coulomb collisions), which are long range collisions.

The present paper is organized as follows. In Section 2, we introduce the splitting methods for the model problem. In Section 3, we discuss the improvement of the splitting method based on the method of multiple scales. The extension to a multiscale splitting scheme is discussed in Section 4. The numerical results are discussed in Section 5 and we draw some conclusions in Section 6.

2. SPLITTING METHODS

Splitting methods are important when we can split differential equations into a sum of two or more parts and solve each parts simpler than the original, see McLachlan et al. (2002).

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Based on our problem, we can decompose the FP equation (3) into two parts with different time-scales:

- Transport Part (slow time-scale):

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} + E(x,\epsilon)\frac{\partial f}{\partial v} = 0, \tag{4}$$

- Collision Part (fast time-scale):

$$\frac{\partial f}{\partial t}|_{coll} = \frac{\partial}{\partial v}(-\gamma v f + \beta^{-1}\gamma\frac{\partial f}{\partial v}). \tag{5}$$

We are following the characteristics of the space x and velocity v of equations (4)-(5) and obtain the Langevin-like equations, which are the following multiscale nonlinear SDE equations, see also Bou-Rabee et al. (2012):

- Ordinary differential equation (ODE)

$$\frac{dx}{dt} = v, \ \frac{dv}{dt} = E(x,\epsilon), \tag{6}$$

- Stochastic differential equation (SDE)

$$\frac{dx}{dt} = 0, \ dv = -\gamma v dt + \sqrt{2\beta^{-1}\gamma}dW, \tag{7}$$

  where W is a one-dimensional Brownian motion. For the SDE part, we have the analytical solution: $v(t) = \exp(-\gamma t) + \sqrt{2\beta^{-1}\gamma}\int_0^t \exp(-\gamma(t-s))\, dW(s)$.

For the splitting method, we apply the numerical methods for the transport part, see Hockney et al. (1985), and fast SDE solver or analytical solutions for the collision part, see Kloeden (1992).

Then, we result in the full equation:

$$\frac{dx}{dt} = v, \tag{8}$$

$$dv(t) = E(x,\epsilon)dt - \gamma v dt + \sqrt{2\beta^{-1}\gamma}dW, \tag{9}$$

where W is a one-dimensional Brownian motion.

In the following, we present some standard methods, see Geiser (2013), to solve the full equations (8)-(9) with respect to the discussed splitting ideas. We apply an AB splitting and semi-analytical method (later called analytical method):

- AB-Splitting:

$$v(t^{n+1}) = v(t^n) + \Delta t\ E(x(t^n),\epsilon) \tag{10}$$
$$-\Delta t\ \gamma v(t^n) + \sqrt{2\beta^{-1}\gamma}\Delta W,$$
$$x(t^{n+1}) = x(t^n) + \Delta t\ v(t^{n+1}), \tag{11}$$

  where $\Delta W = W(t^{n+1} - W(t^n)) = \text{rand}\sqrt{\Delta t}$ and rand is the Gaussian normal distribution $N(0,1)$.
- Semi-analytical method:

$$x(t^{n+1}) = x(t^n) + \Delta t\ v(t^n), \tag{12}$$
$$v(t^{n+1}) = \exp(-\gamma\Delta t v(t^n) \tag{13}$$
$$+\sqrt{2\beta^{-1}\gamma}\int_{t^n}^{t^{n+1}} \exp(-\gamma(t^{n+1}-s)\ dW(s)$$
$$+\Delta t/2\Big(E(x(t^{n+1}),\epsilon) + \exp(-\gamma\Delta t)\ E(x(t^n,\epsilon)\Big),$$

  where we have applied the stochastic integral as

$$\int_{t^n}^{t^{n+1}} \exp(-\gamma(t^{n+1}-s)dW_s \tag{14}$$
$$= \sum_{j=0}^{N-1} \exp(-\gamma(\frac{t^{n,j}+t^{n,j+1}}{2}))\ (W(t^{n,j+1}) - W(t^{n,j})),$$
$$\Delta t = (t^{n+1}-t^n)/N, t^{n,j} = \Delta t + t^{n,j-1}, t^{n,0} = t^n.$$

For both methods, we have the problems, that we do not take into account the multiscale problem, see Le Bris (2009) and Geiser (2013). Here, we discuss the extensions, that are necessary to consider and contribute the multiple time-scales to a novel method:

- Symplecticity for the harmonic oscillator for particles in the electric field with $\epsilon \to 0$).
- Higher order resolution for the singular oscillator (impact oscillator) for particles in the electric field with $\epsilon \to 1$).

3. THE METHOD OF MULTIPLE SCALES

In the following, we discuss the method of multiple scales, which is used for problems in which the solutions depend simultaneously on widely different scales, see Kevorkian et al. (1996) and Murdock (1991). Typical examples are highly oscillatory solutions over time scales that are greater than the period of the known oscillations, see Johnson (2005).

We apply the method of multiple scale and rewrite the equations (8)-(9) to the second order SDE:

$$\frac{d^2x}{dt^2} = E(x,\epsilon) - \gamma\frac{dx}{dt} + \sqrt{2\beta^{-1}\gamma}\frac{dW}{dt}, \tag{15}$$

where $x(0)$ and $\frac{dx(0)}{dt}$ are the initial conditions (e.g., $(x(0),v(0))^\top = (0.5,0.5)^\top$) and $E(x,\epsilon) = \epsilon\frac{2}{x^3} - 2x$.

Based on the nonlinear and singular perturbed electric field, we have a switch between an harmonic oscillator $E(x,0) = -2x$, and a highly oscillatory solutions related to $E(x,1) = \frac{2}{x^3} - 2x$ for $x \to 0$. Here, we have to employ multiscale modelling to take into account the different scales and develop a new method based on a splitting approach.

For the multiscale problem, we look for solutions $x(t,\epsilon)$ and apply the following hierarchical ordering:

$$x(t,\epsilon) = x_0(t) + \epsilon x_1(t) + O(\epsilon^2), \tag{16}$$

with the initial conditions $x(0,\epsilon) = x(0)$ and $\frac{dx(0,\epsilon)}{dt} = v(0)$ to the multiple scale equation (15).

The leading order perturbation equation with $\mathcal{O}(1)$ is

$$\frac{d^2x_0}{dt^2} = -2x_0 - \gamma\frac{dx_0}{dt}dt + \sqrt{2\beta^{-1}\gamma}\frac{dW}{dt}, \tag{17}$$

$$x_0(0) = x(0), \frac{dx_0}{dt} = v(0). \tag{18}$$

The next order perturbation equation with $\mathcal{O}(\epsilon)$ is

$$\frac{d^2x_1}{dt^2} = -2x_1 + \frac{2}{x_0^3} - \gamma\frac{dx_1}{dt}dt + \sqrt{2\beta^{-1}\gamma}\frac{dW}{dt}, \tag{19}$$