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based on modified equations**

by

**Assyr Abdulle, David Cohen, Gilles Vilmart, and Konstantinos C.
Zygalakis**



Oxford Centre for Collaborative Applied Mathematics
Mathematical Institute
24 - 29 St Giles'
Oxford
OX1 3LB
England

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Assyr Abdulle¹, David Cohen², Gilles Vilmart^{1,3}, and Konstantinos C. Zygalakis⁴

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Abstract

Inspired by recent advances in the theory of modified differential equations, we propose a new methodology for constructing numerical integrators with high weak order for the time integration of stochastic differential equations. This approach is illustrated with the constructions of new high order weak methods, in particular, implicit integrators well suited for stiff stochastic problems, and integrators that exactly conserve all quadratic first integrals of a stochastic dynamical system. Numerical examples confirm the theoretical results and show the versatility of the methodology.

Keywords: Stochastic differential equations, weak convergence, modified equations, backward error analysis.

AMS subject classification (2010): 65C30, 60H35

1 Introduction

The problem of computing the expectation of some functional of a random process appears in many practical situations, for example: in finance [33], in random mechanics [38], in nonlinear filtering [9] or bio-chemical processes [12], to mention a few examples. Here, we are interested in the situation where the random process is the solution of an Itô stochastic differential equations (SDE)

$$dX = f(X)dt + g(X)dW(t), \quad X(0) = X_0, \quad (1)$$

where $X(t)$ is a random variable with values in \mathbb{R}^d , $f : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is the drift term, $g : \mathbb{R}^d \rightarrow \mathbb{R}^{d \times m}$ is the diffusion term with $d \times m$ matrix values, and the components $W_j(t), j = 1, \dots, m$ of $W(t) = (W_1(t), \dots, W_m(t))^T$ are independent Wiener processes. We assume that the drift and diffusion terms are smooth enough, Lipschitz continuous and satisfy a growth bound, to ensure an unique (mean-square bounded) solution of (1) [4, 19]. Analytic solutions of SDEs are rarely known and their practical computation must usually be done numerically. A one-step numerical method for the approximation of (1) is given by

$$X_{n+1} = \Psi(f, g, X_n, h, \xi_n), \quad (2)$$

where $\Psi(f, g, \cdot, h, \xi_n) : \mathbb{R}^d \rightarrow \mathbb{R}^d$, $X_n \in \mathbb{R}^d$ for $n \geq 0$, h denotes the timestep size, and ξ_n denotes a random vector. Of interest in this paper is the approximation of $\mathbb{E}(\phi(X(\tau)))$, where $\phi : \mathbb{R}^d \rightarrow \mathbb{R}$ is a smooth function, by $\mathbb{E}(\phi(X_N))$, $N = \tau/h$. For a practical computation,

¹Mathematics Section, École Polytechnique Fédérale de Lausanne, Station 8, CH-1015 Lausanne, Switzerland, Assyr.Abdulle@epfl.ch

²Mathematisches Institut, Universität Basel, CH-4051 Basel, Switzerland, David.Cohen@unibas.ch

³new address: École Normale Supérieure de Cachan, Antenne de Bretagne, av. Robert Schuman, F-35170 Bruz, France, Gilles.Vilmart@bretagne.ens-cachan.fr

⁴Oxford Centre for Collaborative Applied Mathematics (OCCAM), UK, zygalakis@maths.ox.ac.uk

$\mathbb{E}(\phi(X_N))$ is further approximated by a Monte-Carlo method [19]. The efficiency of this later approximation, which is not addressed in the present paper, is very important in practice and is still an active research topic. In particular, the methods developed in this paper could be combined with the recently proposed Multilevel Monte-Carlo method [13].

The accuracy of the approximation can be measured by the weak order of convergence of the numerical method. We recall that a numerical approximation (2), starting from the exact initial condition X_0 of (1) is said to have weak order p if for $\tau > 0$, we have

$$|\mathbb{E}(\phi(X_N)) - \mathbb{E}(\phi(X(t_N)))| \leq Ch^p, \quad (3)$$

for any fixed $t_N = Nh \in [0, \tau]$ with h sufficiently small and all functions $\phi : \mathbb{R}^d \rightarrow \mathbb{R}$ that are $2p + 1$ times continuously differentiable with all partial derivatives with polynomial growth.

