Iterative Splitting Methods for Coulomb Collisions in Plasma Simulations

Jürgen Geiser *

March 19, 2018

Abstract

In this paper, we present splitting methods that are based on iterative schemes and applied to plasma simulations. The motivation arose of solving the Coulomb collisions, which are modeled by nonlinear stochastic differential equations. We apply Langevin equations to model the characteristics of the collisions and we obtain coupled nonlinear stochastic differential equations, which are delicate to solve. We propose well-known deterministic splitting schemes that can be extended to stochastic splitting schemes, by taking into account the stochastic behavior. The benefit decomposing the different equation parts and solve such parts individual is taken into account in the analysis of the new iterative splitting schemes. Numerical analysis and application to various Coulomb collisions in plasma applications are presented.

Keywords: splitting methods, stochastic differential equations, iterative splitting schemes, particle simulations, Coulomb collisions, convergence analysis, Langevin equation.

AMS subject classifications. 35K25, 35K20, 74S10, 70G65.

1 Introduction

We are motivated to develop fast algorithms to solve Coulomb collisions in plasma simulations. Such modeling equations results in characteristics equations, which are nonlinear stochastic differential equations with different time-scales. Based on the nonlinearities and multiscale problems such differential equations are solved by higher order stochastic solvers, e.g., Milstein scheme, see [15] and [2]. Such solvers are direct or non-iterative and have the drawback in missing relaxations of such nonlinear parts, see [7] and [13].
Therefore, we propose new iterative splitting schemes, see [11], which allow to obtain higher order accuracy with a nonlinear solver effect which is related to the fixpoint scheme, see [12].

In the paper, we discuss the two directions of solver methods for the nonlinear stochastics differential equations

- Direct methods: Euler-Maruyama and Milstein schemes, see [15],
- Indirect methods: Iterative splitting schemes, see [7].

From the methodological point of the methods, we have historically two ideas for algorithms to solve the Coulomb collisions in particle simulations. Such methods are based on finite-sized particles, whose characteristics are lying on a grid (e.g. particle-in-cell (PIC) simulation). Here, we have the following methods:

- Binary algorithm: Particles in a finite cell are organized into discrete pairs of interacting particles. The collision is based on the scattered velocities through an angle whose statistical variance is dictated by the theory of Coulomb collisions [18] and [24].
- Test particle algorithm: The collisions are modeled by defining test and field particles. The velocity of the test-particle is modeled by Langevin equations with drag and diffusion coefficients, influenced by the moments of the field-particle velocity distribution, which are deposited on the space mesh [1], [13], [16], [17] and [23].

The underlying model equation for the particle simulation is the Fokker-Planck equation, which is given as

\[ \frac{\partial}{\partial t} f(v) = - \frac{\partial}{\partial v} (F_d(v) f(v)) + \frac{1}{2} \frac{\partial^2}{\partial v \partial v} (D(v) f(v)), \]  
\( (1) \)

where \( F_d = \langle \Delta v/\Delta t \rangle \) and \( D = \langle \Delta vv/\Delta t \rangle \), and \( \langle \cdot \rangle \) are the expected values, which are given as ensemble-averaged drag and diffusion coefficients (see the derivation in [3] and [4]).

Based on the Fokker-Planck equation, we can shift to the velocity dependent Langevin equation with an embedded collision operator, which is related to an explicit derivation, e.g., [5].

For a test particle with velocity \( v \) we have the following equation:

\[ dv(t) = F_d(v)dt + \sqrt{2D_v(v)}dW_v(t), \]  
\( (2) \)
\[ d\mu(t) = -2D_a(v)\mu dt + \sqrt{2D_a(v)(1 - \mu^2)}dW_\mu(t), \]  
\( (3) \)
\[ d\phi(t) = \sqrt{2D_a(v)} \left( \frac{1}{1 - \mu^2} \right) dW_\phi(t), \]  
\( (4) \)
\[ v_0 = 1.0, \mu(0) = 0, \phi(0) = 1.0, \]  
\( (5) \)

where the coordinates \( (v, \mu = \cos(\theta), \phi) \) are the underlying spherical coordinates given as \( (v, \theta, \phi) \) of the test particle. \( F_d \) is an ensemble-averaged drag, and
$D_v$ and $D_a$ are the diffusion coefficients. Furthermore, $W_v$, $W_\mu$ and $W_\phi$ are independent of the Wiener processes and $v_0$, $\mu_0$ and $\phi_0$ are the initial-conditions.

The paper is outlined as following. In the Section 2, we discuss the iterative splitting method for the stochastic differential equations and the convergence analysis. The numerical algorithms of the direct and indirect methods are presented in Section 3. The numerical results are discussed in Section 4 and we conclude our results in Section 5.

2 Iterative Splitting Method for Stochastic Ordinary Differential Equations

The following algorithm is based on the iteration with a fixed-splitting discretization step-size $\tau$. For the time-interval $[t^n, t^{n+1}]$, we solve the following sub-problems consecutively for $i = 1, 3, \ldots, 2m+1$, (cf. [6]):

$$
\begin{align*}
 dc_i(t) &= Ac_i(t)dt + Bc_{i-1}dW_t(t), \text{ with } c_i(t^n) = c^n \\
\text{and } c_i(t^n) &= c^n, \quad c_0 = 0.0, \\
dc_{i+1}(t) &= Ac_i(t)dt + Bc_{i+1}(t)dW_t, \\
\text{with } c_{i+1}(t^n) &= c^n,
\end{align*}
$$

where $c^n$ is the known split approximation at the time-level $t = t^n$. The split approximation at the time-level $t = t^{n+1}$ is defined as $c^{n+1} = c_{2m+2}(t^{n+1})$. Furthermore, $W$ is a Wiener process, see [15].

We can rewrite this into the form of the following ordinary differential equation (ODE):

$$
\begin{align*}
 \frac{\partial c_i(t)}{\partial t} &= Ac_i(t) + Bc_{i-1}\dot{W}_t, \text{ with } c_i(t^n) = c^n \\
\text{and } c_i(t^n) &= c^n, \quad c_0 = 0.0, \\
\frac{\partial c_{i+1}(t)}{\partial t} &= Ac_i(t) + Bc_{i+1}(t)\dot{W}_t, \\
\text{with } c_{i+1}(t^n) &= c^n,
\end{align*}
$$

where $\dot{W}_t = \frac{dW_t}{dt}$.

We present the results of the consistency of our iterative method extended to stochastic operators, see [11]. For simplicity, we assume the system of operators are generators of a $C_0$-semigroup based on their underlying operator norms.

**Theorem 2.1.** Let us consider the abstract Cauchy problem in a Banach space $X$

$$
\begin{align*}
 \partial_t c(x,t) &= Ac(x,t) + Bc(x,t)\dot{W}_t, \quad x \in \Omega \times [0,T], \\
 c(x,0) &= c_0(x) \quad x \in \Omega, \\
c(x,t) &= c_1(x,t) \quad x \in \partial \Omega \times [0,T],
\end{align*}
$$

where $A, B : X \to X$ are given linear operators that are generators of the $C_0$-semigroup and $c_0 \in X$ is a given element.
The iterative operator splitting method has the following splitting error:

\[
||S_i - \exp(At + BW)|| \leq C\tau^{\frac{1}{2}},
\]

where \( S_i \) is the approximated solution for the i-th iterative step and \( C \) is a constant that can be chosen uniformly on bounded time intervals.

**Proof.** The iterative steps are given in the following.

- For the first iterations, we have:
  \[
  \partial_t c_1(t) = Ac_1(t) + BW_t c_0, \quad t \in (t^n, t^{n+1}],
  \]
  where we have the solution given as:

  \[
  c_1(t) = \exp(At) c(t^n) + \int_0^t \exp(A(t-s))B W_s c(t^n) ds, \quad t \in (t^n, t^{n+1}],
  \]
  \[
  = \exp(At) c(t^n)
  + (I + At) \int_0^t \exp(-As)B \exp(BW_s) dW_s + O(t^{3/2}),
  \]
  \[
  = \exp(At) c(t^n)
  + (I + At) \left( BW_t - ABtW_t + \frac{1}{2} BB^t W_t^2 - \frac{1}{2} BB^t t \right) + O(t^{3/2}),
  \]
  \[
  = (I + At + BW_t + \frac{1}{2} BB^t W_t^2 - \frac{1}{2} BB^t t) c(t^n) + O(t^{3/2}),
  \]

where \( c_0(t) = \exp(BW_t) c(t^n) \).

