Workshop: *Particle transport with emphasis on Stochastics* Lecture: Splitting Methods for Particle Transport: Theory and Application in Plasma Simulations

Jürgen Geiser, Ruhr University of Bochum,
Department of Electrical Engineering and Information Technology,
Universitätsstr. 150, D-44801 Bochum, Germany

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Splitting methods for particle transport problems are interesting tools to solve deterministic/stochastic partial differential equations.

- Reduction of computational amount (decomposition into a deterministic and stochastic part).
- Concentrating on each individual term (e.g., transport and collision part).
- Multiscale-Splitting: Decomposing to slow- and fast time or spatial scales (dynamical view-point).
- Parallelisation-Idea

Solver-Toolbox and Idea

- Splitting schemes are solver methods for deterministic and stochastic differential equations
- Main idea of the schemes: partitioning of full operators into a quantity of simpler and faster computable operators, e.g., partitioning into deterministic and stochastic parts

Numerical Challenges of Splitting schemes

- Reduction of the numerical error: Each splitting method has a numerical error (splitting error). To reduce the error, we apply adaptivity or higher order splitting schemes.
- Conservation of the underlying physics: for example particle transport problems need long term evolutions, means conservation of the dynamics, e.g., symplecticity of the schemes

Particle Transport: Characterizing the Model problem

- Microscopic model (each particle is treated via an individual equation (transport and collision operators)).
- Plasma simulations are done with particle transport models, where ionized particles are transported via an electromagnetic field and particles can be collide.

Different problems:

- Forward problem: All parameters of the model-equation (e.g. stochastic differential equation) are known, e.g., physical laws, heuristics etc.
- Backward problem: An experimental data-set of the particles are given and we reconstruct the parameters, e.g., drag, diffusion, potential, etc. of the underlying model-equation (e.g., ambit stochastics, inverse modeling)

Classification of Decomposition Methods based on the Splitting Aspect

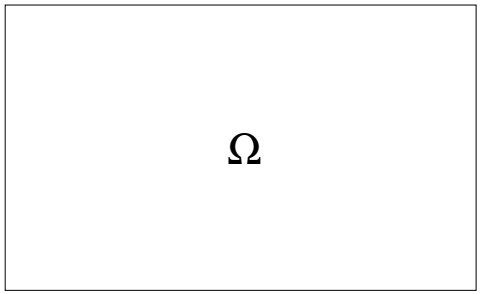
We have the three different methodological ideas:

- Domain-Decomposition, i.e., Partitioning of large spatial-domains in smaller and computable spatial-domains, each smaller domain can be computed parallel, e.g., Schwartz-Waveform-Relaxation (Relaxation-Idea)
- Time-Decomposition, i.e., Partitioning of large time-intervals in smaller and computable time-intervals, each smaller time-intervals can be computed parallel, e.g., Parareal-algorithm (Predictor-Corrector-Idea)
- Operator-Splitting, i.e., Partitioning of the large operator (e.g., deterministic and stochastic operator) into simpler and smaller operators, which can be handled in separate operator equations and can also be computed in parallel, e.g., Splitt-up algorithms.

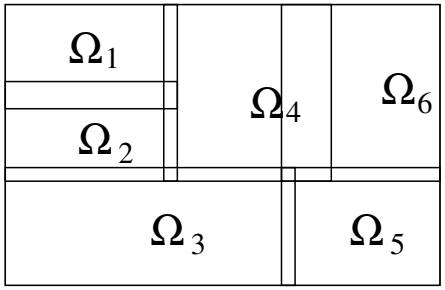
Domain-Decomposition (Overlapping and Nonoverlapping)

Domain Decomposition

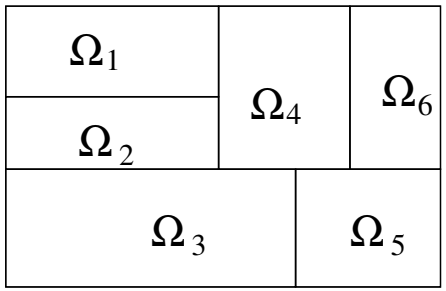
Unique Domains



Overlapping domains



Non−Overlapping domains



Time-Decomposition (Partitioning and Windowing of Time-Intervals)

1.) Windowing:

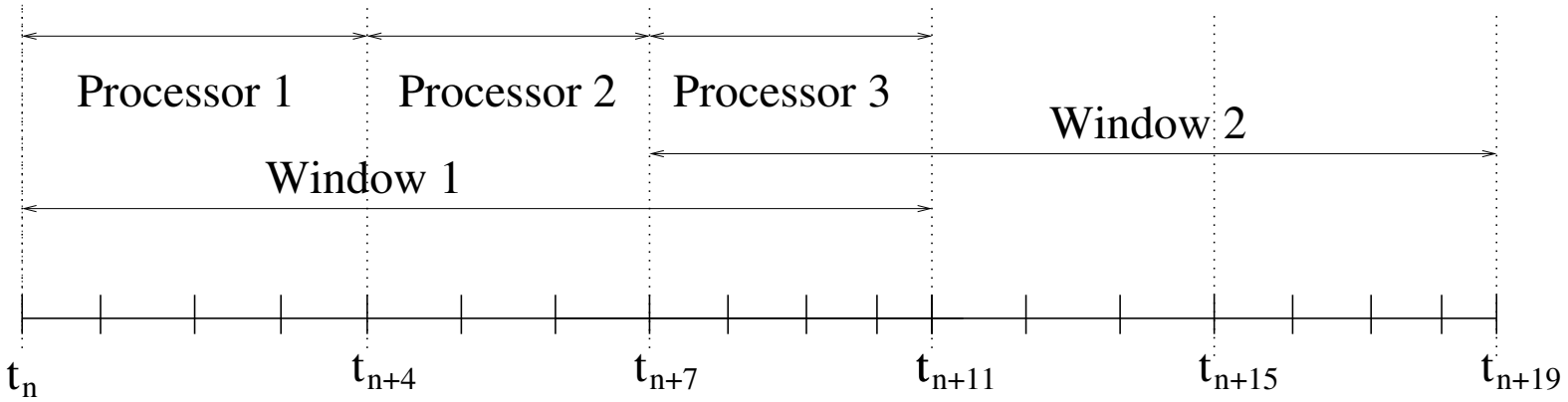


Figure: Parallelization with Parareal, windowing of the parallel process.

Splitt-up Algorithms (Parallelisation of Operators)

2.) Splitting-up of a full operator $A_{full} = \sum_{i=1}^{m} A_i$.
We deal with m parallel sub-problem given as:

$$\frac{\partial c_1(t)}{\partial t} = A_1 c_1(t) , \quad \text{with } c_1(t^n) = c(t^n) , \tag{1}$$

$$\frac{\partial c_2(t)}{\partial t} = A_2 c_2(t) , \quad \text{with } c_2(t^n) = c(t^n) , \tag{2}$$

$$\vdots \tag{3}$$

$$\frac{\partial c_m(t)}{\partial t} = A_m c_m(t) , \quad \text{with } c_m(t^n) = c(t^n) , \tag{4}$$

and one additive step that couples the independent sub-steps:

$$c(t^{n+1}) = c(t^n) + \sum_{i=1}^{m} (c_i(t^{n+1}) - c(t^n)), \; n = 1, 2, \ldots, N, \; c(0) = c_0.$$

The local splitting error of the parallel scheme is $\mathcal{O}(\tau)$.

Particle Transport Model: Langevin-like Equations

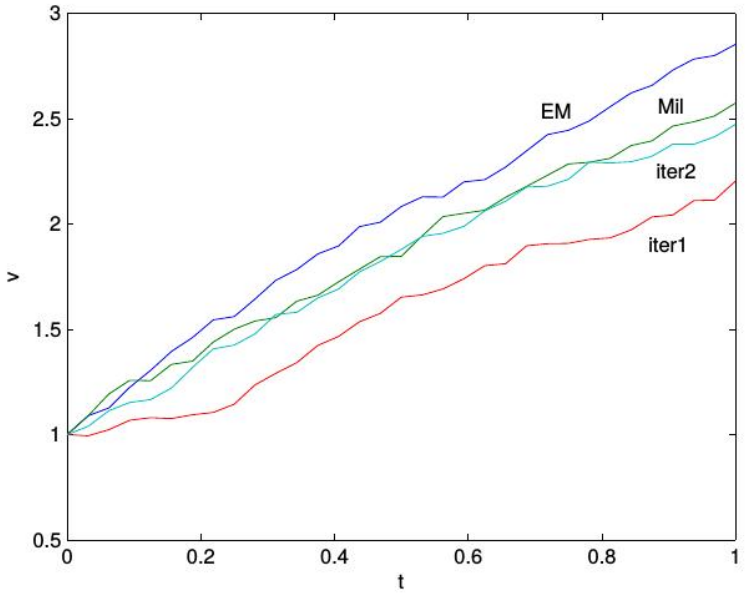
Idea: Particle Simulation Algorithms for Coulomb-Collision in Plasmas with Langevin equations.
Coulomb Collision Approach:

Remark

Coulomb Collisions can be approximated via defining test and field particles. The test-particle velocity is subjected to drag and diffusion in three velocity dimensions using Langevin Equations, see [Cohen2010][1] .

