Qualitative behaviour of numerical methods for SDEs and application to homogenization

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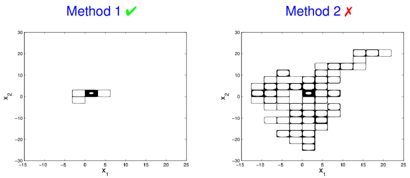
Outline

1. Modified Equations
   - ODE theory.
   - Main idea for SDEs.
   - Different numerical methods and Associated Modified Equations.
   - Numerical examples.
2. Application to Homogenization
   - Long time behaviour and homogenization.
   - Numerical algorithms/results.
   - From homogenization to averaging in cellular flows.
3. Higher order numerical methods based on modified equations.
   - Key idea.
   - One simple example.

Motivating example



Interesting Question

- The two numerical methods have the same order of convergence but completely different qualitative behaviour.
- Is there a way to distinguish between these two methods?
- A very powerful tool for addressing this question is backward error analysis (modified equations).

Modified equations for ODEs

$$\frac{dx}{dt} = f(x),$$

and let x_n be a numerical approximation of x of order p:

$$|x(nh) - x_n| = \mathcal{O}(h^p).$$

Can I find $X(t)$ satisfying another ODE (modified equation) such that:

$$|X(nh) - x_n| = \mathcal{O}(h^{p+q}).$$

Euler method-one dimension

$$\boxed{x_{n+1} = x_n + hf(x_n).}$$

Modified equation:

$$\frac{dX}{dt} = f(X) - \frac{h}{2} f'(X) f(X),$$

since

$$|X(nh) - x_n| = \mathcal{O}(h^2).$$

Sketch proof

$$\frac{dX}{dt} = f(X) + hg(X).$$

$$\begin{aligned} X(h) &= X(0) + \int_0^h \left(f(X(s)) + hg(X(s))\right) ds \\ &= X(0) + hf(X(0)) + h^2 g(X(0)) + \frac{h^2}{2} f(X(0))f'(X(0)) + \mathcal{O}(h^3). \end{aligned}$$

Assume $x_0 = X(0)$ then

$$X(h) - x_1 = h^2 \left(g(X(0)) + \frac{1}{2} f(X(0))f'(X(0)) \right) + \mathcal{O}(h^3),$$

and thus

$$\boxed{g(x) = -\frac{1}{2} f(x)f'(x).}$$

Stochastic Differential Equations and Numerical Methods

$$dx = u(x)dt + \sigma(x)dW_t,$$

- Euler method:

$$x_{n+1} = x_n + hu(x_n) + \sqrt{h}\sigma(x_n)\xi_n,$$

- θ-Milstein method:

$$x_{n+1} = x_n + \theta hu(x_{n+1}) + (1-\theta)hu(x_n) + \sqrt{h}\sigma(x_n)\xi_n + \frac{h}{2}\sigma(x_n)\sigma^{(1)}(x_n)(\xi_n^2 - 1),$$

where $\xi_n \sim \mathcal{N}(0,1)$.

Weak and Strong Convergence

- Weak convergence: We look at $|\mathbb{E}(\phi(x(nh))) - \mathbb{E}(\phi(x_n))|$.
- Strong convergence: We look at $\mathbb{E}|x(nh) - x_n|$.
- In general the weak and strong order of convergence of a numerical method NEEDS NOT to be the same!!!

Statement of the Problem

Let $x(t)$ satisfy the following SDE:

$$dx = u_1(x)dt + \sigma_1(x)dW_t,$$

and x_n be its numerical approximation at $T = nh$ by a weak p-order method i.e

$$|\mathbb{E}(\phi(x(T))) - \mathbb{E}(\phi(x_n))| = \mathcal{O}(h^p),\ \forall \phi \in C^\infty.$$

We want to develop a procedure that allows us to evaluate the properties of our weak numerical scheme.

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First Modified Equation

We want to find a modified SDE of the form (*i.e.*, find v_2 and σ_2)

$$d\tilde{x} = [u_1(\tilde{x}) + hu_2(\tilde{x})] + [\sigma_1(\tilde{x}) + h\sigma_2(\tilde{x})]\, dW_t,$$

for which

$$|\mathbb{E}(\phi(\tilde{x}(T))) - \mathbb{E}(\phi(x_n))| = \mathcal{O}(h^{p+1}),\ \forall \phi \in C^{\infty}.$$

For the rest of the talk we concentrate in the case where $p = 1$.