Remark 1.1 *A well-known theorem of Milstein [26] allows to infer the weak order from the error after one step. Assuming that f, g are Lipschitz continuous and satisfy $f, g \in C^{2p+1}$, with all partial derivatives up to order $2p + 1$ having polynomial growth, that the moments of the exact solution of the SDE (1) exist and are bounded (up to a sufficiently high order) and that $\phi \in C^{2p+1}$, then, the local error bound*

$$|\mathbb{E}(\phi(X_1)) - \mathbb{E}(\phi(X(t_1)))| \leq Ch^{p+1},$$

implies the global error bound (3).

The simplest method to approximate solutions to (1) is the so-called Euler-Maruyama method [24], which has weak order one. In many applications, it is of interest to approximate the moments of the solution of an SDE (or a functional of its solution) with a better accuracy. The construction of higher order schemes has been pursued by many authors. Classical approaches for getting high weak order numerical schemes for stochastic differential equations are based on weak Taylor approximation or Runge-Kutta type methods [6, 10]. For example, second order weak methods were proposed by Milstein [25, 26], Platen [32], Mackevicius [23], Talay [39] (see also [19, 28]) and Tocino and Vigo-Aguiar [41]. We mention also the extrapolation methods of Talay and Tubaro [40] and of [20] that combines methods with different stepsizes to achieve higher order weak convergence.

In this paper we propose yet another approach inspired by the construction of high order numerical integrators for deterministic problems proposed in [8] and the newly developed theory of modified equations for stochastic differential equations [11, 42]. The basic idea of our new approach can be summarized as follows. Instead of applying the numerical method (2) to the SDE (1), we apply it to a suitably modified differential equation (a perturbation of (1)) so that the resulting numerical scheme yields a higher order approximation of the original SDE. This permits to fulfill automatically the order conditions, which can be very numerous for SDEs (for instance, 59 weak order two conditions have been listed for a class of stochastic Runge-Kutta type methods in [36, Thm. 5.1]). We present a criterion (see Theorem 2.3) to construct weak methods of arbitrary order. Classical methods (Milstein or Talay methods) can be derived in a new way with our methodology. New methods will also be derived.

As an example, we propose a second weak-order mean-square stable method suitable for the integration of so-called stiff problems. We also show how the methodology can be used to construct high weak order methods for random mechanical problems. In particular, we derive new second order weak method preserving exactly all quadratic first integrals of the underlying SDE. As an illustration, we study the stochastic rigid body problem.

The paper is organized as follows. In Section 2, we present our new methodology and give a criterion for the construction of high order weak methods. In Section 3, we give explicit constructions of second order weak methods with emphasis on the numerical integration of stiff problems and random mechanical problems. Numerical examples illustrate the behavior of our new methods and corroborate the claimed weak orders of convergence.

2 Integrators based on modified equations

The general idea of constructing high order integrators based on modifying equation for SDEs can be summarized as follows. Consider a numerical method (2) for problem (1) and assume that its weak order of convergence (3) is $p \geq 1$. We then consider (1) with suitably modified drift and noise functions

$$d\tilde{X} = f_h(\tilde{X})dt + g_h(\tilde{X})dW(t), \quad \tilde{X}(0) = X_0, \quad (4)$$

where ¹

$$f_h(x) = f(x) + hf_1(x) + h^2f_2(x) + \dots, \quad (5)$$

$$g_h(x) = g(x) + hg_1(x) + h^2g_2(x) + \dots, \quad (6)$$

and apply the numerical method to (4), i.e.,

$$\tilde{X}_{n+1} = \Psi(f_h, g_h, \tilde{X}_n, h, \xi_n).$$

The goal is to choose f_h, g_h in such a way that $(\tilde{X}_n)_{n \geq 0}$ is a better weak approximation to the solution of the original SDE (1), i.e.,

$$|\mathbb{E}(\phi(\tilde{X}_N)) - \mathbb{E}(\phi(X(t_N)))| \leq Ch^{p+r},$$

with $r > 0$.

Remark 2.1 *The above procedure should not be confused with a procedure called backward error analysis for SDEs [11, 42] or the related approach [37], developed to study the long time behavior of numerical methods for SDEs. There, one tries to find a modified equation*

$$d\hat{X} = a_h(\hat{X})dt + b_h(\hat{X})dW(t), \quad \hat{X}(0) = X_0, \quad (7)$$

such that its exact solution is closer to the numerical solution (2), i.e.,

$$|\mathbb{E}(\phi(X_N)) - \mathbb{E}(\phi(\hat{X}(t_N)))| \leq Ch^{p+q},$$

with $q > 0$. In general, the modified SDEs (7) and (4) are different (see Remark 2.4 below).