[1] B.I. Cohen, et al, Time-Step Considerations in Particle Simulation Algorithms for Coulomb Collisions in Plasmas, IEEE Transactions on Plasma Science, 38(9): 2394-2406, 2010.

Particle Trajectories in Plasma (Work with Th. Zacher, Humboldt University of Berlin, Germany)



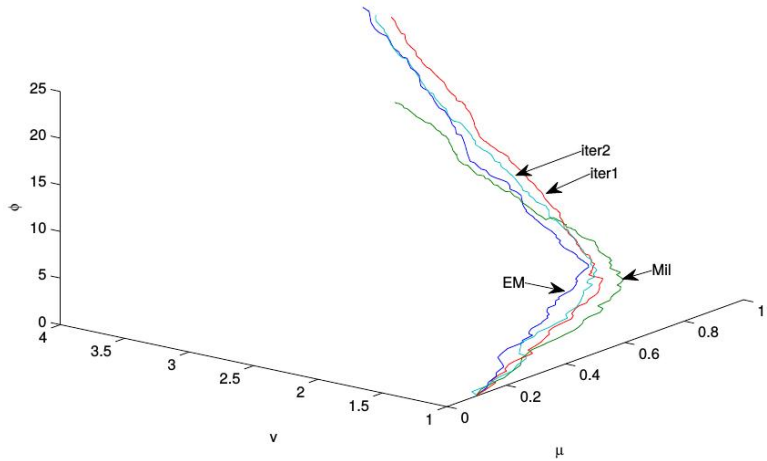


Figure: Velocity v of a particle and 3D presentation of the velocity components for one underlying particle (see [Geiser 2014, submitted to JMAA]).

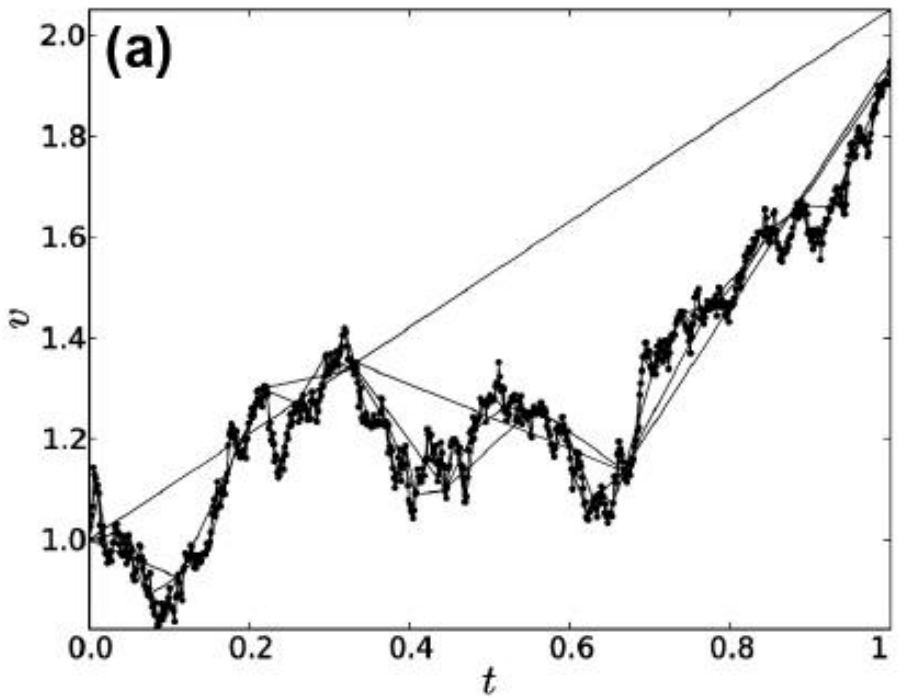


Figure: Velocity v of a particle for one underlying particle (see [Dimits et al 2013]).

Introduction to the Particle Model

We deal with the Fokker-Planck-equation with collision operator given as:

$$\frac{\partial f_\alpha}{\partial t} + \mathbf{v} \cdot \frac{\partial f_\alpha}{\partial \mathbf{x}} + \frac{q_\alpha}{m_\alpha}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \frac{\partial f}{\partial \mathbf{v}} = \frac{\partial f_\alpha}{\partial t}|_{coll}, \tag{5}$$

where $f_\alpha(\mathbf{x}, \mathbf{v})$ is the phase-space distribution function (density) of a charged plasma species α submitted to electromagnetic field $(\mathbf{E}, \mathbf{B})$.

Landau's collision term

The Landau's collision term is given as:

$$\frac{\partial f_\alpha}{\partial t}|_{coll} = \frac{\partial}{\partial \mathbf{v}} \cdot \left(\pi \; q_\alpha^2 \; \lambda \sum_\beta q_\beta^2 \int (f_\alpha \frac{\partial f'_\beta}{\partial \mathbf{v}'} - f'_\beta \frac{\partial f_\alpha}{\partial \mathbf{v}'}) \; \frac{u^2 I - \mathbf{u}\mathbf{u}}{u^3} \right) \; d^3\mathbf{v}' (6)$$

where the sum is over the index β of the plasma charged-particle species, q_β is the charge of species β, $f_\beta(\mathbf{x}, \mathbf{v}')$, $\mathbf{u} = \mathbf{v} - \mathbf{v}'$, $u = |\mathbf{u}|$ and λ is the Coulomb logarithm.

Langevin equation for the Coulomb scattering test-particle problem

We apply the equation (6) with respect to a consistent test-particle, isotropic Maxwellian-background reduction, see [Dimits et al 2013].
We obtain the following test-particle equation:

$$\frac{\partial f_t}{\partial t}|_{coll} = -\frac{\partial}{\partial v}(F_D(v)f_t) + \frac{\partial^2}{\partial v^2}(D_v(v)f_t) \tag{7}$$
$$+\frac{\partial}{\partial \mu}(2D_a(v)\mu f_t) + \frac{\partial^2}{\partial \mu^2}(D_a(v)(1-\mu^2)f_t) + \frac{\partial^2}{\partial \phi^2}(\frac{D_a(v)}{(1-\mu^2)}f_t)$$

where v is the speed, $\mu = \cos(\theta)$, with θ is the angle of the axial direction and ϕ is the azimuthal angle

SDE system of the Coulomb scattering test-particle problem

The SDE system is given as:

$$dv(t) = F_D(v)dt + \sqrt{2D_v(v)}dW_v(t), \tag{8}$$

$$d\mu(t) = -2D_a(v)\mu\, dt + \sqrt{2D_a(v)(1-\mu^2)}dW_\mu(t), \tag{9}$$

$$d\phi(t) = \sqrt{\frac{D_a(v)}{(1-\mu^2)}}dW_\phi(t). \tag{10}$$

One-dimensional Example: Decomposition Idea

The 1D-Fokker-Planck equation with collision term is given as

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} - E(x)\frac{\partial f}{\partial v} = \frac{\partial f}{\partial t}|_{coll} \tag{11}$$

$$\frac{\partial f}{\partial t}|_{coll} = \frac{\partial}{\partial v}(-\gamma v f + \beta^{-1}\gamma\frac{\partial f}{\partial v}), \tag{12}$$

where we could decouple such a FP equation into the PIC (particle in cell) part and the SDE part.

- PIC-part

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} - E(x)\frac{\partial f}{\partial v} = 0, \tag{13}$$

- SDE part

$$\frac{\partial f}{\partial t} = \frac{\partial}{\partial v}(-\gamma v f + \beta^{-1}\gamma\frac{\partial f}{\partial v}). \tag{14}$$

Then we solve the characteristics of the particles:

- PIC-part

$$\frac{dx}{dt} = v, \tag{15}$$

$$\frac{dv}{dt} = -E(x) = \frac{\partial U}{\partial x}, \tag{16}$$

where U is the potential.