Generators for ODEs and SDEs

- ODE:

$$\begin{aligned} dx &= h(x)dt, \\ \mathcal{L}u &:= h(x) \cdot \nabla_x u. \end{aligned}$$

- SDE:

$$\begin{aligned} dx &= h(x)dt + \sigma(x)dW_t, \\ \mathcal{L}u &:= h(x) \cdot \nabla_x u + \frac{1}{2}\sigma(x)\sigma^T(x) : \nabla_x \nabla_x u. \end{aligned}$$

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Backward Kolmogorov Equation

$$\begin{aligned} \frac{\partial u}{\partial t} &= \mathcal{L}u, \\ u(x,0) &= \phi(x). \end{aligned}$$

Then

$$u(x,t) = \mathbb{E}(\phi(x(t))|x(0) = x).$$

Stochastic B-series

By integrating over time the backward Kolmogorov Equation and taking a Taylor expansion of $u(x, s)$ around $s = 0$, we obtain, (assuming appropriate smoothness of the drift and diffusion term)

$$u(x, h) - \phi(x) = \sum_{k=0}^{\infty} \frac{h^{k+1}}{(k+1)!} \mathcal{L}^{k+1}\phi(x).$$

Note that in the case where $\phi(x) = x$, $\sigma(x) = 0$, this expansion correspond to the B-series expansion of the ODE

$$dx = v_1(x)dt.$$

Local Error/Global Error

A weak first order numerical method has the following expansion

$$u_{num}(x,h) - \phi(x) = h\mathcal{L}\phi(x) + h^2\mathcal{L}_e\phi(x) + \mathcal{O}(h^3),$$

and so

$$u(x,h) - u_{num}(x,h) = h^2\left(\frac{1}{2}\mathcal{L}^2\phi(x) - \mathcal{L}_e\phi(x)\right), \quad \text{Local Error}$$

which implies that

$$u(x,T) - u_{num}(x,T) = \mathcal{O}(h). \quad \text{Global Error}$$

Generator of the Modified Equation

Remember that the 1-st modified equation is of the form

$$d\tilde{x} = [u_1(\tilde{x}) + hu_2(\tilde{x})] + [\sigma_1(\tilde{x}) + h\sigma_2(\tilde{x})]\, dW_t.$$

Its generator $\mathcal{L}$ can be written as

$$\mathcal{L} = \mathcal{L}_0 + h\mathcal{L}_1 + h^2\mathcal{L}_2,$$

where $\mathcal{L}_0$ is the generator of the original SDE and

$$\mathcal{L}_1\phi := u_2(x)\frac{d\phi}{dx} + \sigma_1(x)\sigma_2(x)\frac{d^2\phi}{dx^2}.$$

Main Equation

If we now subtract the Taylor expansion of the numerical method from the stochastic B-series of the modified equation we see that in order for the local error to be $\mathcal{O}(\Delta t^3)$ we need

$$\boxed{\mathcal{L}_1\phi = \mathcal{L}_e\phi - \frac{1}{2}\mathcal{L}_0^2\phi, \ \forall\phi \in C^\infty.}$$

Euler-Maryama Method

In the case of Euler-Maryama method in the case of multiplicative noise it turns out that a modified equation does not exist since

$$\mathcal{L}_1\phi \neq \cdots + \frac{\sigma_1^3(x)}{2}\sigma_1^{(1)}(x)\phi^{(3)}(x).$$

as $\mathcal{L}_1$ is a second order partial differential operator!!!