A natural way of looking at expectations of functionals of the path for SDEs is by using the backward Kolmogorov equation associated to (1), which is the (deterministic) partial differential equation

$$\frac{\partial u}{\partial t} = \mathcal{L}u, \quad u(x, 0) = \phi(x), \quad (8)$$

where $\phi : \mathbb{R}^d \rightarrow \mathbb{R}$ is a smooth function, and the differential operator \mathcal{L} , called the generator of the SDE, is given by

$$\mathcal{L} := f \cdot \nabla_x + \frac{1}{2}(gg^T) : \nabla_x^2. \quad (9)$$

In (9), ∇_x and ∇_x^2 denote respectively the gradient and the Hessian matrix operator ² with respect to x . In the case $m = d = 1$, the generator reduces to

$$\mathcal{L} = f \frac{\partial}{\partial x} + \frac{1}{2}g^2 \frac{\partial^2}{\partial x^2}.$$

¹Here, h is the timestep size of the numerical method (2).

²Here, we consider the usual scalar product on matrices defined by $A : B = \text{trace}(A^T B)$.

The probabilistic interpretation (see for example [29, 30, 34]) of the solution $u = u^{f,g}(\phi, x, t)$ to (8) is that

$$u^{f,g}(\phi, x, t) = \mathbb{E}(\phi(X(t)) | X(0) = x),$$

where $X(t)$ solves (1). Using (8) one can easily derive the following formal Taylor expansion [11, 42]

$$u^{f,g}(\phi, x, h) - \phi(x) = \sum_{j=1}^{\infty} \frac{h^j}{j!} \mathcal{L}^j \phi(x).$$

Under appropriate smoothness assumptions on f, g and ϕ one can prove that

$$u^{f,g}(\phi, x, h) - \phi(x) = \sum_{j=1}^k \frac{h^j}{j!} \mathcal{L}^j \phi(x) + \mathcal{O}(h^{k+1}), \quad (10)$$

for all integer k . By defining

$$U^{f,g}(\phi, x, h) = \mathbb{E}(\phi(\Psi(f, g, X_0, h, \xi_0)) | X(0) = x), \quad (11)$$

for the numerical integrator (2), we see that the local weak error of the numerical integrator applied to (1) after one step is given by

$$\mathbb{E}(\phi(X_1)) - \mathbb{E}(\phi(X(t_1))) = U^{f,g}(\phi, x, h) - u^{f,g}(\phi, x, h). \quad (12)$$

Motivated by an expansion of (11) in Taylor series, we assume

Assumption 1 *The numerical solution (11) has the following expansion*

$$U^{f,g}(\phi, x, h) = \phi(x) + hA_1(f, g)\phi(x) + h^2A_2(f, g)\phi(x) + \dots, \quad (13)$$

where $A_i(f, g)$, $i = 0, 1, 2, \dots$ are differential operators depending on the drift and diffusion functions of the SDE to which the numerical integrator is applied to. We further assume that these differential operators $A_i(f, g)$, $i = 1, 2, \dots$ satisfy for all $\varepsilon > 0$, f, \hat{f}, g, \hat{g}

$$A_i(f + \varepsilon \hat{f}, g + \varepsilon \hat{g}) = A_i(f, g) + \varepsilon \hat{A}_i(f, \hat{f}, g, \hat{g}),$$

where \hat{A}_i , $i = 1, 2, \dots$ are again differential operators.

The above smoothness assumption is usually satisfied by numerical integrators. For the expansion in integer powers of the stepsize h , special care has to be taken, as explained in the following remark.