Then, the consistency of the first iterative step is given in the following. For \( e_1 \), we have:

\[
  c_1(t) = (I + At + BW_t + \frac{1}{2} BB^t W_t^2 - \frac{1}{2} BB^t t) c(t^n) + O(t^{3/2}),
  \]
\[
  c(t) = \exp((A - BB^t/2)t + BW_t) c(t^n)
  = (I + At + BW_t + \frac{1}{2} BB^t W_t^2 - \frac{1}{2} BB^t t) c(t^n) + O(t^{3/2}).
  \]

We obtain:

\[
  ||e_1|| = ||c - c_1|| \leq ||O(t^{3/2})||.
\]

- For the second iteration, we have:
  \[
  \partial_t c_2(t) = Ac_2(t) + BW_t c_1, \quad t \in (t^n, t^{n+1}],
  \]
where we have the solution given as:

\[
c_2(t) = \exp(At)c(t^n) + \int_0^t \exp(A(t-s))BW.tc_1(s)ds, \quad t \in (t^n, t^{n+1}],
\]

\[
= (I + At)c(t^n) + (I + At)\int_0^t (I - As)B(I + As)dW_s + \mathcal{O}(t^2),
\]

\[
= (I + At)c(t^n) + (I + At)\int_0^t (I - As)B(I + As)\int_0^s (I - As_1)B(I + As_1)dW_{s_1} dW_s + \mathcal{O}(t^2),
\]

\[
= (I + At)c(t^n) + (I + At)\int_0^t (BW_t - tABW_t + \frac{1}{2}ABW_t t + BAtW_t s - \frac{1}{2}BAW_t t + \frac{1}{2}B^2\frac{1}{2}W^2_t - \frac{1}{2}B^2 t) + \mathcal{O}(t^2),
\]

\[
= (I + At)(B^2\frac{1}{2}W^2_t - \frac{1}{2}B^2 t) + \mathcal{O}(t^2),
\]

and we apply the second order accurate integration of \(\int_0^t ABW_s ds = \frac{1}{2}ABtW_t\).

Then, the consistency of the second iterative step is given in the following.

For \(e_2\), we have:

\[
c_2(t) = (I + At + BW_t + \frac{1}{2}BB^tW^2_t - \frac{1}{2}BB^t t + \frac{1}{2}BAtW_t + \frac{1}{2}AtW_t)c(t^n) + \mathcal{O}(t^2))
\]

\[
c(t) = \exp((A - BB^t/2)t + BW_t)c(t^n)
\]

\[
= (I + At + BW_t + \frac{1}{2}BB^tW^2_t - \frac{1}{2}BB^t t + \frac{1}{2}BAtW_t + \frac{1}{2}AtW_t - \frac{1}{2}B^3tW_t)c(t^n) + \mathcal{O}(t^2))
\]

where we assume \(\frac{1}{2}B^3tW_t \approx 0\).

We obtain:

\[
||e_2|| = ||c - c_2|| \leq \mathcal{O}(t^2).
\]

With the next iterative step \(i = 3\), we gain \(\frac{1}{2}B^3tW_t\) and we obtain a full second order scheme.

**Remark 2.1.** We obtain a higher order scheme for the iterative splitting method. For each iterative step, we obtain additional a half order accuracy, means \(\mathcal{O}(t^{1 + \frac{1}{2}i})\), where \(i = 1, 2, 3, \ldots\), is the number of iterative steps.
3 Numerical Algorithms for the Nonlinear Stochastic Ordinary Differential Equations

In the following, we deal with the different numerical algorithms to solve the nonlinear stochastics differential equations.

We deal with the underlying nonlinear stochastics differential equation, which is given as:

\[
dX = A(X)Xdt + B(X)XdW, \tag{27}
\]

where \(A, B\) are matrices in \(\mathbb{R}^{m \times m}\) with \(m\) is the number of unknown. Further, the components of the matrices are dependent of the solution \(X\). Further, the initial values are given as \(X_{t_0} = X_0\) and \(W\) is Wiener process, see [15].

In the following, we deal with the direct and indirect algorithms, which are implemented in the numerical experiments. The direct methods are numerical standard methods, which are used in the numerical approximation of stochastic differential equations. They are simply to implement and obtain direct the numerical solutions (one-step methods), while they have their drawback in the resolution of the nonlinear solutions, while the linearization is given by the time-step. Instead the indirect methods are iterative solvers and obtain higher order resolutions with additional iterative cycles (multi-step methods), such that they allow to resolve the nonlinear solution in the time-step approach, see [7] and [12].

3.1 Direct Algorithms

In the following, the standard numerical schemes for solving the nonlinear stochastics equation (27) are given:

- Euler-Maruyama scheme is given as:

\[
X_{n+1} = X_n + A(X_n)X_n\Delta t + B(X_n)X_n(W_{t_{n+1}} - W_{t_n}), \tag{28}
\]

for \(n = 0, 1, \ldots, N - 1\), \(X_0 = X_{t_0}\), and \(\Delta t = t_{n+1} - t_n\) is the time-step. Further, \(\Delta W = W_{t_{n+1}} - W_{t_n}\) is the stochastic step based on a Wiener process, see [15].

- Milstein scheme is given as:

\[
X_{n+1} = X_n + A(X_n)X_n\Delta t + B(X_n)X_n(\Delta W) + \frac{1}{2}B(X_n)X_n \left. \frac{\partial B(X)}{\partial X} \right|_{X_n} ((\Delta W)^2 - \Delta^2), \tag{29}
\]

for \(n = 0, 1, \ldots, N - 1\), \(X_0 = X_{t_0}\) and \(\Delta t = t_{n+1} - t_n\) is the time-step. Further, \(\Delta W = W_{t_{n+1}} - W_{t_n}\) is the stochastic step based on a Wiener process, see [15].

- A-B Splitting method, see the ideas in [19], which is given as:
We assume that we have an approximated solution of the nonlinear stochastic differential equation (27). We assume the following fixed point of the operators, which are given as $A(X^n) \to \tilde{A}$ and $B(X^n) \to \tilde{B}$ for $n \to \infty$, where $X^n = X(t^n)$.

Then, we obtain:

$$X_{n+1} = X_0 \exp((\tilde{A} - \frac{\tilde{B}^t}{2})(n + 1)\Delta t + \tilde{B} \sum_{i=1}^{n+1} \Delta W_{i-1}),$$ (30)

where we assume $W = \{W_t, t \geq 0\}$ and $\Delta W_{i-1} = W_{i-1}(t_{n+1}) - W_{i-1}(t_n)$, where $\Delta t = t_{n+1} - t_n$ and we assume an equidistant grid.

Then, we obtain the following A-B splitting approach:

$$\tilde{X}_n = X_{n-1} \exp((\tilde{A} - \frac{\tilde{B}^t}{2})\Delta t),$$ (31)

$$X_n = \tilde{X}_n \exp(\tilde{B} \Delta W),$$ (32)

for $n = 0, 1, \ldots, N - 1$, $X_0 = X_{t_0}$.

**Remark 3.1.** The direct methods are fast to implement and obtain lower order results. The numerical scheme have the following accuracy: $O(t^k)$ for the Euler-Maruyama scheme, $O(t)$ for the Milstein scheme and $O(t^{2k})$ for the AB-splitting scheme for large $n \to \infty$. Here, the approach to higher order schemes are delicate, see [173].

### 3.2 Indirect Algorithms (iterative splitting)

In the following, we discuss the iterative splitting methods for the nonlinear stochastic equation (27).

- **First iterative step**

  $$X_{1,n}(t) = \phi_1(t)X_{n-1},$$ (33)

  where $\phi_1(t) = \exp(A(X_{n-1})\Delta t)$ is the first order approximation of the non-linear Magnus-expansion.

- **Second iterative step**

  $$X_{2,n}(t) = X_{1,n}(t)
  + X_{1,n}(t)[B(X_{n-1}), \int_0^t \exp(A(X_{n-1})s)dW_s], \quad t \in (t^n, t^{n+1}],
  $$

  $$X_{2,n}(t) = X_{1,n}(t) + X_{1,n}(t)[B(X_{n-1}), C_1(t)], \quad t \in (t^n, t^{n+1}],
  $$

  $$X_{2,n}(t) = X_{1,n}(t) + X_{1,n}(t)C_2(t), \quad t \in (t^n, t^{n+1}],$$ (34)
where \( C_1(t) = \int_0^t \exp(A(X_{n-1})s)dW_s \Delta W_i = (W_{t_i+1} - W_{t_i}) \), for \( n = 0, 1, \ldots, N - 1, X_0 = X_{t_0} \).

The stochastic integral is computed as Stratonovich integral:

\[
C_1(\tilde{t}) = \int_0^{\tilde{t}} \exp(A(X_{n-1})s)dW_s \\
= \sum_{j=0}^{N-1} \exp(A(X_{n-1})\frac{(t_j + t_{j+1})}{2}) (W(t_{j+1}) - W(t_j)), \\
\Delta t = \tilde{t}/N, t_j = \Delta t + t_{j-1}, t_0 = 0,
\]

and the commutator \([\cdot, \cdot]\) is computed as:

\[
C_2(t) = [B(X_{n-1}), C_1(t)] = B(X_{n-1})C_1(t) - C_1(t)B(X_{n-1}),
\]

which is based on the different random variables of \( C_1(t) \). Additionally, in the scalar case, the commutator is not equal to zero.