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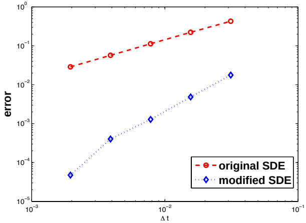
θ-Milstein Method

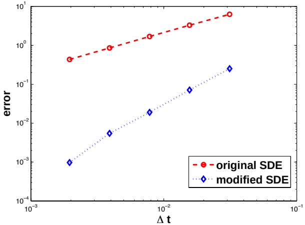
$$
\begin{aligned}
u_2(x) &= \left(\theta - \frac{1}{2}\right)\left(v_1(x)v_1^{(1)}(x) + \frac{\sigma_1^2(x)}{2}v_1^{(2)}(x)\right), \\
\sigma_2(x) &= \left(\theta - \frac{1}{2}\right)\sigma_1(x)v_1^{(1)}(x) - \frac{1}{2}v_1(x)\sigma_1^{(1)}(x) - \frac{\sigma_1^2(x)}{4}\sigma_1^{(2)}(x).
\end{aligned}
$$

Geometric Brownian motion

$$
\begin{aligned}
dx &= \mu x dt + \sigma x dW_t, \\
d\tilde{X} &= \left[\left(\mu - \frac{h}{2}\mu^2\right)\tilde{X}\right] dt + \sigma \tilde{X}\left(1 - h\mu\right) dW_t.
\end{aligned}
$$



First moment



Second moment

Linear SDEs with additive noise

$$dx = Axdt + \Sigma dW_t,$$

Numerical Approximation:

$$x(h) = A(h)x + f(h, \omega).$$

Example (Euler-Maryama):

$$\begin{aligned} A(h) &= (I + hA), \\ f(h, \omega) &= \Sigma \sqrt{h} \xi. \end{aligned}$$

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∞ Modified Equation and its coefficients

$$dx = \tilde{A}xdt + \tilde{\Sigma}dW_t,$$

$$\begin{aligned} \tilde{A} &= \frac{\log(A(h))}{h}, \\ e^{\tilde{A}h}\tilde{\Sigma}\tilde{\Sigma}^T e^{\tilde{A}^T h} - \tilde{\Sigma}\tilde{\Sigma}^T &= \tilde{A}J + J\tilde{A}^T, \end{aligned}$$

where

$$J = \mathbb{E}(ff^T).$$

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Orstein Uhlenbeck Process

$$dx = -\gamma x dt + \sigma dW_t.$$

Forward Euler:

$$\begin{aligned}\tilde{A} &= \frac{\log(1-\gamma h)}{h},\\ \tilde{\Sigma} &= \sigma\sqrt{\frac{2\log(1-\gamma h)}{(1-\gamma h)^2-1}}.\end{aligned}$$

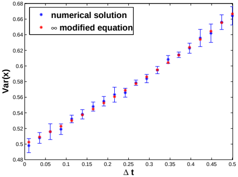
Backward Euler:

$$\begin{aligned}\tilde{A} &= -\frac{\log(1+\gamma h)}{h},\\ \tilde{\Sigma} &= \sigma\sqrt{\frac{2\log(1+\gamma h)}{1-(1+\gamma h)^{-2}}}.\end{aligned}$$

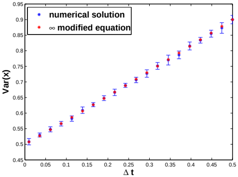
Invariant Measure

$$\lim_{t\to\infty} \mathbb{E}(x^2(t)) = \frac{\sigma^2}{2\gamma - \gamma^2 h}, \quad \text{Forward Euler}$$

$$\lim_{t\to\infty} \mathbb{E}(x^2(t)) = \frac{\sigma^2(1+\gamma h)}{2\gamma + \gamma^2 h}, \quad \text{Backward Euler}.$$



Forward Euler



Backward Euler

Figure: $\lim_{t\to\infty} \mathbb{E}(x^2(t))$ as a function of h.

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Passive Tracers, Effective Diffusivity

$$dx = v(x)dt + \sigma dW_t,$$

where $v(x)$ is a periodic function. It is possible to show using homogenization that

$$\lim_{t\to\infty} \frac{\mathbb{E}(x(t)\otimes x(t))}{2t} = \mathcal{K}.$$

We will refer to $\mathcal{K}$ as the *effective diffusivity matrix*

Velocity Field of Interest

Example

We are interested in the following 2-dimensional incompressible velocity field

$$v(x) = \nabla^{\perp}\Psi(x), \text{ where } \Psi(x) = \sin x_1 \sin x_2$$

Result

In this case it is known that $\mathcal{K} = DI_2$, where $D \in \mathbb{R}$ depending on σ for passive tracers and that the following result is true for passive tracers

$$D(\sigma) \sim \sigma, \quad \sigma \ll 1$$

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Key Property of the Velocity Field