Remark 2.2 *The assumption that the expansion (13) holds with integer powers of the timestep h is essential to avoid non integer powers of h in the modified equation (4). For instance, let us consider the scalar θ -Milstein method*

$$X_{n+1} = X_n + (1 - \theta)hf(X_n) + \theta hf(X_{n+1}) + g(X_n)\Delta W_n + \frac{1}{2}g'(X_n)g(X_n)((\Delta W_n)^2 - h),$$

where ΔW_n are independent $\mathcal{N}(0, h)$ distributed random variables and θ is a fixed parameter. More details on this scheme will be given in Section 3. The assumption (13) is not satisfied if one uses the Platen [19] approximation

$$\frac{1}{2}g'(X_n)g(X_n) \approx \frac{1}{2\sqrt{h}} \left(g(X_n + \sqrt{h}g(X_n)) - g(X_n) \right),$$

for approximating the derivative of the noise function in the θ -Milstein method, because (13) would contain a term of size $\mathcal{O}(h^{5/2})$. However, if one considers instead the approximation used by Rößler [35] in which the noise part is evaluated as

$$\frac{1}{2}g'(X_n)g(X_n) \approx \frac{1}{4\sqrt{h}} \left(g(X_n + \sqrt{h}g(X_n)) - g(X_n - \sqrt{h}g(X_n)) \right),$$

then, the assumption (13) is satisfied. This can be checked by observing that the substitution $\sqrt{h} \leftrightarrow -\sqrt{h}$ leaves the definition of the method unchanged.

Construction of modified equations For a numerical method (2) with an expansion (13) satisfying (see (12))

$$U^{f,g}(\phi, x, h) - u^{f,g}(\phi, x, h) = \mathcal{O}(h^{p+1}),$$

i.e., of weak order p in view of Remark 1.1, the task now is to find a modified SDE (4) such that

$$U^{f_h, g_h}(\phi, x, h) - u^{f,g}(\phi, x, h) = \mathcal{O}(h^{p+r+1}), \quad (14)$$

i.e., a numerical method $(\tilde{X}_n)_{n \geq 0}$ of weak order $p+r$ with $r > 0$ for the original problem (1). A second assumption that we make on the numerical integrator is that it is consistent, i.e. of weak order at least one. This assumption implies $A_1(f, g)\phi = \mathcal{L}\phi$ and $A_1(f_h, g_h)\phi = \tilde{\mathcal{L}}\phi$, where

$$\tilde{\mathcal{L}}\phi := f_h \cdot \nabla_x \phi + \frac{1}{2}(g_h g_h^T) : \nabla_x^2 \phi, \quad (15)$$

for all function ϕ . Substituting f_h, g_h given by (5),(6), respectively, in (15) yields the following expansion for $\tilde{\mathcal{L}}$

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

where for $j = 0, 1, 2, \dots$, \mathcal{L}_j is given by

$$\mathcal{L}_j = f_j \cdot \nabla_x + \frac{1}{2} \sum_{k=0}^j (g_k g_{j-k}^T) : \nabla_x^2. \quad (16)$$

Here and in what follows, we used the notation $\mathcal{L}_0 := \mathcal{L}$, $f_0 := f$ and $g_0 := g$. We will also sometimes write $\mathcal{L}_j = \mathcal{L}_j(f_j, g, g_1, \dots, g_j)$ to emphasize on the dependency of these operators towards the functions f_j, g, g_1, \dots, g_j .

We may now state in this section the main result of this paper. We show that under suitable assumptions, the weak order p of the numerical integrator (2) can be increased to $p+r$ with $r \geq 1$ by applying it to a suitably modified SDE (4), with modified drift and noise of the form

$$f_{h,s}(x) = f(x) + hf_1(x) + \dots + h^s f_s(x), \quad (17)$$

$$g_{h,s}(x) = g(x) + hg_1(x) + \dots + h^s g_s(x), \quad (18)$$

where $s = p+r-1$. The integrator with improved weak order r can be written as

$$\tilde{X}_{n+1} = \Psi(f_{h,p+r-1}, g_{h,p+r-1}, \tilde{X}_n, h, \xi_n). \quad (19)$$

Theorem 2.3 *Assume that the numerical scheme (2) has order $p \geq 1$ and that Assumption 1 holds. Let $r \geq 1$ and assume that the functions f_j and g_j for $j = 1, \dots, p+r-2$ have been constructed such that $\tilde{X}_{n+1} = \Psi(f_{h,p+r-2}, g_{h,p+r-2}, \tilde{X}_n, h, \xi_n)$ has weak order $p+r-1$. Consider the differential operator defined as*

$$\mathcal{L}_{p+r-1} := \lim_{h \rightarrow 0} \frac{u^{f,g}(\cdot, x, h) - U^{f_{h,p+r-1}, g_{h,p+r-1}}(\cdot, x, h)}{h^{p+r}}, \quad (20)$$