- Third iterative step

\[
X_{3,n}(t) = X_{2,n}(t) + X_{1,n}(t) \int_0^t [B(X_{n-1}), \exp(sA(X_{n-1}))] \cdot [B(X_{n-1}), \int_0^s \exp(A(X_{n-1})s_1)ds_1] ds,
\]

\[
X_{3,n}(t) = X_{2,n}(t) + X_{1,n}(t) \int_0^t [B(X_{n-1}), \exp(sA(X_{n-1}))] C_2(s) ds,
\]

\[
X_{3,n}(t) = X_{2,n}(t) + X_{1,n}(t) C_3(t),
\]

where \( \Delta W_i = (W_{t_i+1} - W_{t_i}) \), for \( n = 0, 1, \ldots, N - 1, X_0 = X_{t_0} \).

The operator \( C_3(t) \) is computed as:

\[
C_3(t) = \sum_{j=0}^{N-1} \left( B(X_{n-1}) \exp(A(X_{n-1})\frac{(t_j + t_{j+1})}{2}) C_2(B(\frac{t_j + t_{j+1}}{2})) \right), \\
\Delta t = t/N, t_j = \Delta t + t_{j-1}, t_0 = 0,
\]

where \( C_2(B(\frac{t_j + t_{j+1}}{2})) \) is computed with (37), for each \( \tilde{t} = \frac{t_j + t_{j+1}}{2}, j = 0, \ldots, N - 1 \).

**Remark 3.2.** The indirect methods are based on the iterative approaches related to fixedpoint-schemes and obtained higher order accuracy: \( O(t^{i+4}) \), where \( i \) is the number of iterative steps. Based on their recursive behavior numerical approaches in previous iterative steps can be used. Such a clever combination of the previous computed iterative cycles allows to obtain fast iterative methods, see [8] and [9].
4 Numerical Examples

In the following numerical examples, we verify the theoretical results and the benefits of the novel iterative solvers for the stochastic differential equations.

We deal with the following examples and discuss the methodological sense of the different schemes:

- Scalar benchmark problem (scalar multiplicative noise): The stochastic differential equations are based on $m \times m$ operator matrices, while we have a scalar stochastic term. For such a benchmark examples, we can detailed analyze the benefit of the iterative scheme, which is related to the higher order approach.

- Vectorial benchmark problems (vectorial multiplicative noise): The stochastic differential equations are based on $m \times m$ operator matrices and we have vectorial stochastic terms. Such vectorial examples need additional, so called outer-diagonal entries for the standard scheme, see [15] and [4]. For the iterative schemes, we have also an extension to resolves such multiple integrals based on the vectorial stochasticstics, see [25]. Here, we can analyze the benefit of the additional terms and the higher accuracy of the novel methods. Further, we also extend such problems to larger operator matrices to see the computational amount of the different schemes.

- Real-life problem (Coulomb test-particle): Here, we test a system of non-linear stochastic differential equations with vectorial stochastic terms. Such examples are delicate to solve and we apply the different standard and novel schemes. For such problems, we see the benefit of the iterative splitting methods, which combine the linear and nonlinear solvers. We relax the solution based on the iterative approach and obtain much more accurate results.

4.1 Scalar multiplicative noise

In the following, we deal with a simple chemical reaction model, while the reaction part is influenced via stochastic noise.

We deal first with an ordinary differential equation and separate the complex operator into two simpler operators: the $m \times m$ ordinary differential equation
4 NUMERICAL EXAMPLES

system given as:

\[ dy(t) = Ay(t) + Py(t) \, dW(t), \]  
\[ A = \begin{pmatrix} -\lambda_{1,1} & \lambda_{2,1} & \cdots & \lambda_{1,10} \\ -\lambda_{2,1} & -\lambda_{2,2} & \cdots & \lambda_{2,10} \\ \vdots \\ -\lambda_{10,1} & \lambda_{10,2} & \cdots & -\lambda_{10,10} \end{pmatrix} = \begin{pmatrix} -1 & 0 & \cdots & 0 \\ 0.1 & -1 & \cdots & 0 \\ \vdots \\ 0.1 & 0.1 & \cdots & -1 \end{pmatrix} \]

\[ P = \begin{pmatrix} \sigma_{1,1} & \sigma_{1,2} & \cdots & \sigma_{1,10} \\ \sigma_{2,1} & \sigma_{2,2} & \cdots & \sigma_{2,10} \\ \vdots \\ \sigma_{10,1} & \sigma_{10,2} & \cdots & \sigma_{10,10} \end{pmatrix} = \begin{pmatrix} 0.01 & 0 & \cdots & 0 \\ 0.005 & 0.01 & \cdots & 0 \\ \vdots \\ 0.005 & 0.005 & \cdots & 0.01 \end{pmatrix} \]

\[ dW(t) = dW_1(t) \text{(stochastic scalar)}, \]

\[ y(0) = (1, \ldots, 1)^t \text{(initial conditions)}, \]

where \( \lambda_{11} \ldots \lambda_{10,10} \in \mathbb{R}^+ \) are the decay factors and \( \sigma_{11} \ldots \sigma_{10,10} \in \mathbb{R}^+ \) are the parameters of the perturbations. We deal with non-commutation matrices \([A, P] = AP - PA\) as given with the tridiagonal matrices in the experiment.

We have the time interval \( t \in [0, T] \) and \( m \in \mathbb{N} \).

We apply the following numerical schemes:

- The application of the standard Euler-Maruyama scheme is given as:
  \[
y_{n+1} = y_n + Ay_n \Delta t + Py_n \Delta W,
  \]
  for \( n = 0, 1, \ldots, N - 1, y_0 = y_0, \Delta t = t_{n+1} - t_n, \Delta W = W_{t_{n+1}} - W_{t_n} = \sqrt{\Delta t}N(0, 1), \) where \( N(0, 1) \) is \( \text{rand} \) is a normally distributed random variable.

- Milstein scheme is given as:
  \[
y_{n+1} = y_n + Ay_n \Delta t + Py_n (\Delta W) + \frac{1}{2} PP^t y_n ((\Delta W)^2 - \Delta t),
  \]
  for \( n = 0, 1, \ldots, N - 1, y_0 = y_0. \)

- Recursive Splitting scheme is given as:
  \[
y_{n+1} = \exp(A - PP^t) y_n, \quad \hat{y}_{n+1} = \exp(P \Delta W) \hat{y}_{n+1},
  \]
  for \( n = 0, 1, \ldots, N - 1, y_0 = y_0. \)

- Summative Splitting scheme is given as:
  \[
y_{n+1} = \exp(A - PP^t) y_n, \quad y_{n+1} = \exp(P \frac{1}{\sqrt{N}} \sum_{j=1}^{N} \Delta W_j) y_{n+1},
  \]
  for \( n = 0, 1, \ldots, N - 1, y_0 = y_0. \)
\[ \Delta W_j = (W(\tilde{t}_{j+1}) - W(\tilde{t}_j)) = \sqrt{\delta t} N(0, 1), \] where \( N(0, 1) = \text{rand} \) is a normally distributed random variable. Further the intermediate time-steps are given as \( \delta t = \Delta t/N, \tilde{t}_{j+1} = \delta t + \tilde{t}_j, \tilde{t}_1 = t_n \) and the time-intervals are given as \( n = 0, 1, \ldots, N - 1, y_0 = y_{t_0} \).

- Iterative splitting scheme:

**Version 1: 2 iterative steps**

Second iterative step:

\[ X_{2,n}(t) = X_{1,n}(t) + X_{1,n}(t)C_2(t), \quad t \in (t^n, t^{n+1}], \] (49)

where the commutator is given as:

\[ C_2(t) = [P, C_1(t)] = PC_1(t) - C_1(t)P, \] (50)

where \( C_1(t) = \int_0^t \exp(As)dW_s \)

The stochastic integral is computed as a Stratonovich integral:

\[ C_1(\tilde{t}) = \int_0^{\tilde{t}} \exp(As)dW_s \] (51)

\[ = \sum_{j=0}^{N-1} \exp(A(\frac{t_j + t_{j+1}}{2})) (W(t_{j+1}) - W(t_j)), \]

\[ \Delta t = \tilde{t}/N, t_j = \Delta t + t_{j-1}, t_0 = 0, \] (52)

where \( \Delta W_i = (W_{t_{i+1}} - W_{t_i}) \), for \( n = 0, 1, \ldots, N - 1, X_0 = X_{t_0} \).