- SDE part (Langevin-like equation)

$$\frac{dx}{dt} = 0, \tag{17}$$

$$dv = -\gamma v dt + \sqrt{2\beta^{-1}\gamma} dW, \tag{18}$$

We apply the following nonlinear SDE problem:

$$\frac{dx}{dt} = v, \tag{19}$$

$$dv(t) = \frac{\partial}{\partial x} U(x) - \gamma v dt + \sqrt{2\beta^{-1}\gamma} dW, \tag{20}$$

where W is a Wiener process, γ is the thermostat parameter, β the inverse Temperature.
A long solution to the SDE is distributed according to a probability measure with density π satisfying:

$$\pi(x, v) = C^{-1} \exp(-\beta(\frac{v^2}{2} + U(x)), \tag{21}$$

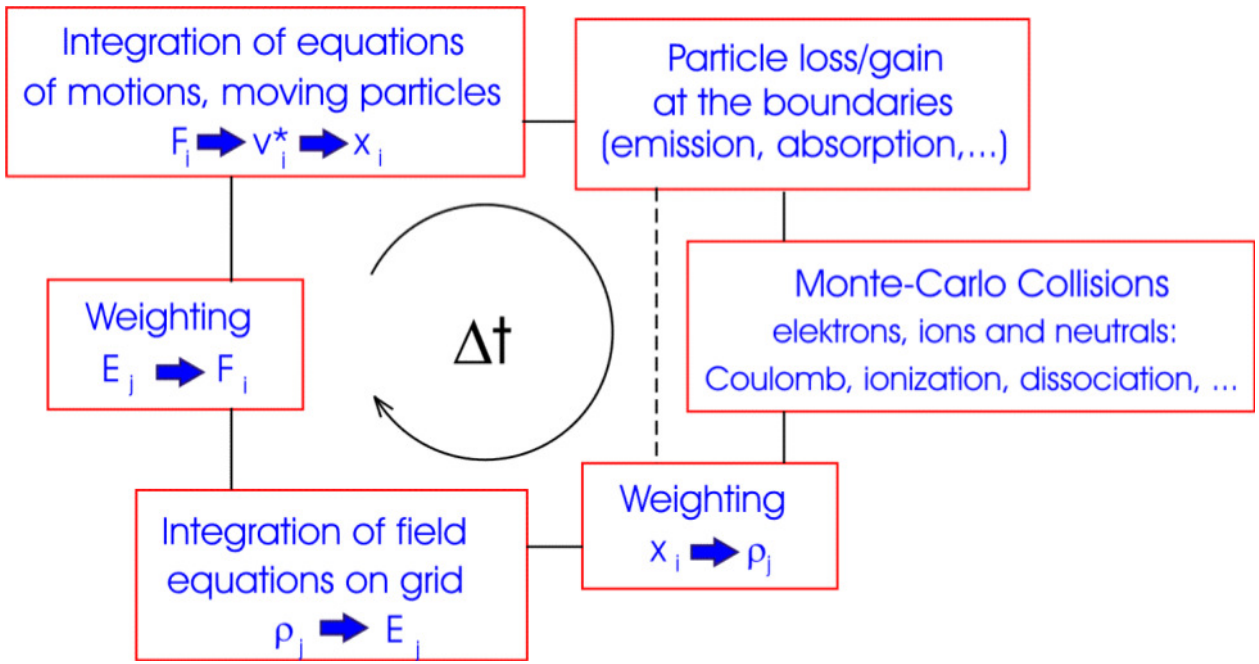
where $x > 0.0$, $v \in \mathbb{R}$.

Splitting of Deterministic and Stochastic Parts

- Deterministic Part (PIC-Cycle with particle motion and electromagnetic field)
- Stochastic Part (Collision: Langevin-equation)

Standard PIC-Cycle

Decomposition to a mesh-free (equation of motion) and mesh equation (electromagnetic field). Such a decomposition allows to accelerate the solver-process.



PIC-Cycle

Pusher-Part (equation of Motion)

$$\frac{dx_p}{dt} = v_p, \ \frac{dv_p}{dt} = \frac{q_s}{m_s} E_p(x_p), \tag{22}$$

Approximation particle to grid:

$$\rho_s(x,t) = \sum_p q_s N_p S_x(x - x_p), \tag{23}$$

Solver-Part

$$\nabla \cdot \nabla U(x) = -\frac{\rho_s(x,t)}{\epsilon_0}, \tag{24}$$

$$\nabla U(x) = -E(x), \tag{25}$$

Approximation grid to particle:

$$E_p = \int S_x(x - x_p) E(x) \, dx, \tag{26}$$

where S_x is a spline function.

Introduction to Splitting Methods

We deal with semidiscretized PDE systems and assume, that we have derived an abstract Cauchy problem:

$$\begin{aligned} \frac{\partial c}{\partial t} &= Ac + Bc \ , \text{ in } \Omega \times (0,T) \ , \\ c(x,0) &= c_0(x) \ , \text{ in } \Omega \text{ (Initial Conditions)} \ , \end{aligned} \tag{27}$$

where $c = (c_1, \ldots, c_n)^t$ and the spatial-discretized matrices have embedded the boundary conditions.

Decomposition-Methods (Non-iterative)

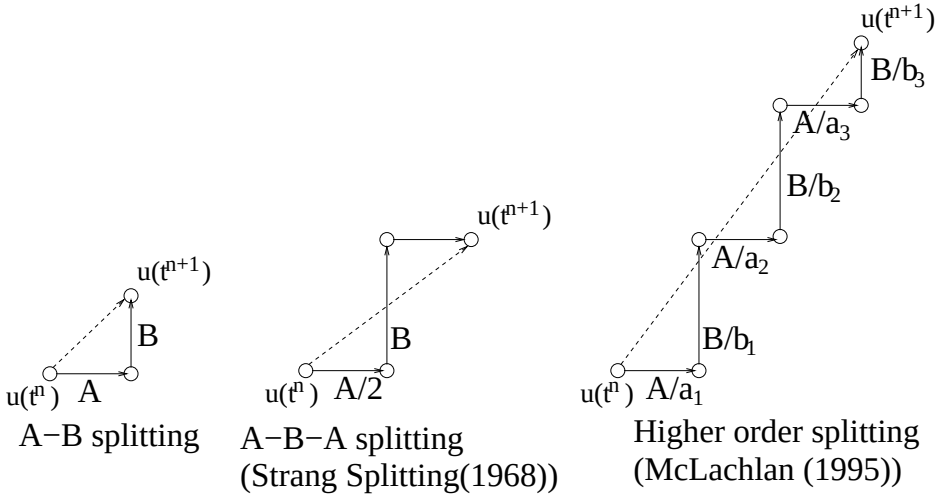


Figure: Visualization of the Splitting Methods (non-iterative).

Decomposition-Methods (iterative)

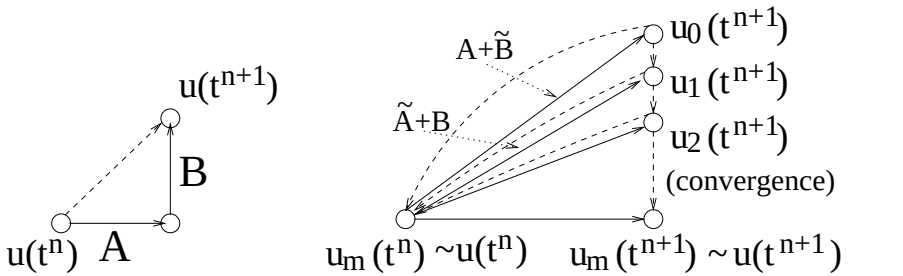


Figure: Visualization of the Splitting Methods (iterative).

Simple Results (sequential Splitting)

A-B Splitting (Lie-Trotter Splitting):

$$\partial_t c^* = Ac^* \quad \text{with} \quad c^*(t^n) = c^n \ ,$$
$$\partial_t c^{**} = Bc^{**} \quad \text{with} \quad c^{**}(t^n) = c^*(t^{n+1}) \ ,$$

where $c(t^{n+1}) = c^{**}(t^{n+1})$ (e.g. [Strang 68], [Karlsen et al 2001]).
The splitting error $err_{global} = c - c_{AB}$ is is given

$$err_{global} = \frac{1}{2}\tau(BA - AB)c(t^n) + O(\tau^2) \ ,$$

error is related to the commutator $[B, A]$, see [Strang 68], [Sheng1993].