where $u^{f,g}(\phi, x, h)$ is expanded in (10) and $U^{f,g}(\phi, x, h)$ is defined in (11). If there exist functions $f_{p+r-1} : \mathbb{R}^d \rightarrow \mathbb{R}^d$ and $g_{p+r-1} : \mathbb{R}^d \rightarrow \mathbb{R}^{d \times m}$ such that the differential operator (20) can be written in the form (16), then the numerical integrator (19) applied to the SDE with the modified drift and noise (17),(18) has weak order of accuracy $p+r$ for the original system of SDEs (1) provided $f_{h,p+r-1}, g_{h,p+r-1} \in C^{2(p+r)+1}$. The error bound

$$|\mathbb{E}(\phi(\tilde{X}_N)) - \mathbb{E}(\phi(X(t_N)))| \leq Ch^{p+r},$$

holds for any fixed $t_N = Nh \in [0, \tau]$ with h sufficiently small and for all functions $\phi : \mathbb{R}^d \rightarrow \mathbb{R}$ that are $2(p+r)+1$ times continuously differentiable with all partial derivatives with polynomial growth.

Proof. By induction hypothesis, $\tilde{X}_{n+1} = \Psi(f_{h,p+r-2}, g_{h,p+r-2}, \tilde{X}_n, h, \xi_n)$ is an integrator of weak order $p+r-1$. Thus, it has a weak expansion of the form

$$\begin{aligned} U^{f_{h,p+r-2}, g_{h,p+r-2}}(\phi, x, h) &= \phi(x) + hA_1(f_{h,p+r-2}, g_{h,p+r-2})\phi(x) + \dots \\ &+ h^{p+r}A_{p+r}(f_{h,p+r-2}, g_{h,p+r-2}) + \mathcal{O}(h^{p+r+1}) \\ &= \phi(x) + h\mathcal{L}(f, g)\phi(x) + \dots + \frac{h^{p+r-1}}{(p+r-1)!}\mathcal{L}^{p+r-1}(f, g)\phi(x) \\ &+ h^{p+r}B_{p+r}(f, g)\phi(x) + \mathcal{O}(h^{p+r+1}), \end{aligned}$$

where $B_{p+r}(f, g)$ is a certain differential operator. Using Assumption 1, we have the relation $A_i(f_{h,p+r-1}, g_{h,p+r-1}) = A_i(f_{h,p+r-2}, g_{h,p+r-2}) + \mathcal{O}(h^{p+r-1})$. The weak expansion of the modified integrator (19) can then be written as

$$\begin{aligned} U^{f_{h,p+r-1}, g_{h,p+r-1}}(\phi, x, h) &= \phi(x) + h\mathcal{L}(f, g)\phi(x) + \dots + \frac{h^{p+r-1}}{(p+r-1)!}\mathcal{L}^{p+r-1}(f, g)\phi(x) \\ &+ h^{p+r}(\mathcal{L}_{p+r}(f_{p+r-1}, g, g_1, \dots, g_{p+r-1}) + B_{p+r}(f, g))\phi(x) + \mathcal{O}(h^{p+r+1}), \end{aligned}$$

where \mathcal{L}_{p+r-1} is defined in (16). If f_{p+r-1} and g_{p+r-1} are such that

$$\mathcal{L}_{p+r-1}(f_{p+r-1}, g, g_1, \dots, g_{p+r-1}) = \frac{\mathcal{L}^{p+r}}{(p+r)!} - B_{p+r}(f, g),$$

then (14) holds for $U^{f_{h,p+r-1}, g_{h,p+r-1}}(\phi, x, h)$. Now observing that the right-hand side of the above equality is equal to the right-hand side of (20) together with Remark 1.1 proves the theorem. \square

Relation with backward error analysis. We close this section by relating the previous construction of modified integrators with the backward error analysis for SDEs [11, 42] mentioned in Remark 2.1. Applying the numerical integrator (2) to the original SDE (1), we search for a modified differential equation (7) such that

$$U^{f, g}(\phi, x, h) - u^{\hat{f}_h, \hat{g}_h}(\phi, x, h) = \mathcal{O}(h^{p+q+1}) \quad (21)$$

with $q > 0$. The aim in such a procedure is to better understand the behavior of the numerical method (2) (applied to (1)) by studying the modified SDE (7). The modified SDE (7), with \hat{f}_h, \hat{g}_h given by an expansion