**Version 2: 3 iterative steps**

\[ X_{3,n}(t) = X_{2,n}(t) + X_{1,n}(t)C_3(t), \] (53)

where \( \Delta W_i = (W_{t_{i+1}} - W_{t_i}) \), for \( n = 0, 1, \ldots, N - 1, X_0 = X_{t_0} \).

The operator \( C_3(t) \) is computed as:

\[
C_3(t) = \sum_{j=0}^{N-1} \left( B \exp(A(\frac{t_j + t_{j+1}}{2})) C_2(\frac{t_j + t_{j+1}}{2}) - \exp(A(\frac{t_j + t_{j+1}}{2})) B C_2(\frac{t_j + t_{j+1}}{2}) (W(t_{j+1}) - W(t_j)) \right),
\]

\[ \Delta t = t/N, t_j = \Delta t + t_{j-1}, t_0 = 0, \] (55)

where \( C_2(\frac{t_j + t_{j+1}}{2}) \) is computed with \[34\], for each \( \tilde{t} = \frac{t_j + t_{j+1}}{2}, j = 0, \ldots, N - 1. \)

We compare the following schemes:

- First order (or strong convergence \( O(t^{1/2}) \))
4 NUMERICAL EXAMPLES

- EM (Euler-Maruyama): explicit first order Runge-Kutta scheme, see [15].
- rS (recursive Splitting): modified Lie-Trotter splitting scheme for the stochastic term, see Equation (45)-(46) and [10] and [11].
- sS (summative Splitting): modified Lie-Trotter splitting scheme with improved computation of the stochastic term, see Equation (47)-(48) and [10] and [11].

• Second order (or strong convergence $O(t^1)$)
  - Mil (Milstein): explicit second order Runge-Kutta scheme, see [15].
  - NV (Niomiya-Victori Splitting): modified Strang-Splitting scheme for the stochastic terms, see [19] and [20].
  - iterative splitting ($i = 2$)

• Third order (or strong convergence $O(t^{3/2})$)
  - iterative splitting ($i = 3$): modified iterative splitting scheme for the stochastic terms, see Equation (53) and [11].

In the following, we present the results of the lower order schemes in Figure

Remark 4.1. In the multiplicative noise example, we present the benefits of the iterative splitting schemes, which resolves the stochastic behavior more accurate than the standard schemes. While Euler-Maruyama and Milstein schemes are explicit methods, the iterative approach is based on an implicit idea to relax the oscillations via additional iterative steps, see [7]. Based on these characteristics, we could reduce the numerical errors of the novel schemes with additional iterative steps.

4.2 Vectorial Multiplicative Noise (simple)

In the following, we deal with a reduced 2 simple chemical reaction model, but with non-commuting operators.

We deal first with an ordinary differential equation and separate the complex operator into two simpler operators: the $2 \times 2$ ordinary differential equation
Figure 1: The upper right figure presents the results of the EM, rS, sS-schemes (difference between exact and numerical solutions). The upper left figure presents the results of the mean values (mean value of the difference between the exact and numerical solutions). The lower figure presents the variance of the schemes.

The system is given as:

\[ dy(t) = Ay(t) + \sum_{j=1}^{2} P_j y(t) \, dW_j(t), \]  

(56)

\[ A = \alpha_1 \begin{pmatrix} -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}, \]  

(57)

\[ P_1 = \alpha_2 \begin{pmatrix} \frac{2}{3} & 0 \\ 0 & \frac{1}{3} \end{pmatrix}, \]  

(58)

\[ P_2 = \alpha \begin{pmatrix} 0 & \frac{2}{3} \\ \frac{3}{4} & 0 \end{pmatrix}, \]  

(59)

\[ dW(t) = (dW_1(t), dW_2)(\text{stochastic vector}), \]  

\[ y(0) = (1, \ldots, 1)^t(\text{initial conditions}), \]  

where \([P_1, P_2] \neq 0\). We have the time interval \(t \in [0, T]\) and \(m = 2\).

We apply a weak perturbation with \(\alpha_2 = 0.01\) and a high perturbation with \(\alpha_2 = 1.0\), for \(\alpha_1 = 1.0\) we apply a moderate convection.

We apply \(T = 1\) and we have \(N = 20\) time steps, means \(\Delta t = T/N\).

For the testing the different numerical methods, we have the following ana-
lytical solution, see [21]:

\[
y(t^{n+1}) = \exp \left( A\Delta t - \frac{1}{2} \sum_{j=1}^{m} P_j P_j^t \Delta t + \sum_{j=1}^{m} P_j \Delta W_j \right) y(t^n),
\]

(60)

where \( \Delta W_j = (W_{t_{n+1},j} - W_{t_n,j}) = \sqrt{\Delta t} N_j(0,1) \), where \( N_j(0,1) = \text{rand}_j \), where we have \( j = 1, \ldots, m \) normally distributed random variables.

We apply the following numerical schemes:

- The application of the standard Euler-Maruyama scheme is given as:

\[
y_{n+1} = y_n + A y_n \Delta t + \sum_{j=1}^{m} P_j y_n \Delta W_j,
\]

(61)

for \( n = 0, 1, \ldots, N-1 \), \( y_0 = y_{t_0} \), \( \Delta t = t_{n+1} - t_n \), \( \Delta W = (W_{t_{n+1},1} - W_{t_n,1}, \ldots, W_{t_{n+1},m} - W_{t_n,m}) = (\sqrt{\Delta t} N_1(0,1), \ldots, \sqrt{\Delta t} N_m(0,1)) \), where \( N_i(0,1) = \text{rand}_{i} \), where we have \( i = 1, \ldots, m \) normally distributed random variables.

- Milstein scheme (without outer-diagonal entries) is given as:

\[
y_{n+1} = y_n + A y_n \Delta t + \sum_{j=1}^{m} P_j y_n \Delta W_j + \left( \sum_{i=1}^{m} \frac{1}{2} P_i P_i^t y_n ((\Delta W_i)^2 - \Delta t) \right),
\]

(62)

for \( n = 0, 1, \ldots, N-1 \), \( y_0 = y_{t_0} \).

- Milstein scheme (with outer-diagonal entries) is given as:

\[
y_{n+1} = y_n + A y_n \Delta t + \sum_{j=1}^{m} P_j y_n \Delta W_j + \left( \sum_{i=1}^{m} \frac{1}{2} P_i P_i^t y_n ((\Delta W_i)^2 - \Delta t) \right) + \sum_{i=1}^{m} \sum_{j=i+1}^{m} \frac{1}{2} [P_i, P_j] (J_{ji} - J_{ij}) y_n,
\]

(63)

for \( n = 0, 1, \ldots, N-1 \), \( y_0 = y_{t_0} \). The commutator is given as \([P_i, P_j] = P_i P_j - P_j P_i\).

Further the \( J_{ij} \) are given as:

\[
J_{ji} = \frac{1}{2} f_j J_i - \frac{1}{2} (a_{i0} J_j - a_{j0} J_i),
\]

(64)
with \( J_i = \Delta W_i = (W_{t_n+1,i} - W_{t_n,i}) \) and the coefficients are given as: \( a_{i0} = \Delta \tilde{W}_i \), where \( \Delta \tilde{W}_i = \sqrt{\Delta t} N_i(0,1) \), where \( N_i(0,1) = \text{rand}_i \).

- Iterative splitting scheme:

  **Version 1: 1 iterative steps**

We apply:

\[
X(0) \rightarrow X(\Delta t) \rightarrow X(2\Delta t) \ldots
\]

Zero iterative step:

\[
X_{0,n+1} = \exp(A\Delta t + \sum_{j=1}^{m} P_j \Delta W_j) X_{0,n}, \quad (65)
\]

where \( X_{1,0} = y(0) \) and we have \( N \) time-steps with \( \Delta t = T/n \) and \( t^{n+1} = t^n + \Delta t \) with \( n = 0, \ldots, N - 1 \).

First iterative step:

\[
X_{1,n+1} = \exp(A\Delta t) X_{1,n}
\]

\[
+ \int_0^{\Delta t} \exp(A(t-s)) \left( \sum_{i=1}^{m} P_i X_{1,s} dW_i \right),
\]

\[
= \exp(A\Delta t) X_{1,n}, \quad (66)
\]

\[
+ \int_0^{\Delta t} \exp(A(t-s)) \left( \sum_{i=1}^{m} P_i \exp(As + \sum_{j=1}^{m} P_j W_{j,s}) dW_i \right) X_{1,n}, \quad (67)
\]

\[
= \exp(A\Delta t) X_{1,n}, \quad (68)
\]

\[
+ \sum_{j=1}^{m} P_j X_{1,n} \Delta W_j
\]

\[
+ \sum_{i=1}^{m} \frac{1}{2} P_i P_i X_{1,n} \left( (\Delta W_i)^2 - \Delta t \right),
\]

\[
+ \sum_{i=1}^{m} \sum_{j=i+1}^{m} \frac{1}{2} [P_i, P_j] (J_{ji} - J_{ij}) X_{1,n},
\]

for \( n = 0, 1, \ldots, N - 1 \), \( y_0 = y_{t_0} \). The commutator is given as \([P_i, P_j] = P_i P_j - P_j P_i\). Further the \( J_{ij} \) are given as:

\[
J_{ji} = \frac{1}{2} J_j J_i - \frac{1}{2} (a_{i0} J_j - a_{j0} J_i), \quad (69)
\]

with \( J_i = \Delta W_i = (W_{t_n+1,i} - W_{t_n,i}) \) and the coefficients are given as: \( a_{i0} = \Delta \tilde{W}_i \), where \( \Delta \tilde{W}_i = \sqrt{\Delta t} N_i(0,1) \), where \( N_i(0,1) = \text{rand}_i \).
We obtain the Milstein scheme with outer-diagonal entries.