Our velocity field $v(x)$ can be written as

$$
\begin{aligned}
v(x) &= \begin{pmatrix} -1/2 \\ +1/2 \end{pmatrix} \sin(x_1 + x_2) + \begin{pmatrix} -1/2 \\ -1/2 \end{pmatrix} \sin(x_1 - x_2), \\
&= \sum_{j=1}^{2} d_j v_j(\langle e_j, x\rangle),
\end{aligned}
$$

where $e_j, d_j \in \mathbb{R}^2$ with the property

$$\boxed{\langle e_j, d_j\rangle = 0.}$$

This is a key property for the construction of our method which is a stochastic extension of a **splitting** method proposed by Quispel 2003.

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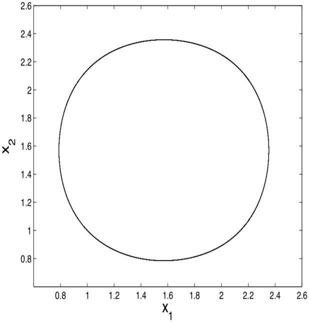
Description of the Method:

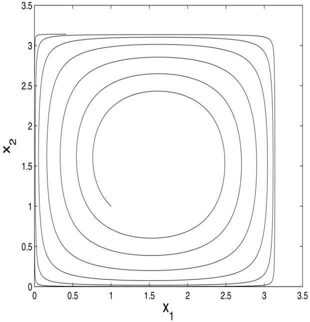
The method in the case of passive tracers involves these 3 steps:

- Step 1: Solve $\dot{x}_1 = d_1 v_1\big(\langle e_1, x_1\rangle\big)$,
- Step 2: Solve $\dot{x}_2 = d_2 v_2\big(\langle e_2, x_2\rangle\big)$,
- Step 3: Solve $\dot{x}_3 = \sigma\dot{\beta}_1$.

The Deterministic Case

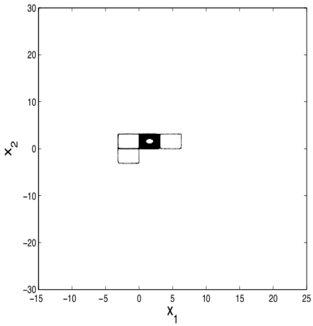


Splitting method for $\sigma = 0$.

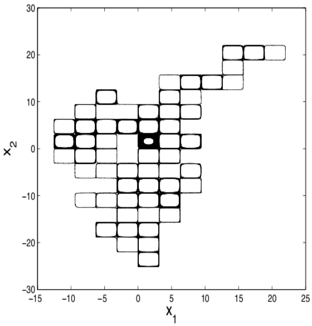


Euler method for $\sigma = 0$.

The Case $\sigma \ll 1$

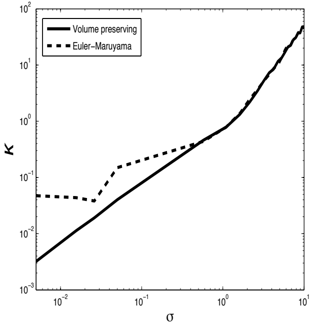


Splitting method for $\sigma = 10^{-2}$.

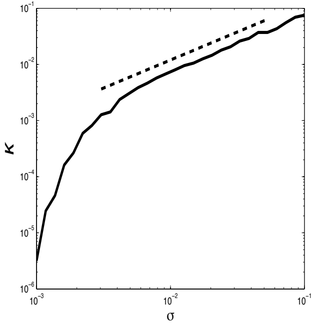


Euler method for $\sigma = 10^{-2}$.

Calculating Effective Diffusivities



Comparison of the two methods.



Splitting Method.