$$\begin{aligned} \hat{f}_h(x) &= f(x) + h\hat{f}_1(x) + h^2\hat{f}_2(x) + \dots, \\ \hat{g}_h(x) &= g(x) + h\hat{g}_1(x) + h^2\hat{g}_2(x) + \dots, \end{aligned}$$

has an associated backward Kolmogorov equation (the formula (8) with \mathcal{L} replaced by $\hat{\mathcal{L}}$) in (9), where

$$\hat{\mathcal{L}} = \mathcal{L} + h\hat{\mathcal{L}}_1 + h^2\hat{\mathcal{L}}_2 + \dots, \quad (22)$$

where for $j = 1, 2, \dots$,³ $\hat{\mathcal{L}}_j$ is given by

$$\hat{\mathcal{L}}_j = \hat{f}_j \cdot \nabla_x + \frac{1}{2} \sum_{k=0}^j (\hat{g}_k \hat{g}_{j-k}^T) : \nabla_x^2.$$

³The same convention as before is used here: $\hat{g}_0 = g$.

The Taylor expansion (10) becomes

$$u^{\hat{f}_h, \hat{g}_h}(\phi, x, h) - \phi(x) = \sum_{j=1}^k \frac{h^j}{j!} \hat{\mathcal{L}}^j \phi(x) + \mathcal{O}(h^{k+1}),$$

which gives in terms of the expansion (22) with $\hat{\mathcal{L}}_0 = \mathcal{L}$ (see [42])

$$u^{\hat{f}_h, \hat{g}_h}(\phi, x, h) - \phi(x) = \sum_{j=1}^k h^j \sum_{i_1+i_2+\dots+i_l=j} \frac{1}{l!} (\hat{\mathcal{L}}_{i_1} \cdots \hat{\mathcal{L}}_{i_l} \phi)(x) + \mathcal{O}(h^{k+1}).$$

The task in this approach is to find \hat{f}_h, \hat{g}_h such that for $U^{f,g}(\phi, x, h)$ given by (13) holds

$$A_j(f, g) = \sum_{i_1+i_2+\dots+i_l=j} \frac{1}{l!} \hat{\mathcal{L}}_{i_1} \cdots \hat{\mathcal{L}}_{i_l},$$

for $j = p + q$. The above relation permits to define by induction the differential operators $\hat{\mathcal{L}}_j$ used to construct the modified equation for backward error analysis. We emphasize once more that the aim and the theory for integrators based on modified equations and backward error analysis are different. In the former approach, the modified SDE constitutes only a surrogate to obtain a better numerical approximation of the solution of the original SDE, in the latter approach, the modified SDE is a tool to study a numerical integrator applied to the original SDE.

Remark 2.4 *In the case $p = r = 1$, the above procedure yields for backward error analysis and for modified integrators the operators $\mathcal{L}_1 = \mathcal{A}_1 - \frac{1}{2}\mathcal{L}^2$ and $\hat{\mathcal{L}}_1 = \frac{1}{2}\mathcal{L}^2 - \mathcal{A}_1$, respectively. Thus, the perturbations \hat{f}_1, \hat{g}_1 in the modified equations for backward error analysis and f_1, g_1 for modified integrators are identical up to the multiplicative factor -1 .*

3 High order weak methods with application to stiff problems and geometric integration

In this section we show two applications of the methodology developed in Section 2. We first derive a class of second weak order methods based on first order methods. Classical methods (Milstein or Talay methods) will be recovered, but new methods will also be derived. In particular, we derive a new second weak-order method which is mean-square stable, suitable for the integration of so-called stiff problems. This method belongs to a general class of second order weak methods derived by Milstein [26], but seems not to have appeared explicitly in the literature. Secondly, we show how our methodology can be applied to structure preserving integrators and derive second weak order methods preserving quadratic invariants. As an example, we consider the stochastic rigid body problem.

3.1 Second order weak scheme with application to stiff stochastic problems

To illustrate our methodology based on modifying equations, we derive here a second order weak method. For that, we pick a first order weak method

$$X_1 = \Psi(f, g, X_0, h, \xi_0),$$

consider the modified equation

$$dX = [f(X) + hf_1(X)] dt + [g(X) + hg_1(X)] dW(t), \quad X(0) = X_0, \quad (23)$$

and apply Theorem 2.3. Accordingly, we have to find f_1, g_1 such that

$$\mathcal{L}_1 = \frac{\mathcal{L}^2}{2} - A_1(f, g), \quad (24)$$

where $\mathcal{L}_1 := f_1 \nabla_x + \frac{1}{2}(g g_1^T + g_1 g^T) : \nabla_x^2$, and where the differential operator A_1 depends on the choice of the first order weak method.