**Version 2: 2 iterative steps**

Second iterative step:

\[
X_{2,n+1} = \exp(A\Delta t)X_{2,n} + \int_0^{\Delta t} \exp(A(t-s)) \left( \sum_{i=1}^{m} P_i X_{1,s} dW_{i,s} \right),
\]

\[
= \exp(A\Delta t)X_{2,n} + \int_0^{\Delta t} \exp(A(t-s)) \left( \sum_{i=1}^{m} P_i \left( \exp(As)X_{1,n} \right) + \int_0^{s} \exp(A(s-s_1)) \left( \sum_{j=1}^{m} P_j X_{1,s_1} dW_{j,s_1} \right) dW_i,s \right),
\]

\[
= \exp(A\Delta t)X_{2,n} + \sum_{j=1}^{m} P_j X_{2,n} \Delta W_j
\]

\[
+\left( \sum_{i=1}^{m} \frac{1}{2} P_i P_i^t X_{2,n} \left( (\Delta W_i)^2 - \Delta t \right) \right),
\]

\[
+ \sum_{i=1}^{m} \sum_{j=i+1}^{m} \frac{1}{2} \left[ P_i, P_j \right] (J_{ji} - J_{ij}) X_{2,n},
\]

\[
+ \sum_{i=1}^{m} \frac{1}{2} \left[ P_i (P_i^t P_i)^{1/2} \right] \left( \frac{1}{3} (\Delta W_i)^2 - \Delta t \right) \Delta W_i \right) X_{2,n},
\]

for \( n = 0, 1, \ldots, N - 1, \ y_0 = y_{t_0}. \) The commutator is given as \([P_i, P_j] = P_i P_j - P_j P_i\).

Further the \( J_{ij} \) are given as:

\[
J_{ji} = \frac{1}{2} J_{ji} J_i - \frac{1}{2} (a_{i0} J_j - a_{j0} J_i),
\]

with \( J_i = \Delta W_i = (W_{t_{n+1}, i} - W_{t_n, i}) = \sqrt{\Delta t} N_i(0, 1) \) and the coefficients are given as: \( a_{i0} = \Delta \tilde{W}_i, \) where \( \Delta \tilde{W}_i = \sqrt{\frac{\Delta t}{2\pi}} N_i(0, 1), \) where \( N_i(0, 1) = \text{rand}_i. \)

We obtain a version which is nearly \( O(\Delta t^{1.5}) \) (and more accurate as the Milstein scheme).

For different case of strong and weak perturbations, we have the following Figures [2].

**Remark 4.2.** We can also verify the benefit of the additional terms, which are necessary to resolve the vectorial stochastics. Here, we obtain for both
4 NUMERICAL EXAMPLES

Figure 2: The upper figures presents the results of the strong perturbations \( \alpha_1 = 1.0, \alpha_2 = 1.0 \) (left figure the numerical error, right figure the numerical solution). The right figures presents the results for the weak perturbations \( \alpha_1 = 1.0, \alpha_2 = 0.1 \) (left figure the numerical error, right figure the numerical solution). We apply the following schemes: EM: Euler-Maruyama, Milstein, Iter1: 1-iterative steps, Iter2: 2-iterative steps.

non-iterative and iterative schemes higher order results for the extension of the schemes. In the numerical implementations, we also receive the benefit of the exponential matrices related to the iterative schemes, see [8].

4.3 Vectorial Multiplicative Noise (non-commutative): Real-life example

In the following, we deal with a simple chemical reaction model, but in a vectorial manner.

We deal first with an ordinary differential equation and separate the complex operator into two simpler operators: the \( m \times m \) ordinary differential equation
system given as:

\[ dy(t) = Ay(t) + \sum_{j=1}^{m} P_j y(t) \, dW_j(t), \]

\[ A = \begin{pmatrix} -\lambda_{1,1} & \lambda_{2,1} & \ldots & \lambda_{1,m} \\ \lambda_{2,1} & -\lambda_{2,2} & \ldots & \lambda_{2,m} \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_{m,1} & \lambda_{m,2} & \ldots & -\lambda_{m,m} \end{pmatrix} = \begin{pmatrix} -1 & 0 & \ldots & 0 \\ \frac{1}{m} & -1 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{m} & \frac{1}{m} & \ldots & -1 \end{pmatrix} \]

\[ P_1 = \begin{pmatrix} \sigma_{1,1} & \sigma_{1,2} & \ldots & \sigma_{1,m} \\ \sigma_{2,1} & \sigma_{2,2} & \ldots & \sigma_{2,m} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{m,1} & \sigma_{m,2} & \ldots & \sigma_{m,m} \end{pmatrix} = 0.05 \begin{pmatrix} 1 & 0 & \ldots & 0 \\ \frac{1}{m} & 1 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{m} & \frac{1}{m} & \ldots & 1 \end{pmatrix} \]

\[ P_2 = 0.05 \begin{pmatrix} \tau_{1,1} & \tau_{1,2} & \ldots & \tau_{1,m} \\ \tau_{2,1} & \tau_{2,2} & \ldots & \tau_{2,m} \\ \vdots & \vdots & \ddots & \vdots \\ \tau_{m,1} & \tau_{m,2} & \ldots & \tau_{m,m} \end{pmatrix} = \begin{pmatrix} 1 & \frac{1}{m} & \ldots & \frac{1}{m} \\ 0 & 1 & \ldots & \frac{1}{m} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & 1 \end{pmatrix} \]

\[ dW(t) = (dW_1(t), dW_2(t))(\text{stochastic vector}), \]

\[ y(0) = (1, \ldots, 1)'(\text{initial conditions}), \]

(75)

where \( \lambda_{1,1} \ldots \lambda_{m,m} \in \mathbb{R}^+ \) are the decay factors and \( \sigma_{1,1}, \ldots, \sigma_{m,m}, \tau_{1,1}, \ldots, \tau_{m,m} \in \mathbb{R}^+ \) are the parameters of the perturbations. We have the time interval \( t \in [0, T] \) and \( m \in \mathbb{N} \).

For the testing the different numerical methods, we have the following analytical solution, see [21]:

\[ y(t^{n+1}) = \exp \left( A\Delta t - \frac{1}{2} \sum_{j=1}^{m} P_j P_j' \Delta t + \sum_{j=1}^{m} P_j \Delta W_j \right) y(t^n), \]

(76)

where \( \Delta W_j = (W_{t_{n+1},j} - W_{t_n,j}) = \sqrt{\Delta t} N_j(0, 1), \) where \( N_j(0, 1) = \text{rand}_j \), where we have \( j = 1, \ldots, m \) normally distributed random variables.

We apply the following numerical schemes:

- The application of the standard Euler-Maruyama scheme is given as:

\[ y_{n+1} = y_n + Ay_n \Delta t + \sum_{j=1}^{m} P_j y_n \Delta W_j, \]

(77)

for \( n = 0, 1, \ldots, N-1 \), \( y_0 = y_0, \Delta t = t_{n+1} - t_n, \Delta W = (W_{t_{n+1},1} - W_{t_n,1}, \ldots, W_{t_{n+1},m} - W_{t_n,m}) = (\sqrt{\Delta t} N_1(0, 1), \ldots, \sqrt{\Delta t} N_m(0, 1), \) where \( N_i(0, 1) = \text{rand}_i \), where we have \( i = 1, \ldots, m \) normally distributed random variables.
• Milstein scheme (without outer-diagonal entries) is given as:

\[
y_{n+1} = y_n + Ay_n \Delta t + \sum_{j=1}^{m} P_j y_n \Delta W_j + \left( \sum_{i=1}^{m} \frac{1}{2} P_i P_i^t y_n \left( (\Delta W_i)^2 - \Delta t \right) \right),
\]

for \( n = 0, 1, \ldots, N - 1, \) \( y_0 = y_{t_0} \).