Improvements: Strang-Splitting

Strang or Strang-Marchuk-Splitting, cf. [Marchuk 68, Strang68]

$$\frac{\partial c^*(t)}{\partial t} = Ac^*(t),\ t^n \leq t \leq t^{n+1/2},\ c^*(t^n) = c^n_{\mathrm{sp}},$$
$$\frac{\partial c^{**}(t)}{\partial t} = Bc^{**}(t),\ t^n \leq t \leq t^{n+1}\ , c^{**}(t^n) = c^*(t^{n+1/2}),$$
$$\frac{\partial c^{***}(t)}{\partial t} = Ac^{***}(t), t^{n+1/2} \leq t \leq t^{n+1}, c^{***}(t^{n+1/2}) = c^{**}(t^{n+1}),$$

where $t^{n+1/2} = t^n + 0.5\tau_n$ and $c^{n+1}_{\mathrm{sp}} = c^{***}(t^{n+1})$.
The splitting error $err_{global} = c - c_{strang}$ is given as

$$err_{global} = \frac{1}{24}\tau_n^2([B,[B,A]] - 2[A,[A,B]])\ c(t^n) + O(\tau_n^3)\ ,$$

error is related to higher commutators $[B,[B,A]]$, see [Strang 68], [Sheng1993].

Iterative Operator Splitting Methods (classical version)

The Cauchy-problem (27) is solved with the following fixpoint-scheme:

$$\frac{\partial c_i(t)}{\partial t} = Ac_i(t) + Bc_{i-1}(t), \text{ with } c_i(t^n) = u^n,$$
$$\frac{\partial c_{i+1}(t)}{\partial t} = Ac_i(t) + Bc_{i+1}(t), \text{ with } c_{i+1}(t^n) = u^n,$$

where $i = 1, 3, \ldots, 2m+1$ are the iterative steps, $c_0(t)$ is fixed function for each iteration. The splitting error is $err_i = c - c_i$.
The splitting error of the iterative splitting is of $2m+1$ order, i.e. $O(\tau^{2m+1})$, with

$$||err_{2m+1}|| = K_m \tau_n^{2m} ||err_0|| + + O(\tau_n^{2m+1}) , \quad (28)$$

where $K_m = ||B^m|| ||A^m||$ (higher order matrix polynomials).

Extension to Splitting Schemes with Deterministic and Stochastic Parts

We discuss some extension to non-iterative splitting schemes.

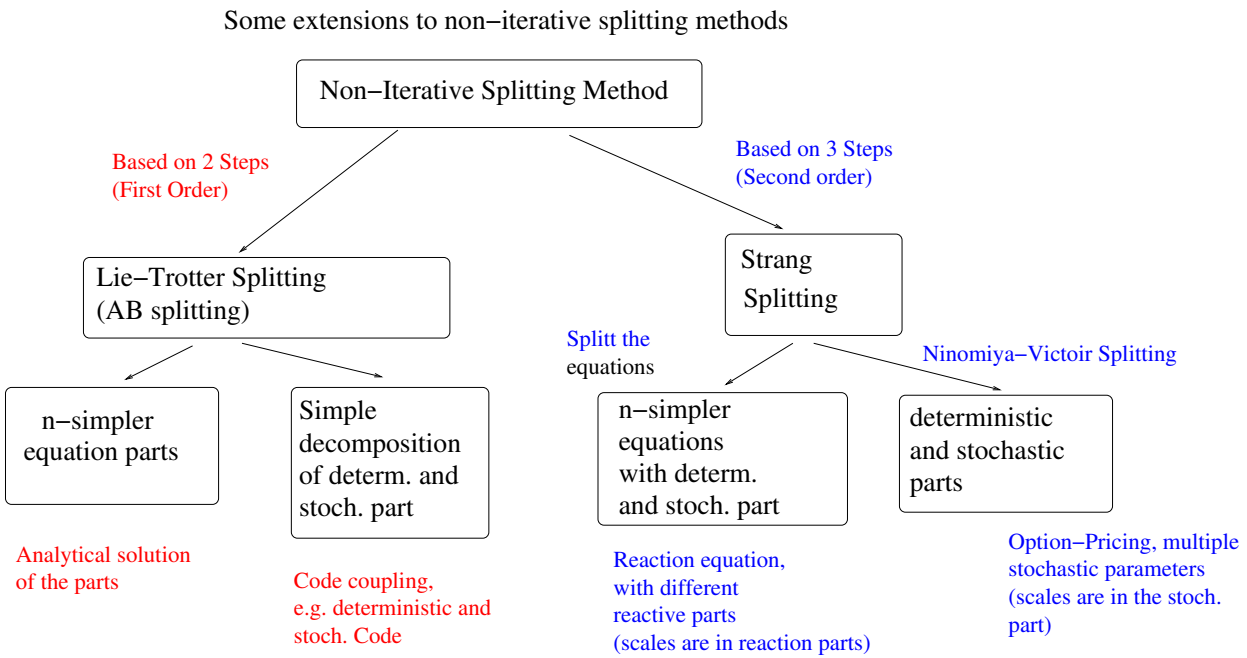


Figure: Some extension to the non-iterative splitting schemes.

Extension to Iterative Splitting Schemes

We discuss some extension to iterative splitting schemes.

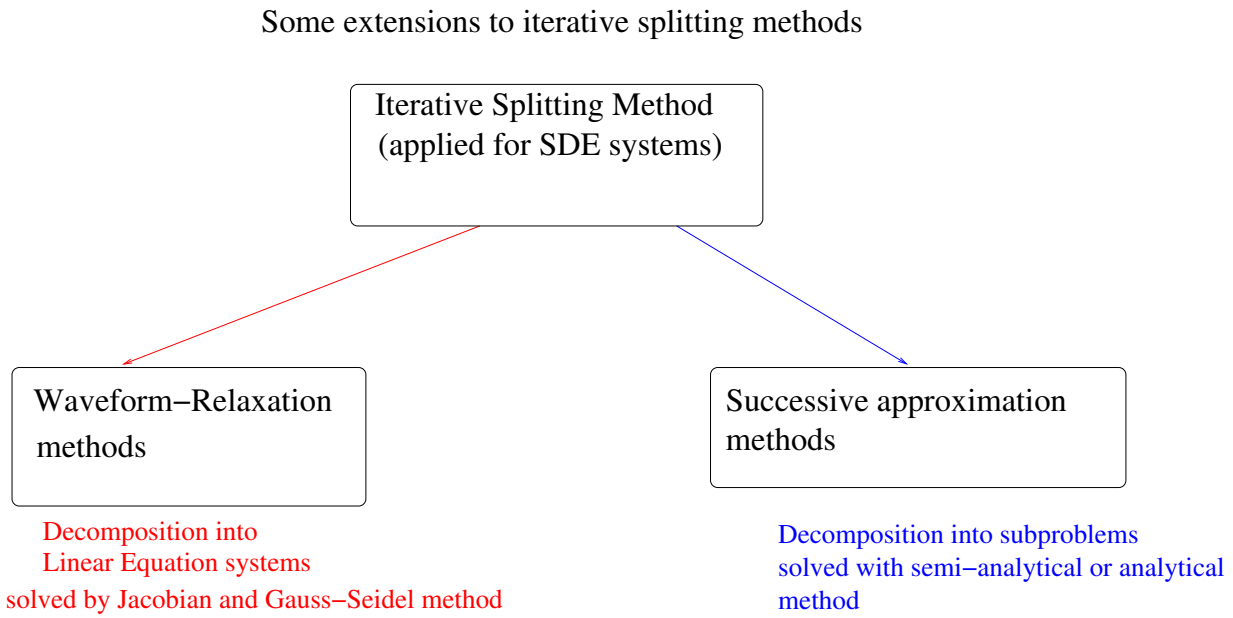


Figure: Some extension to the iterative splitting schemes.

Iterative Splitting Methods for SDE

We propose the following iterative algorithm with step-size τ. For the time-interval $[t^n, t^{n+1}]$, we solve the following sub-problems for $i = 1, 3, \ldots 2m+1$:

$$dc_i(t) = Ac_i(t)dt + Bc_{i-1}dW_t(t), \text{ with } c_i(t^n) = c^n \quad (29)$$
$$\text{and } c_i(t^n) = c^n, \; c_0 = 0.0,$$
$$dc_{i+1}(t) = Ac_i(t)\,dt + Bc_{i+1}(t)\,dW_t, \quad (30)$$
$$\text{with } c_{i+1}(t^n) = c^n,$$

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 [Kloeden 1992].

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

$$\frac{\partial c_i(t)}{\partial t} = Ac_i(t) + Bc_{i-1}\dot{W}_t, \text{ with } c_i(t^n) = c^n \quad (31)$$

$$\text{and } c_i(t^n) = c^n \ , \ c_0 = 0.0,$$

$$\frac{\partial c_{i+1}(t)}{\partial t} = Ac_i(t) + Bc_{i+1}(t)\ \dot{W}_t, \quad (32)$$

$$\text{with } \ c_{i+1}(t^n) = c^n \ ,$$

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

Convergence Results

We present the results of the consistency of our iterative method extended to stochastic operators, see [Geiser 2013].