Mean Hamiltonian

We apply Itô 's formula to $H = \Psi$ we obtain

$$\frac{d\Psi}{dt} = -\sigma^2 \Psi + \mathrm{M.T}$$

which implies that the mean Hamiltonian decays like $e^{-\sigma^2 t}$

Numerical calculation of the mean Hamiltonian with the two methods

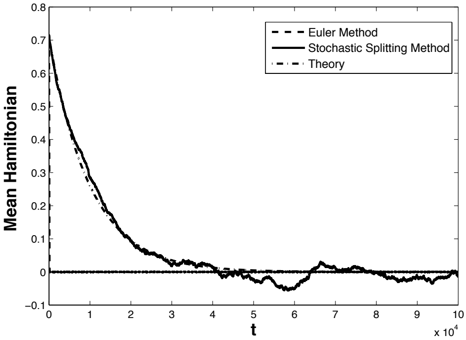


Figure: Mean value of the Hamiltonian as a function of time, for $\Delta t = 10^{-1}, \sigma = 10^{-2}$.

Modified Equations for the Euler Method

$$
\begin{aligned}
dx &= \left(v(x) - \frac{\Delta t}{2} (\nabla v(x)) v(x) - \frac{\sigma^2 \Delta t}{4} \Delta v(x) \right) dt \\
&+ \sigma \left(1 - \frac{\Delta t}{2} \nabla v^T(x) \right) dW_t.
\end{aligned}
$$

$$
\begin{aligned}
\frac{d\Psi}{dt} &= -\frac{\Delta t}{2} (\cos^2 x_1 + \cos^2 x_2) \Psi - \sigma^2 \Psi (1 + \Delta t \cos x_1 \cos x_2) \\
&+ \frac{\sigma^2 \Delta^2 t}{4} (\cos^2 x_1 \cos^2 x_2 \Psi - \Psi^3) + \mathrm{M}_{\Delta t}.
\end{aligned}
$$

Statement of the problem

$$u(x) = \nabla^{\perp}\Psi(x), \quad \Psi(x) = \frac{1}{\pi}\sin \pi x_1 \sin \pi x_2.$$

X_t satisfies the following SDE

$$dX_t = -Au(X_t)dt + \sqrt{2}dW_t.$$

Exit time problem

$$\begin{aligned} -\Delta\tau + Au\cdot\nabla\tau &= 1 \quad \text{in } D, \\ \tau &= 0 \quad \text{on } \partial D, \end{aligned}$$

where $D = [-L/2, L/2] \times [-L/2, L/2]$.

Known results and open questions

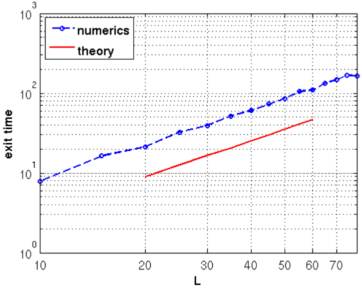
1. A fixed, $L \to \infty$, *homogenization* $(\tau \to \infty)$.
2. L fixed, $A \to \infty$, *averaging* $(\tau \to 0)$.
3. If $D = B_L$ a disk of radius L, then $\tau(x) \sim L^2 - |x|^2$.
4. $A = L^\alpha$ and $L \to \infty$
   - $\alpha < 4$, *homogenization* $(\tau \sim L^{2-\alpha/2})$.
   - $\alpha > 4$, *averaging* $(\tau \sim L^{2-\alpha/2})$.

Question

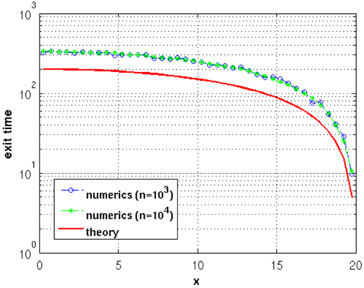
How about $\alpha = 4$?

Numerical investigations I

Define $Y_t = X_{At}$, then $dY_t = u(Y_t)dt + \sqrt{\frac{2}{A}}dW_t$ and $\tau(y) = A\tau(x)$

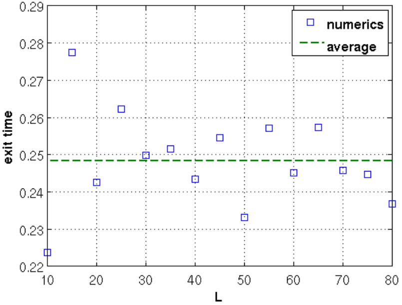


Asymptotic behaviour of exit time ($\alpha = 1$)