• Milstein scheme (with outer-diagonal entries) is given as:

\[
y_{n+1} = y_n + Ay_n \Delta t + \sum_{j=1}^{m} P_j y_n \Delta W_j + \left( \sum_{i=1}^{m} \frac{1}{2} P_i P_i^t y_n \left( (\Delta W_i)^2 - \Delta t \right) \right) + \frac{1}{2} \sum_{i=1}^{m} \sum_{j=i+1}^{m} \frac{1}{2} [P_i, P_j] (J_{ji} - J_{ij}) y_n,
\]

for \( n = 0, 1, \ldots, N - 1, \) \( y_0 = y_{t_0} \). The commutator is given as \([P_i, P_j] = P_i P_j - P_j P_i\).

Further the \( J_{ij} \) are given as:

\[
J_{ji} = \frac{1}{2} J_i J_j - \frac{1}{2} (a_{i0} J_j - a_{j0} J_i),
\]

with \( J_i = \Delta W_i = (W_{t_{n+1},i} - W_{t_n,i}) = \sqrt{\Delta t} N_i(0, 1) \) and the coefficients are given as: \( a_{i0} = \Delta W_i \), where \( \Delta W_i = \frac{\sqrt{2 \pi}}{\Delta t} N_i(0, 1) \), where \( N_i(0, 1) = \text{rand}_i \).

• Iterative splitting scheme is given as in the previous example.

In the following, we have the computations of the non-commutative example. The solution of the 10 species with the iterative scheme (2 steps) and the different schemes for the 10-th species is given in [3].

The errors of the different scheme with respect to the \( L_2 \)-norm, weak and strong error is given in Figure 4.

Remark 4.3. For larger matrices, we also obtain a benefit, when we apply iterative methods. We are more flexible as for the standard schemes, while we can increase the order of the method with additional iterative steps. Further, the computational amount for additional steps are marginal based on the recursive effect of the iterative splitting scheme. Therefore, we can resolve the solution in the same accuracy as a Milstein scheme with additional multiple integral terms, see [15].
4 NUMERICAL EXAMPLES

Figure 3: The solution of the 10 species (left hand side) and the solutions for the 10-th species with the different schemes (right hand side).

Figure 4: The strong error of the numerical solution is given in the left figure. The weak error of the numerical solution is given in the right figure.

4.4 Coulomb test-particle problem (vectorial problem of the linearized Langevin equations)

In the next example, we deal with a real-life problem, which models the characteristics of a collision process, see [4].

We apply the following nonlinear SDE problem:

\begin{align}
    dv(t) &= F_d(v)dt + \sqrt{2D_v(v)}dW_v(t), \\
    d\mu(t) &= -2D_a(v)\mu dt + \sqrt{2D_a(v)(1 - \mu^2)}dW_\mu(t), \\
    d\phi(t) &= \sqrt{\frac{2D_a(v)}{(1 - \mu^2)}}dW_\phi(t),
\end{align}

where the functions and the derivatives of the convection and diffusion operators are given as:

\begin{align}
    D_v(v) &= \frac{1}{2} \frac{1}{v+1}, & \frac{\partial D_v}{\partial v} &= -\frac{1}{2} (v + 1)^{-2}, \\
    F_d(v) &= -\frac{1}{2} \frac{1}{v+1}, & \frac{\partial F_d}{\partial v} &= \frac{1}{2} (v + 1)^{-2}, \\
    D_a(v) &= \frac{1}{2} \frac{1}{v+1}, & \frac{\partial D_a}{\partial v} &= -\frac{1}{2} (v + 1)^{-2},
\end{align}
and where we assume that the initial conditions are given as $v_0 = 1.0$, $\mu_0 = 1.0$ and $\phi_0 = 1.0$.

The notation of the equation in vectorial form is given as:

$$d\mathbf{v}(t) = \mathbf{a}(\mathbf{v})dt + \mathbf{B}(\mathbf{v})dW_{\mathbf{v}}(t),$$

(87)

where $\mathbf{v}(t) = (v, \mu, \phi)^T$ and the vectors and matrix are given as:

$$\mathbf{a}(\mathbf{v}) = \begin{pmatrix} F_d(v) \\ -2D_a(v)\mu \\ 0 \end{pmatrix},$$

$$dW_{\mathbf{v}} = \begin{pmatrix} dW_v \\ dW_\mu \\ dW_\phi \end{pmatrix},$$

(88)

$$\mathbf{B}(\mathbf{v}) = \begin{pmatrix} \sqrt{2D_v(v)} & 0 & 0 \\ 0 & \sqrt{2D_v(v)(1-\mu^2)} & 0 \\ 0 & 0 & \frac{2D_v(v)}{1-\mu^2} \end{pmatrix},$$

(89)

We apply the following numerical schemes:

- The application of the standard Euler-Maruyama scheme is given as:

$$v_{n+1} = v_n + F(v_n)\Delta t + \sqrt{2D(v_n)}\Delta W_v,$$

$$\mu_{n+1} = \mu_n - 2D_a(v_n)\mu_n \Delta t + \sqrt{2D_a(v_n)(1-\mu^2)}\Delta W_\mu,$$

$$\phi_{n+1} = \phi_n + \sqrt{2D_a(v_n)}(1-\mu^2)\Delta W_\phi,$$

(90)

(91)

(92)

for $n = 0, 1, \ldots, N - 1$, $v_0 = v(0), \mu_0 = \mu(0), \phi_0 = \phi(0), \Delta t = t_{n+1} - t_n, \Delta W_i = W_{t_{n+1}} - W_{t_n} = \sqrt{\Delta t}N_i(0,1)$, where $N_i(0,1) = \text{rand}, i = \{v, \mu, \phi\}$ are three independent normally distributed random variables.

- Milstein scheme is given as:

$$v_{n+1} = v_n + F(v_n)\Delta t + \sqrt{2D(v_n)}(\Delta W)$$

$$\quad + \frac{\partial D(v)}{\partial v} \bigg|_{v_n} \frac{1}{2}((\Delta W)^2 - \Delta t),$$

(93)

$$\mu_{n+1} = \mu_n - 2D_a(v_n)\mu_n \Delta t + \sqrt{2D_a(v_n)(1-\mu^2)}\Delta W_\mu - 2\mu_n D_a(v_n)\frac{1}{2}(\Delta W_\mu^2 - \Delta t)$$

$$\quad + \sqrt{D(v_n)}D_a(v_n) \frac{1}{2} \frac{\partial D_a(v)}{\partial v} \bigg|_{v_n} A_{\mu},$$

(94)

$$\phi_{n+1} = \phi_n + \sqrt{2D_a(v_n)}(1-\mu^2)\Delta W_\phi$$

$$\quad + \sqrt{D(v_n)}D_a(v_n) \frac{1}{2} \frac{\partial D_a(v)}{\partial v} \bigg|_{v_n} A_{\phi}$$

$$\quad + \frac{2D_a(v_n)\mu_n}{(1-\mu^2)} A_{\mu, \phi},$$

(95)
for $n = 0, 1, \ldots, N - 1$, $v_0 = v(0), \mu_0 = \mu(0), \phi_0 = \phi(0)$, $\Delta t = t_{n+1} - t_n$, $\Delta W_i = W_{i,t_{n+1}} - W_{i,t_n} = \sqrt{\Delta t} N_i(0,1)$, where $N_i(0,1) = \text{rand}$, $i = \{v, \mu, \phi\}$ are three independent normally distributed random variable.

The iterated Ito integral, which is related to Levy areas \cite{22}, and given as:

$$A_{k,l} = \int_{t_n}^{t_{n+1}} dW_k(s) \int_{t_n}^{s} dW_l(\xi), \quad (96)$$

where we have for the outer-Diagonal case $k \neq l$:

$$A_{k,l} = \frac{1}{2} J_k J_l - \frac{1}{2} (a_{i0} J_k - a_{k0} J_l), \quad (97)$$

with for $i = k, l$, we have $J_i = \Delta W_i = (W_{i,t_{n+1}} - W_{i,t_n}) = \sqrt{\Delta t} N_i(0,1)$ and the coefficients are given as: $a_{i0} = \Delta \tilde{W}_i$, where $\Delta \tilde{W}_i = \sqrt{\frac{\Delta t}{2\pi}} N_i(0,1)$, where $N_i(0,1) = \text{rand}_i$, see \cite{15}.

- Iterative splitting scheme:

  We apply the following linearization techniques of the convective part and iterate via the diffusive part.

  1. Fixpoint iterative version with simple relaxation of the nonlinear part is applied as:

$$dv_{i+1}(t) = \hat{A}(v_i) v_{i+1} dt + B(v_i) dW(t), \quad (98)$$

  with the solution vector $v_i(t) = (v_i(t), \mu_i(t), \phi_i(t))^t$.