Theorem

Let us consider the abstract Cauchy problem in a Banach space $\mathbf{X}$

$$dc(t) = Ac(t)dt + Bc(t)dW_t, \ t \in [0,T], \ c(0) = c_0, \tag{33}$$

where $A, B : \mathbf{X} \to \mathbf{X}$ *are given linear operators in a Banach-space and* $c_0 \in \mathbf{X}$ *is a given element.*
The iterative operator splitting method has the following splitting error:

$$||(S_i - \exp(A\tau + BW_\tau)|| \leq C\tau^{\frac{i+1}{2}}, \tag{34}$$

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:

$$dc_1(t) = Ac_1(t)dt + BdW_t c_0(t), \quad t \in (0, \tau], \tag{35}$$

where we have the solution given as:

$$c_1(\tau) = \exp(A\tau)c(t^n) + \int_{t^n}^{t^{n+1}} \exp(A(t^{n+1} - s))Bc_0(s)dW_s, \tag{36}$$

$$= (I + A\tau + BW_\tau + \frac{1}{2}BB^t W_\tau^2 - \frac{1}{2}BB^t\tau)c(0) + \mathcal{O}(\tau^{3/2}), \tag{37}$$

$$c_0(t) = \exp(BW_t)c(0)$$

□

Proof.

The consistency is given as:
For e_1, we have:

$$c_1(t) = (I + At + BW_t + \frac{1}{2}BB^t W_t^2 - \frac{1}{2}BB^t t)c(t^n) + \mathcal{O}(t^{3/2}), \quad (38)$$

$$c(t) = \exp((A - BB^t/2)t + BW_t)c(0)$$

$$= (I + At + BW_t + \frac{1}{2}BB^t W_t^2 - \frac{1}{2}BB^t t)c(0) + \mathcal{O}(t^{3/2}), \quad (39)$$

We obtain:

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

□

The same idea is done for the second iteration and we obtain:
We obtain:

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

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

Drawback and Problems to overcome with Iterative Splitting Schemes

- One have to compute exp-matrices and exp-integrals
- For higher order schemes we have to apply double stochastic integrals as:

$$c_2(\tau) = \exp(A\tau)c(t^n) + \int_{t^n}^{t^{n+1}} \exp(A(t^{n+1}-s))B\exp(As)dW_s$$

$$+ \int_{t^n}^{t^{n+1}} \exp(A(t^{n+1}-s))B\int_{t^n}^{s} \exp(A(s-s_1))B\exp(As)dW_{s_1}dW_s$$

- For systems of SDE's we have to deal with the iterative Taylor-Expansion of the stochastic terms and obtain double area integrals, e.g.

$$A_{ij} = \int_{t^n}^{t^{n+1}} \left(\int_{t^n}^{s} dW_i(s_1) \right) dW_j(s).$$

Non-iterative Splitting Method for SDE

We deal with the following equations:

$$\frac{dX}{dt} = V, \tag{40}$$
$$dV = -E(x)dt - AVdt + BdW, \tag{41}$$
$$\text{with } X(0) = X_0,\ V(0) = V_0\ ,$$

where W is a Wiener process with the $N(0, \sqrt{\Delta t})$ distributed.
We rewrite to a linear operator and a nonlinear and stochastic operator.

$$\begin{pmatrix} dX \\ dV \end{pmatrix} = \underbrace{\begin{pmatrix} V \\ 0 \end{pmatrix} dt}_{X} + \underbrace{\begin{pmatrix} 0 \\ -E(X) \end{pmatrix} dt}_{Y} + \underbrace{\begin{pmatrix} 0 \\ -AVdt + BdW \end{pmatrix}}_{Z}.$$

Means we can decouple into 3 different parts of the evolution operator:

$$P_{\Delta t} = \exp(\Delta t Z) \exp(\Delta t Y) \exp(\Delta t X) \tag{42}$$

Means, we decouple into two deterministic and stochastic operators.

Example

We could decouple into three pieces, while each piece could be solved independently. We assume to related the stochastic term to the Ornstein-Uhlenbeck equation and solve it exactly, if we deal with scalar parameters, i.e., $A = a, B = b$:

$$\tilde{V}(t^{n+1}) = V(t^n) - E(X(t^n))\Delta t, \tag{43}$$

$$X(t^{n+1}) = X(t^n) + \tilde{V}(t^{n+1})\Delta t, \tag{44}$$

$$V(t^{n+1}) = \exp(-a\,\Delta t)\tilde{V}(t^{n+1}) + \frac{b}{\sqrt{2a}}\sqrt{1-\exp(-2a\,\Delta t)}R_n, \tag{45}$$

where $R_n \approx N(0,1)$ is a Gaussian distributed random variable.

Improved Splitting Schemes

Numerical Improvements

In the numerical viewpoint, we have the following two improvements for the schemes:

- Higher accuracy of the scheme, means we reduce the numerical error, e.g. Störmer-Verlet scheme is of second order accuracy
- Conservation of the long term evolution of dynamical systems (symplecticity)

Example: Improved AB-splitting scheme: Predictor-Correct Idea

In the following, we present an semi-implicit AB-scheme, which is related to the deterministic symplectic Störmer-Verlet methods, see [Hairer2003].
We deal with the following approach:

$$X_1(t^{n+1}) = X(t^n) + \int_{t^n}^{t^{n+1}} V(s)\, ds, \tag{46}$$

$$V_1(t^{n+1}) = \mathcal{E}(t)V(t^n) + \int_{t^n}^{t^{n+1}} \mathcal{E}(t^{n+1}-s)B\, dW_s \tag{47}$$

$$V_2(t^{n+1}) = V_1(t^{n+1}) + \int_{t^n}^{t^{n+1}} (-E(X_1(s)))\, ds, \tag{48}$$

$$X_2(t^{n+1}) = X(t^n) + \int_{t^n}^{t^{n+1}} V_2(s)\, ds, \tag{49}$$

where $\mathcal{E}(\Delta t) = \exp(-A\Delta t)$.

- The forth step of the algorithm improves the method to a semi-implicit Euler which is a symplectic ABA-splitting (related to a Störmer-Verlet method).
- The idea is based on the midpoint-scheme, which allows to conserve the long term stability (symplectic scheme).

Application of the predictor-corrector scheme

Example

We deal with the first order approximation and we have:

$$X(t^{n+1}) = X(t^n) + \Delta t\ V(t^n), \tag{50}$$

$$V(t^{n+1}) = V(t^n) - \Delta t\ E(X(t^n)) - \Delta t\ AV(t^n) + B\Delta W, \tag{51}$$

$$X(t^{n+1}) = X(t^n) + \Delta t\ V(t^{n+1}), \tag{52}$$

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

Proof of the Symplecticity of the Numerical Scheme

Theorem

The predictor-corrector AB splitting scheme is symplectic, means:

$$dx_{n+1} \wedge dy_{n+1} = dx_n \wedge dy_n. \tag{53}$$

Means determinant of the solution operator is given as $Det(S_{PC-AB}) = 1$.

Proof.

The predictor-corrector Euler-Maruyama scheme is given as:

$$x(t^{n+1}) = x(t^n) + \Delta t\ y(t^n), \tag{54}$$
$$y(t^{n+1}) = y(t^n) - \Delta t\ x(t^n) + \sigma \Delta W, \tag{55}$$
$$x(t^{n+1}) = x(t^n) + \Delta t\ y(t^{n+1}), \tag{56}$$

and we have:

$$x(t^{n+1}) = (1 - (\Delta t)^2) x(t^n) + \Delta t\ y(t^n) + \Delta t \sigma \Delta W \tag{57}$$
$$y(t^{n+1}) = y(t^n) - \Delta t\ x(t^n) + \sigma \Delta W. \tag{58}$$

□

Proof.

and the algorithm is given as:

$$\begin{pmatrix} x(t^{n+1}) \\ y(t^{n+1}) \end{pmatrix} = \begin{pmatrix} (1-(\Delta t)^2) & \Delta t \\ -\Delta t & 1 \end{pmatrix} \begin{pmatrix} x(t^n) \\ y(t^n) \end{pmatrix} + \begin{pmatrix} r_n \\ s_n \end{pmatrix} \Delta W,$$

where $a_n = (1-\Delta t^2), b_n = \Delta t, c_n = -\Delta t, d_n = 1$ and $r_n = \Delta t \sigma, s_n = \sigma$.

□

Proof.