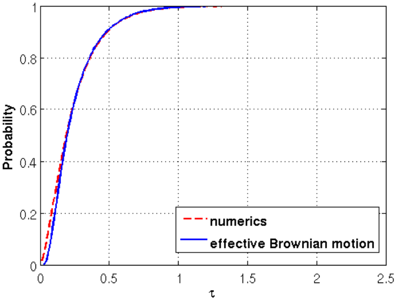


Exit problem from a disk ($L = 40$)

Numerical investigations II, Case $\alpha = 4$



Asymptotic behaviour of exit time ($\alpha = 4$)



Comparison of c.d.f

Key idea

i) Choose a numerical method for the original SDE.

ii) Write down a suitably chosen SDE different than the original one (this SDE depends on the choice of the method from step i).

iii) Apply the numerical method from step i to the SDE from step ii.

Example

$$dX_t = u_1(X_t)dt + \sigma_1(X_t)$$

i) $x_{n+1} = x_n + \theta h u_1(x_{n+1}) + (1-\theta)hu_1(x_n) + \sqrt{h}\sigma_1(x_n)\xi_n + \frac{h}{2}\sigma_1(x_n)\sigma_1^{(1)}(x_n)(\xi_n^2 - 1)$

ii) $dX_t = \tilde{u}(X_t)dt + \tilde{\sigma}(X_t), \tilde{u} = u_1 - hu_2, \quad \tilde{\sigma} = \sigma_1 - h\sigma_2$

iii) $x_{n+1} = x_n + \theta h\tilde{u}(x_{n+1}) + (1-\theta)h\tilde{u}(x_n) + \sqrt{h}\tilde{\sigma}(x_n)\xi_n + \frac{h}{2}\sigma_1(x_n)\sigma_1^{(1)}(x_n)(\xi_n^2 - 1)$

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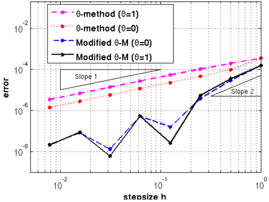
Application to an economy model for asset prices

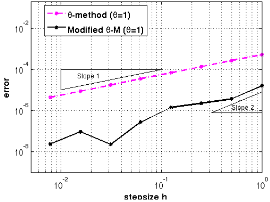
$$
\begin{aligned}
dX_1 &= \beta_1 X_1 X_2 dW_1, \\
dX_2 &= -(X_2 - X_3)dt + \beta_2 X_2 dW_2, \\
dX_3 &= \alpha(X_2 - X_3)dt,
\end{aligned}
$$

N. Hofmann, E. Platen, M. Schweizer. Option pricing under incompleteness and stochastic volatility. *M*athematical Finance, 2(3):153–187, (1992).

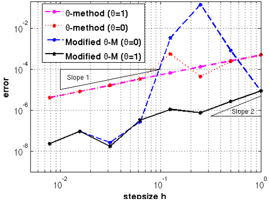
Numerical Investigations



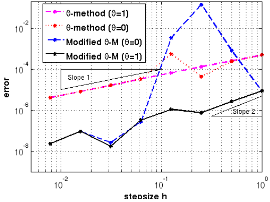
Error for $\mathbb{E}(X_1^2)$. Nonstiff case $\alpha = 1$.



Error for $\mathbb{E}(X_1^2)$. Very stiff case $\alpha = 100$.



Error for $\mathbb{E}(X_1^2)$. Stiff case $\alpha = 25$.



Error for $\mathbb{E}(X_2^2)$. Stiff case $\alpha = 25$.

Conclusions

1. It is not always possible to write down a modified Itô SDE for a given numerical method.
2. In the case of linear SDEs with additive noise it is possible to write down an ∞-modified equation that the numerical method satisfy exactly in the weak sense.
3. It is possible to generalize ideas from the backward error analysis of ODEs to SDEs.
4. Modified equations can be used as a tool for constructing higher order methods.

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Future work

1. Find modified equations for numerical methods with respect to strong convergence.
2. Give a rigorous explanation for failing to find a modified SDE for the Euler method in case of multiplicative noise.
3. Use modified equations to characterize the invariant measure approximated by different numerical schemes.
4. Compare exit times from a square for different starting points, with the ones of the effective Brownian motion.
5. Study exit times in case where the inertia is important (inertial particles).

Thank for your attention!

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