  Furthermore, the linearized matrix is given as

$$\hat{A}(v_i) = \begin{bmatrix}
  \frac{F_{v_i}(v_i)}{v_i} & 0 & 0 \\
  0 & -2D_a(v_i) & 0 \\
  0 & 0 & 0
\end{bmatrix}, \quad (99)$$

  Then the fixpoint scheme is given as:

$$v_{i+1}(t^{n+1}) = \exp(\hat{A}(v_i(t^{n+1}))) \Delta t \ v(t^n)$$

$$+ \int_{t_n}^{t_{n+1}} \exp(\hat{A}(v_i(t^{n+1}))) \ (t^{n+1} - s) \ B(v_i(s)) dW_v(s). \quad (100)$$

where the integral is computed as:

1.) Trapezoidal-rule:

$$\int_{t_n}^{t_{n+1}} \exp(\hat{A}(v_i(t^{n+1}))) \ (t^{n+1} - s) \ B(v_i(s)) dW_v(s)$$

$$= \frac{1}{2} (W_v(t^{n+1}) - W_v(t^n)) \left( B(v_i(t^{n+1})) \right)$$

$$+ \exp(\hat{A}(v_i(t^{n+1}))) \Delta t \ B(v_i(t^n)), \quad (101)$$
$\Delta t = t^{n+1} - t^n$ and

$(W(t^{n+1}) - W(t^n)) = (\text{rand}_1\sqrt{\Delta t}, \text{rand}_2\sqrt{\Delta t}, \text{rand}_3\sqrt{\Delta t})^t$,

2.) Simpson-rule

$$
\int_{t^n}^{t^{n+1}} \exp(\hat{A}(v_i(t^{n+1}))) \left( t^{n+1} - s \right) B(v_i(s)) dW_v(s) \quad (103)
$$

$$
= \frac{1}{6} (W_v(t^{n+1}) - W_v(t^n)) \left( B(v_i(t^{n+1})) + 4 \exp(\hat{A}(v_i(t^n + \Delta t/2)) \Delta t/2) B(v_i(t^n + \Delta t/2)) + \exp(\hat{A}(v_i(t^{n+1})) \Delta t) B(v_i(t^n)) \right) ,
$$

$\Delta t = t^{n+1} - t^n$ and

$(W(t^{n+1}) - W(t^n)) = (\text{rand}_1\sqrt{\Delta t}, \text{rand}_2\sqrt{\Delta t}, \text{rand}_3\sqrt{\Delta t})^t$,

2. Fixpoint iterative version with Taylor expansion of the nonlinear part is applied as:

$$
dv_{i+1}(t) = \tilde{a}(v(t^n)) dt + A(v(t^n))dv_{i+1} dt + B(v_i) dW(t),
$$

where we have $v_i = (v_i, \mu_i, \phi_i)^t$ as the solution vector in the $i$-th version, $\tilde{a}$ is the vector and $A(t^n)$ is the Jacobian matrix coming from the linearization, and $dW(t) = (dW_v(t), dW_\mu(t), dW_\phi(t))^t$ is a 3-dimensional Wiener-process. We apply the linearization of the convective part, where the matrices are given as:

$$
a(v) = a(v(t^n)) + J(v)|_{t^n}(v - v(t^n)),
$$

$$
= \left( a(v(t^n)) - J(v)|_{t^n}v(t^n) \right) + J(v)|_{t^n}v, \quad (107)
$$

$$
= \tilde{a}(v(t^n)) + J(v)|_{t^n}v. \quad (108)
$$
The Jacobian matrix is given as:

\[
J(v) = \begin{bmatrix}
\frac{\partial a_1}{\partial v} & \frac{\partial a_1}{\partial \mu} & \frac{\partial a_1}{\partial \phi} \\
\frac{\partial a_2}{\partial v} & \frac{\partial a_2}{\partial \mu} & \frac{\partial a_2}{\partial \phi} \\
\frac{\partial a_3}{\partial v} & \frac{\partial a_3}{\partial \mu} & \frac{\partial a_3}{\partial \phi}
\end{bmatrix}
= \begin{bmatrix}
\frac{\partial F_v(v)}{\partial v} & 0 & 0 \\
-2\mu \frac{\partial D_a(v)}{\partial v} & -2D_a(v) & 0 \\
0 & 0 & 0
\end{bmatrix}, \tag{109}
\]

\[
J(v)|_{t^n} = \begin{bmatrix}
\frac{\partial F_v(v)|_{t^n}}{\partial v} & 0 & 0 \\
-2\mu \frac{\partial D_a(v)|_{t^n}}{\partial v} & -2D_a(v)|_{t^n} & 0 \\
0 & 0 & 0
\end{bmatrix}, \tag{110}
\]

\[
A(v(t^n)) = J(v)|_{t^n}. \tag{111}
\]

The fixpoint scheme is given as:

\[
v_{t+1}(t^{n+1}) = \exp(A(v(t^n)) \Delta t) \left( v(t^n) + A(v(t^n))^{-1}(I - \exp(A(v(t^n)) \Delta t)) \tilde{a}(t^n) \right)
+ \int_{t^n}^{t^{n+1}} \exp(A(v(t^n))(t^{n+1} - s))B(v_i)(s)dW_v(s), \tag{112}
\]

We rewrite this with the singular term $A^{-1}$ and obtain:

\[
v_{t+1}(t^{n+1}) = \exp(A(v(t^n)) \Delta t) \left( v(t^n) + \left( I \Delta t + A(v(t^n)) \frac{\Delta t^2}{2} + A^2(v(t^n)) \frac{\Delta t^3}{3!} \right) \tilde{a}(t^n) \right)
+ \int_{t^n}^{t^{n+1}} \exp(A(v(t^n))(t^{n+1} - s))B(v_i)(s)dW_v(s), \tag{113}
\]

where $\tilde{a}(v(t^n)) = \left( a(v(t^n)) - A(v(t^n))v(t^n) \right)$

The stochastic integral is computed as a Stratonovich integral, e.g., Trape-
4 NUMERICAL EXAMPLES

Zoidal rule:

\[ c(\Delta t) = \int_0^{t_{n+1}} \exp(A(v(t^n))(t^{n+1} - s))B(v_i)(s)dW_s \]  

(114)

\[ = \frac{1}{2}(W_v(t^{n+1}) - W_v(t^n))\left( B(v_i(t^{n+1})) + \exp(A(v(t^n)) \Delta t) B(v_i(t^n)) \right) \]  

(115)

\[ \Delta t = t^{n+1} - t^n, \]  

(116)

\[ (W(t_{j+1}) - W(t_j)) = (rand_1 \sqrt{\Delta t}, rand_2 \sqrt{\Delta t}, rand_3 \sqrt{\Delta t})^t \]  

(117)

where \( rand_1, rand_2 \) and \( rand_3 \) are three independent random numbers given with \( N(0, 1) \).

We apply the following errors:

- The errors are computed as:
  \[ err_{v, \Delta t, t=1} = ||v_{\Delta t, Scheme}(t = 1) - v_{\Delta t, fine, Mil}(t = 1)||, \]  

(118)

where \( || \ldots || \) is the \( L_2 \)-norm, \( v_{\Delta t, Scheme}(t = 1) \) is the solution of the applied schemes, which means \( Scheme = \{ EM, Mil, Iter1, Iter2 \} \). \( \Delta t = \{ 10^{-4}, 10^{-3}, 10^{-2}, 10^{-1} \} \) are the different time-steps and \( t = 1.0 \) is the evaluated end-time-point. \( v_{\Delta t, fine, Mil}(t = 1) \) is a reference solution based on the Milstein-scheme at \( t = 1.0 \) and time-steps \( 10^{-5} \).

The same errors are encountered with the solutions of \( \mu \) and \( \phi \) (see \( err_{\mu, \Delta t, t=1}, err_{\phi, \Delta t, t=1} \)).

- The statistical errors are given as:
  - Strong convergence is based on the errors:
    \[ err_{v, \Delta t, t=1}, err_{\mu, \Delta t, t=1}, err_{\phi, \Delta t, t=1}. \]  

(119)

- Weak convergence is based on the mean values of the errors:
  \[ err_{v, \Delta t, t=1, weak} = \frac{1}{N} \sum_{i=1}^{N} err_{i, v, \Delta t, t=1}, \]  

(120)

where \( err_{i, v, \Delta t, t=1} \) are \( i = 1, \ldots, N \) independent errors of the solution \( v \).

- The derivation of the mean value or variance is given as:
  \[ \sigma_{v, \Delta t, t=1}^2 = \frac{1}{N - 1} \sum_{i=1}^{N} (err_{i, v, \Delta t, t=1} - err_{v, \Delta t, t=1, weak})^2. \]  

(121)
– Time-averaged mean-square value over the time (scan over the time-
space):

\[
\sigma_v^2,\Delta t = \frac{1}{T} \sum_{i=1}^{N} \Delta t (v_{\Delta t,\text{Scheme}}(i \Delta t) - v_{\Delta t,\text{Mil}}(i \Delta t))^2. \quad (122)
\]

where the time-space is given as \(i = 1, \ldots, N, \Delta t N = T = 1\).