Based on the symplecticity, we have:

$$dx_{n+1} \wedge dy_{n+1} = (a_n d_n - b_n c_n) dx_n \wedge dy_n \tag{59}$$

$$dx_{n+1} \wedge dy_{n+1} = ((1 - (\Delta t)^2) - (\Delta t)^2) x_n \wedge dy_n \tag{60}$$

$$dx_{n+1} \wedge dy_{n+1} = x_n \wedge dy_n \tag{61}$$

□

Benefits of Non-Iterative Splitting Methods

The non-iterative or operator splitting scheme have the following benefits

- the deterministic and stochastic operators can be fully decoupled, means we can solve them independently;
- we have a modular behavior, means we add new operators without recoding, e.g. ABCD etc.

Drawbacks of Non-Iterative Splitting Methods

The traditional splitting scheme have the following problems:

- for non-commuting operators we may have a very large constant in the local splitting error which requires the use of unrealistically small splitting time step;
- within a full splitting step in one sub-interval the inner values aren't approximate to the solution of the original problem;
- splitting the original problem into the different sub-problems with one operator (i.e. neglect the other components) is physically questionable, e.g., nonlinearities.

Coulomb test-particle problem (Work with Th. Zacher)

A coulomb test particle is described with the following Langevin equation (nonlinear SDE problem):

$$dv(t) = F_d(v)dt + \sqrt{2D_v(v)}dW_v(t), \tag{62}$$

$$d\mu(t) = -2D_a(v)\mu dt + \sqrt{2D_a(v)(1-\mu^2)}dW_\mu(t), \tag{63}$$

$$d\phi(t) = \sqrt{\frac{2D_a(v)}{(1-\mu^2)}}dW_\phi(t), \tag{64}$$

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

$$D_v(v) = \frac{1}{2}\frac{1}{v+1}, \quad \frac{\partial D_v}{\partial v} = -\frac{1}{2}(v+1)^{-2}, \tag{65}$$

$$F_d(v) = -\frac{1}{2}\frac{1}{v+1}, \quad \frac{\partial F_d}{\partial v} = \frac{1}{2}(v+1)^{-2}, \tag{66}$$

$$D_a(v) = \frac{1}{2}\frac{1}{v+1}, \quad \frac{\partial D_a}{\partial v} = -\frac{1}{2}(v+1)^{-2}, \tag{67}$$

where we assume, that the initial condition are given as $v_0 = 1.0, \mu_0 = 1.0, \phi_0 = 1.0$.

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

$$d\mathbf{v}(t) = \mathbf{a}(\mathbf{v})dt + B(\mathbf{v})d\mathbf{W}_{\mathbf{v}}(t), \tag{68}$$

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

$$\mathbf{a}(\mathbf{v}) = \begin{pmatrix} F_d(v) \\ -2D_a(v)\mu \\ 0 \end{pmatrix}, d\mathbf{W}_{\mathbf{v}} = \begin{pmatrix} dW_v \\ dW_\mu \\ dW_\phi \end{pmatrix}, \tag{69}$$

$$B(\mathbf{v}) = \begin{pmatrix} \sqrt{2D_v(v)} & 0 & 0 \\ 0 & \sqrt{2D_a(v)(1-\mu^2)} & 0 \\ 0 & 0 & \sqrt{\frac{2D_a(v)}{(1-\mu^2)}} \end{pmatrix}, \tag{70}$$

Standard Euler-Maruyama scheme

1.) Standard Euler-Maruyama scheme is given as:

$$v_{n+1} = v_n + F(v_n)\Delta t + \sqrt{2D(v_n)}\Delta W_v, \tag{71}$$

$$\mu_{n+1} = \mu_n - 2D_a(v_n)\mu_n\Delta t + \sqrt{2D_a(v_n)(1-\mu_n^2)}\Delta W_\mu, \tag{72}$$

$$\phi_{n+1} = \phi_n + \sqrt{\frac{2D_a(v_n)}{(1-\mu_n^2)}}\Delta W_\phi, \tag{73}$$

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 $N_i(0,1) = rand$, $i = \{v, \mu, \phi\}$ are three independent normally distributed random variable.

Iterative splitting scheme: Fixpoint Idea

Relaxation of the nonlinear part is applied as:

$$d\mathbf{v}_{i+1}(t) = \hat{A}(\mathbf{v}_i)\mathbf{v}_{i+1}dt + B(\mathbf{v}_i)d\mathbf{W}(t), \tag{74}$$

with the solution vector $\mathbf{v}_i(t) = (v_i(t), \mu_i(t), \phi_i(t))^t$.

$$\hat{A}(\mathbf{v}_i) = \begin{bmatrix} \frac{F_v(v_i)}{v_i} & 0 & 0 \\ 0 & -2D_a(v_i) & 0 \\ 0 & 0 & 0 \end{bmatrix}, \tag{75}$$

Then the fixpoint scheme is given as:

$$\mathbf{v}_{i+1}(t^{n+1}) = \exp(\hat{A}(\mathbf{v}_i(t^{n+1}))\Delta t)\ \mathbf{v}(t^n)$$
$$+ \int_{t^n}^{t^{n+1}} \exp(\hat{A}(\mathbf{v}_i(t^{n+1}))\ (t^{n+1} - s)\ B(\mathbf{v}_i(s))d\mathbf{W}_{\mathbf{v}}(s). \tag{76}$$

Fixpoint iterative version with Taylor expansion of the nonlinear part

$$\begin{aligned} d\mathbf{v}_{i+1}(t) &= \tilde{\mathbf{a}}(\mathbf{v}(t^n))dt + A(\mathbf{v}(t^n))\mathbf{v}_{i+1}dt \\ &+ B(\mathbf{v}_i)d\mathbf{W}(t), \end{aligned} \tag{77}$$

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

$$\begin{aligned} \mathbf{a}(\mathbf{v}) &= \mathbf{a}(\mathbf{v}(t^n)) + J(\mathbf{v})|_{t^n}(\mathbf{v} - \mathbf{v}(t^n)), && (78) \\ &= \left(\mathbf{a}(\mathbf{v}(t^n)) - J(\mathbf{v})|_{t^n}\mathbf{v}(t^n)\right) + J(\mathbf{v})|_{t^n}\mathbf{v}, && (79) \\ &= \tilde{\mathbf{a}}(\mathbf{v}(t^n)) + J(\mathbf{v})|_{t^n}\mathbf{v}. && (80) \end{aligned}$$

The fixpoint scheme is given as:

$$\mathbf{v}_{i+1}(t^{n+1}) = \exp(A(\mathbf{v}(t^n))\Delta t) \left(\mathbf{v}(t^n) \right.$$

$$\left. + A(\mathbf{v}(t^n))^{-1}(I - \exp(A(\mathbf{v}(t^n))\Delta t))\, \tilde{\mathbf{a}}(t^n) \right)$$

$$+ \int_{t^n}^{\Delta t^{n+1}} \exp(A(\mathbf{v}(t^n))(t^{n+1} - s))B(\mathbf{v}_i)(s)d\mathbf{W}_{\mathbf{v}}(s) \Big).$$

We apply the following errors:

- Strong Convergence:

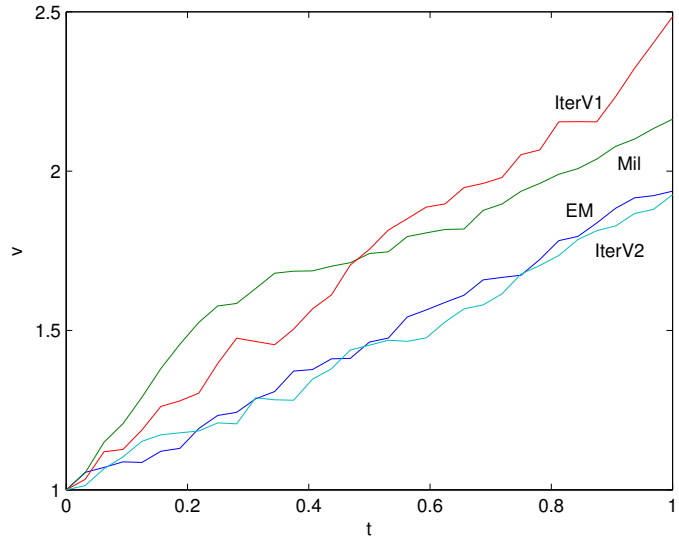
$$err_{v,\Delta t,t=1} = ||v_{\Delta t,Scheme}(t=1) - v_{\Delta t_{fine},Mil}(t=1)||, \quad (81)$$

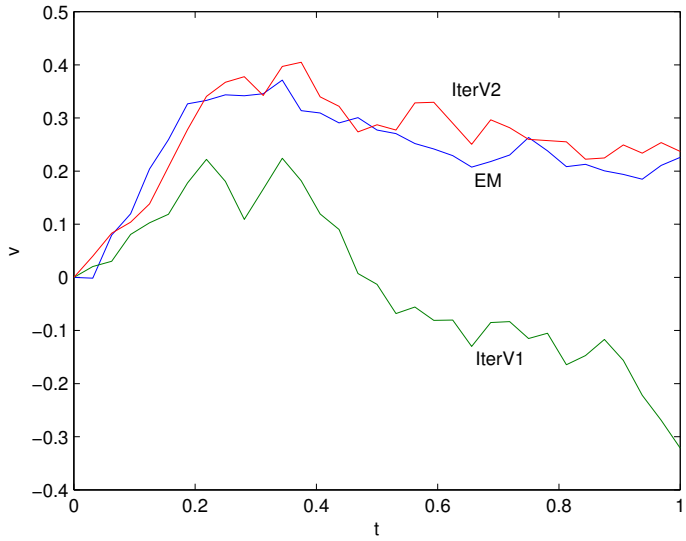
- Weak Convergence:

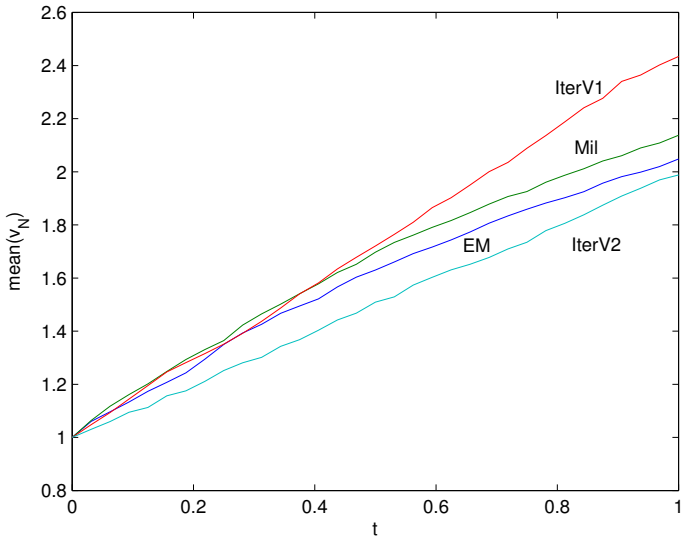
$$err_{v,\Delta t,t=1,weak} = \frac{1}{N}\sum_{i=1}^{N} err_{i,v,\Delta t,t=1}, \quad (82)$$

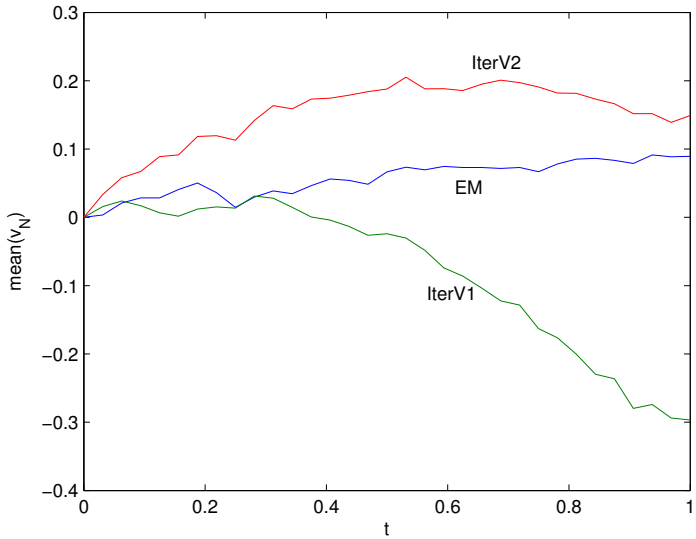
where $err_{i,v,\Delta t,t=1}$ are $i = 1,\ldots,N$ independent errors of the solution v.

Results of the different Schemes

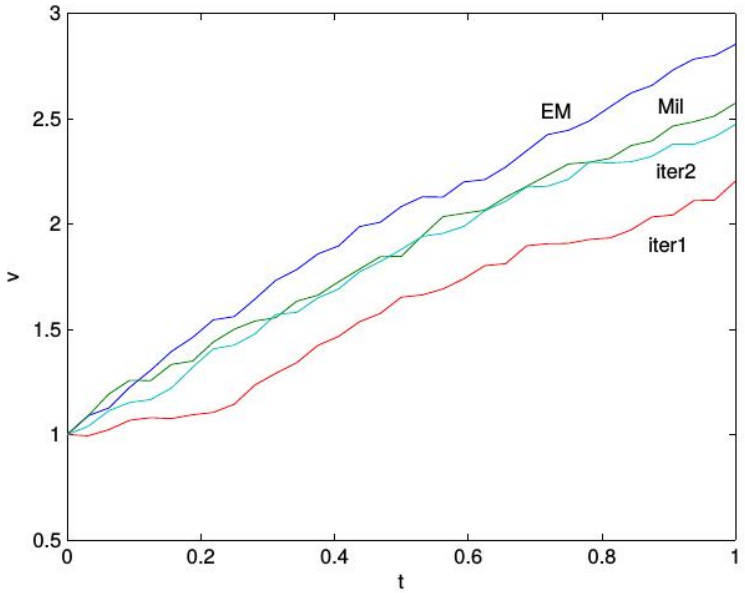








Particle Trajectories in Plasma



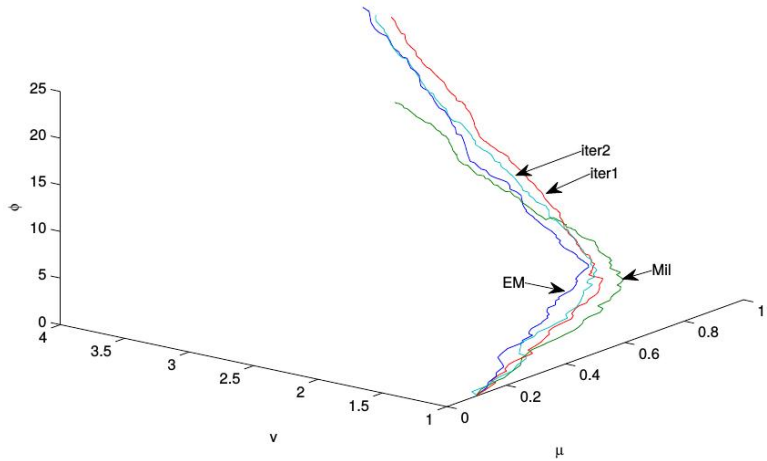


Figure: Velocity v of a particle and 3D presentation of the velocity components for one underlying particle (see [Geiser 2014, submitted to JMAA]).

Particle transport: Impact Oscillator (Work with Th. Zacher)

We deal with the following nonlinear SDE problem (applied in the particle transport models):

$$\frac{dx}{dt} = v, \tag{83}$$

$$dv(t) = \frac{\partial}{\partial x} U(x) - \gamma v dt + \sqrt{2\beta^{-1}\gamma} dW, \tag{84}$$

where W is a Wiener process, γ is the thermostat parameter, β the inverse Temperature.

A long solution to the SDE is distributed according to a probability measure with density π satisfying:

$$\pi(x, v) = C^{-1} \exp(-\beta(\frac{v^2}{2} + U(x)), \tag{85}$$

where $x > 0.0$, $v \in \mathbb{R}$.
We test the following methods:

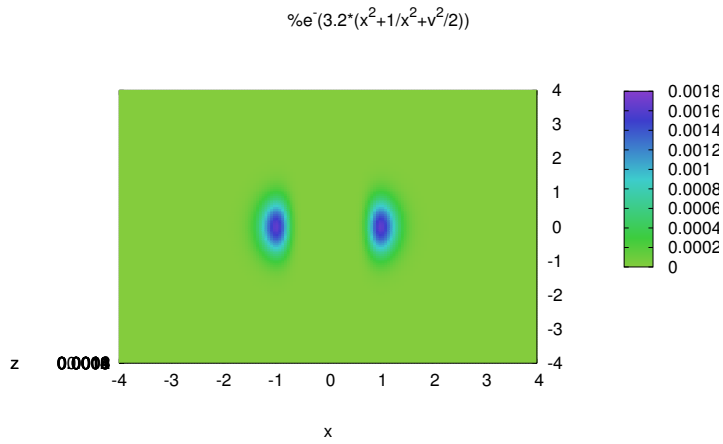
- Verlet
- Semi-analytical method,
- AB splitting and improved AB splitting method,
- Euler-Maruyama scheme and improved EM scheme,
- Milstein scheme.