The same errors and variances are also encountered with the solutions of \(\mu\) and \(\phi\).

The solutions of the equations are given for the different schemes in Figure 5.

Figure 5: The figures present the results of the different splitting schemes (EM: Euler-Maruyama, Iter1: Splitting Version 1, Iter2: Splitting Version 2. The upper left figure presents the solutions of \(v\), the upper right figure presents the solutions of \(\mu\) and the lower figure presents the solution of \(\phi\).

The convergence results of the different schemes and the three dimensional plots are given in Figure 6.

In the following, the computational time of the different schemes are given (see Table 1). We obtain, that the explicit schemes, i.e., Euler-Maruyama and Milstein scheme, are faster but they have only their restrictions to small time-steps. Therefore, the benefit of the implicit-iterative schemes, i.e., iterative splitting (iter1 and iter2), is given based on large time-steps, e.g., \(\Delta t \leq 10^{-1}\), where the explicit scheme are oscillating.
5 Conclusion

We discuss the problems of using novel iterative splitting schemes to solve stochastic differential equations, which are applied to Langevin equations. We derive convergence results to the iterative schemes and see the benefit of higher order reconstruction based on the number of iterative steps. The numerical examples present the advantages of the iterative schemes and their computational costs with respect to their relaxation effects. A real-life problem based on a collision model is presented. The novel schemes can be applied to nonlinear problems and they allow to use larger time steps without losing their numer-

Figure 6: The figures present the results of the different splitting schemes (EM: Euler-Maruyama, Iter1: Splitting Version 1, Iter2: Splitting Version 2. The upper left figure presents the weak convergence of \( v \); the upper right figure presents variance of \( v \) and the lower figure presents the three dimensional plot of all the solutions.

Remark 4.4. The examples show the important selections of the linearization method, which is related to the iterative schemes. Some small benefits are obtained with the Version 1, see Equation (112), that applied a simple relaxation of the nonlinear part. Here, we take into account the relaxation effect of the iterative schemes as a function of time step. We see an improvement with larger time-steps, e.g. see the variance-errors in Figure 6. On the other hand, we have taken into account the costs of the new algorithms, that are acceptable, e.g., 2-3 times that of the standard schemes.


| Method         | $\Delta t$ | $10^{-1}$ | $10^{-2}$ | $10^{-3}$ | $10^{-4}$ |
|---------------|------------|-----------|-----------|-----------|-----------|
| Euler-Maruyama| 7.7248e-04s| 0.0018s   | 0.0132s   | 0.1517s   |           |
| Milstein      | 0.0012s    | 0.0032s   | 0.0286s   | 0.3215s   |           |
| iter1         | 0.0080s    | 0.0536s   | 0.5302s   | 6.1977s   |           |
| iter2         | 0.0078s    | 0.0472s   | 0.4497s   | 5.1896s   |           |

Table 1: Computational time of the different solver methods.

Theoretical accuracy. Here, we can optimize the application of such novel schemes, while the computational costs for the standard schemes are higher with smaller time steps. In future, we see an area to optimize such novel schemes with their benefit of relaxing the nonlinear solutions and to apply larger time steps.

References

[1] B.I. Cohen, L. Divol, A.B. Langdon, and E.A. Williams. Effects of ion-ion collisions and inhomogeneity in two-dimensional kinetic ion simulations of stimulated Brillouin backscattering. Phys. Plasmas, 13(2), 022705, 2006.

[2] B.I. Cohen, A.M. Dimits, A. Friedman and R.E. Caflisch. Time-Step Considerations in Particle Simulation Algorithms for Coulomb Collisions in Plasmas. IEEE Transactions on Plasma Science, 38(9): 2394-2406, 2010.

[3] A.M. Dimits, B.I. Cohen, R.E. Caflisch, L. Ricketson and M.S. Rosin. Higher-order and Multi-Level Time Integration of Stochastic Differential Equations and Application to Coulomb Collisions. Lecture at the Workshop III: Mathematical and Computer Science Approaches to High Energy Density Physics, May 7-11, 2012, IPAM, UCLA, USA, 2012.

[4] A.M. Dimits, B.I. Cohen, R.E. Caflisch, M.S. Rosin, and L.F. Ricketson. Higher-order time integration of Coulomb collisions in a plasma using Langevin equations. Journal of Computational Physics, 242:561-580, 2013.

[5] L.G. Eriksson and P. Helander. Monte Carlo operators for orbitaveraged FokkerPlanck equations. Phys. Plasmas, 1(2):308-314, 1994.

[6] J. Geiser. Decomposition Methods for Partial Differential Equations: Theory and Applications in Multiphysics Problems. Numerical Analysis and Scientific Computing Series, CRC Press, Chapman & Hall/CRC , edited by Magoules and Lai, 2009.

[7] J. Geiser. Iterative Splitting Methods for Differential Equations. Numerical Analysis and Scientific Computing Series, CRC Press, Chapman & Hall/CRC , edited by Magoules and Lai, 2011.
[8] J. Geiser. *Computing Exponential for Iterative Splitting Methods*. Journal of Applied Mathematics, Vol. 2011, Article ID 193781, 2011.

[9] J. Geiser. *An Iterative Splitting Method via Waveform Relaxation*. International Journal of Computer Mathematics, Taylor and Francis, New York, 88(7):3646-3665, 2011.

[10] J. Geiser. *Iterative Splitting Methods for Multiscale Problems*. Proceeding of the Distributed Computing and Applications to Business, Engineering & Science (DCABES), 12th International Symposium, London, 2-4 Sept. 2013, pp. 3-6, 2013.

[11] J. Geiser. *Multiscale splitting for stochastic differential equations: applications in particle collisions*. Journal of Coupled Systems and Multiscale Dynamics, American Scientific Publishers, Valencia, CA, USA, August 2013.

[12] J. Geiser. *Picard’s Iterative method for nonlinear Multicomponent Transport Equations*. Cogent Mathematics, Taylor and Francis, 3(1): 1158510, 2016.

[13] M.E. Jones, D.S. Lemons, R.J. Mason, V.A. Thomas, and D. Winske. *A grid-based Coulomb collision model for PIC codes*. J. Comput. Phys., 123(1):169-181, 1996.

[14] C.T. Kelley. *Iterative Methods for Linear and Nonlinear Equations*. SIAM Frontiers in Applied Mathematics, no. 16, SIAM, Philadelphia, 1995.

[15] P.E. Kloeden and E. Platen. *The Numerical Solution of Stochastic Differential Equations*. Springer-Verlag, Berlin-Heidelberg-New York, 1992.

[16] D.S. Lemons, D. Winske, W. Daughton, and B. Albright. *Small-angle Coulomb collision model for particle-in-cell simulations*. J. Comput. Phys., 228(5):1391-1403, 2009.

[17] W.M. Manheimer, M. Lampe, and G. Joyce. *Langevin representation of Coulomb collisions in PIC simulations*. J. Comput. Phys., 138(2):563-584, 1997.

[18] K. Nanbu. *Theory of cumulative small-angle collisions in plasmas*. Phys. Rev. E, Stat. Phys. Plasmas Fluids Relat. Interdiscip. Top., 55(4):4642-4652, 1997.

[19] S. Ninomiya and N. Victoir. *Weak approximation of stochastic differential equations and application to derivative pricing*. Appl. Math. Finance, 15:107-121, 2008.

[20] M. Ninomiya and S. Ninomiya. *A new higher-order weak approximation scheme for stochastic differential equations and the Runge-Kutta method*. Finance and Stochastics, 13(3):415-443, 2009.
[21] E. Platen and N. Bruti-Liberati. *Numerical Solution of Stochastic Differential Equations with Jumps in Finance.* Series: Stochastic Modelling and Applied Probability, Volume 64, Springer-Verlag Berlin Heidelberg, 2010.

[22] K. Scheicher. *Complexity and effective dimension of discrete Levy areas.* Journal of Complexity, 23(2):152-168, 2007.

[23] M. Sherlock. *A Monte-Carlo method for Coulomb collisions in hybrid plasma models.* J. Comput. Phys., 227(4):2286-2292, 2008.

[24] T. Takizuka and H. Abe. *A binary collision model for plasma simulation with a particle code.* J. Comput. Phys., 25(3):205-219, 1977.

[25] A. Tocino *Multiple stochastic integrals with Mathematica.* Mathematics and Computers in Simulation, 79(5): 1658-1667, 2009.
\[10^{-3}, 10^{-2}, 10^{-1}, 10^0, 10^1\]

\[\delta v, \delta t\]


diagram showing \(\delta v\) vs. \(\delta t\) with labels iter1, iter2, and EM.