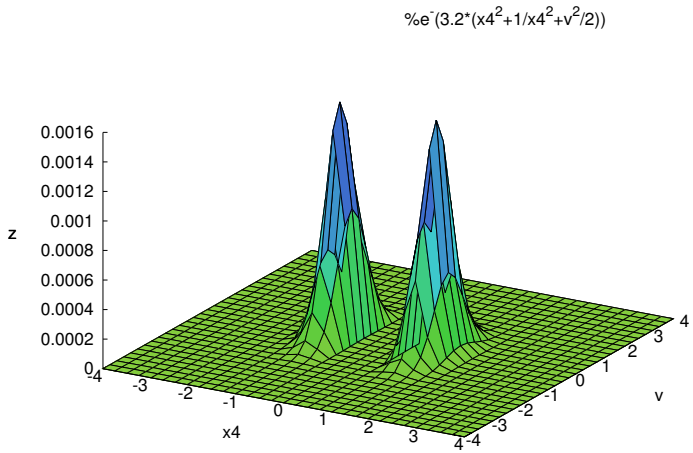
We deal with the impact oscillator $U(x) = \frac{1}{x^2} + x^2, E(x) = 2\frac{1}{x^3} - 2x$. The equilibrium distribution of the impact oscillator is given as:

$$\pi(\beta, x, v) = \exp(-\beta(\frac{v^2}{2}) + U(x)), \tag{86}$$

where $\beta = 3.2$ and $U(x) = \frac{1}{x^2} + x^2$.

The distribution of the impact oscillator is given as





Numerical results of the different schemes

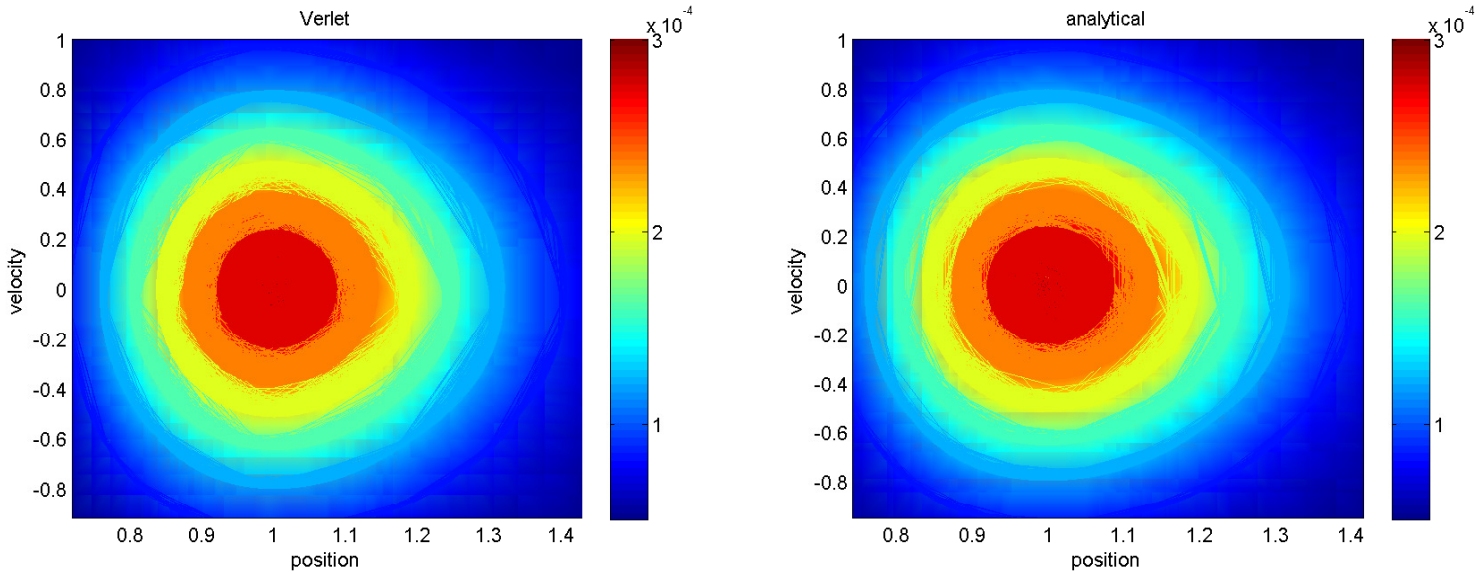


Figure: We apply $U(x) = \frac{1}{x^2} + x^2, E(x) = 2\frac{1}{x^3} - 2x$ and the starting points $(x, v)^t = (1.0, 1.0)^t$. The figures present the contours of the Hamiltonian with the Verlet-algorithm (left figure) and the analytical-algorithm (right figure).

Numerical results of the different schemes

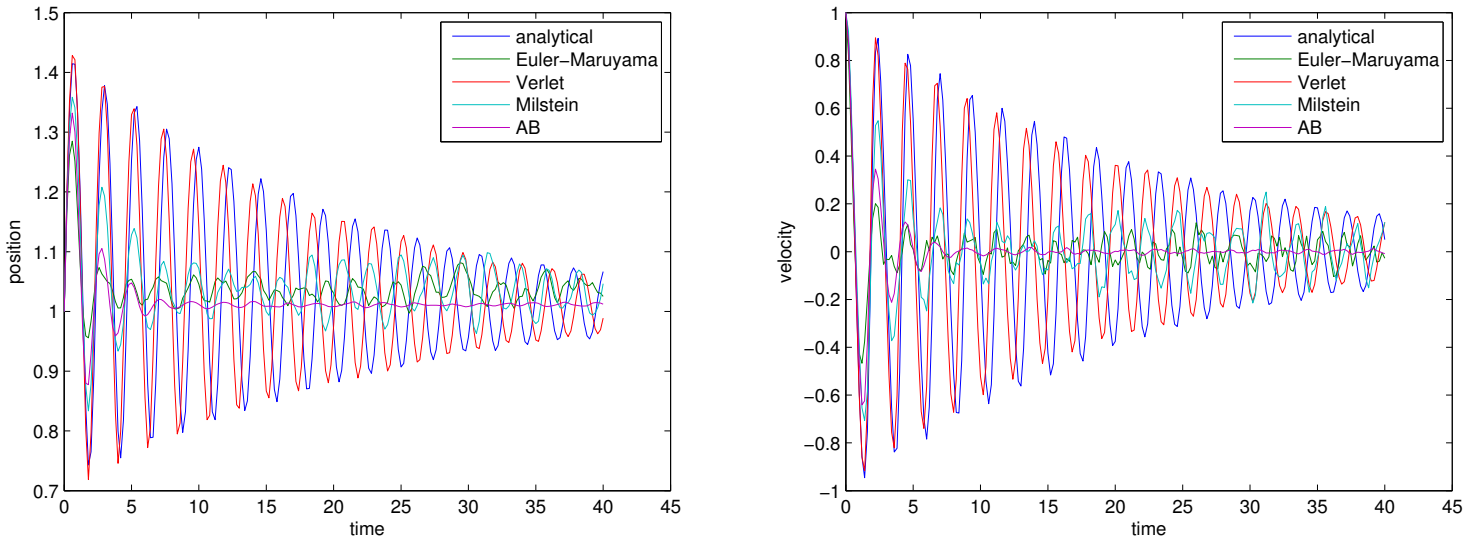


Figure: We apply $U(x) = \frac{1}{x^2} + x^2$, $E(x) = 2\frac{1}{x^3} - 2x$ and the starting points $(x, v)^t = (1.0, 1.0)^t$. The figures presents the x (left) and v (right) solutions of the Verlet algorithm, where $A = 0.1, B = 0.25$.

Remark

The optimal method is the predictor-corrector AB splitting method, which combines higher order and symplecticity. The other methods have drawback in controlling the singularity in a long term evolution.

Conclusions

Conclusion

1) Splitting scheme can be extended to stochastic differential equations.
2) The convergence order of the stochastic splitting schemes is lower than the deterministic splitting (e.g. $O(\Delta t) \rightarrow O(\sqrt{\Delta t})$.
3) Iterative splitting schemes can gain a higher order accuracy as the non-iterative splitting schemes.
4) Non-iterative splitting schemes are simpler to implement.

Future Works

Outview

1) Numerical analysis of the novel splitting schemes.
2) Combination with alternative schemes, e.g., Metropolis Monte Carlo schemes.
3) Combination of non-iterative and iterative splitting schemes.
4) Real-life applications in Coulomb-Collisions.