3.1.1 One-dimensional case

For the sake of simplicity let us first consider a one dimensional SDE with one dimensional noise. The simplest first order weak method is the Euler-Maruyama method. However, for reasons explained in Remark 3.2 below, this is not a suitable method to start with. A fairly general class of first order weak methods that can be used for our purpose is the θ -Milstein (θ -M) method [15]

$$X_{n+1} = X_n + (1 - \theta)hf(X_n) + \theta hf(X_{n+1}) + g(X_n)\Delta W_n + \frac{1}{2}g'(X_n)g(X_n)((\Delta W_n)^2 - h), \quad (25)$$

where ΔW_n are independent $\mathcal{N}(0, h)$ distributed random variables and $X_0 = x$. We Taylor expand ϕ up to 4th order $\phi(X_1) = \sum_{i=0}^4 \frac{1}{i!}\phi^{(i)}(x)F^i + \dots$, where

$$F = (1 - \theta)hf(x) + \theta hf(x_1) + g(x)\Delta W_0 + \frac{1}{2}g(x)g^{(1)}(x)((\Delta W_0)^2 - h),$$

and obtain ⁴

$$u^{f,g}(\phi, x, h) = \mathbb{E}(\phi(X_1)|X_0 = 0) = \phi(x) + h\mathcal{L}\phi(x) + h^2 A_1(f, g)\phi(x) + \mathcal{O}(h^3),$$

where

$$\begin{aligned} A_1(f, g)\phi(x) &= h^2\theta \left[f(x)f^{(1)}(x) + \frac{1}{2}f^{(2)}(x)g^2(x) \right] \phi^{(1)}(x) \\ &+ \frac{h^2}{2} \left[f^2(x) + \theta g^2(x)f^{(1)}(x) + \frac{1}{2}(g(x)g^{(1)}(x))^2 \right] \phi^{(2)}(x) \\ &+ \frac{h^2}{2} \left[g^3(x)g^{(1)}(x) + g^2 f(x) \right] \phi^{(3)}(x) + \frac{h^2}{8}g^4(x)\phi^{(4)}(x). \end{aligned}$$

Applying the method (25) to the modified equation (23) we obtain $U^{f_h, g_h}(\phi, x, h)$ which is a second order approximation of $u^{f,g}(\phi, x, h)$ if we can find f_1, g_1 such that (24) holds. A simple computation reveals that

$$\begin{aligned} \left(\frac{1}{2}\mathcal{L}^2\phi - A_1\phi \right)(x) &= \left(\frac{1}{2} - \theta \right) \left(f'(x)f(x) + \frac{1}{2}f''(x)g^2(x) \right) \phi^{(1)}(x) \\ &+ \left(\left(\frac{1}{2} - \theta \right) f'(x)g(x) + \frac{1}{2}g'(x)f(x) + \frac{1}{4}g^2(x)g''(x) \right) g(x)\phi^{(2)}(x). \end{aligned}$$

We see from the above formula that we can define the appropriate operator \mathcal{L}_1 with

$$\begin{aligned} f_1(x) &= \left(\frac{1}{2} - \theta \right) f'(x)f(x) + \frac{1}{2} \left(\frac{1}{2} - \theta \right) f''(x)g^2(x), \\ g_1(x) &= \left(\frac{1}{2} - \theta \right) f'(x)g(x) + \frac{1}{2}g'(x)f(x) + \frac{1}{4}g^2(x)g''(x). \end{aligned}$$

⁴Recall that $\mathbb{E}(\Delta W_0) = \mathbb{E}(\Delta W_0^3) = 0$ and $\mathbb{E}(\Delta W_0^2) = h^2, \mathbb{E}(\Delta W_0^4) = 3h^2$.

Now setting $f_{h,1} = f + hf_1$ and $g_{h,1} = g + hg_1$, we obtain the following new integrator

$$\begin{aligned} X_{n+1} &= X_n + (1 - \theta)hf_{h,1}(X_n) + \theta hf_{h,1}(X_{n+1}) + g_{h,1}(X_n)\Delta W_n \\ &+ \frac{1}{2}g'(X_n)g(X_n)((\Delta W_n)^2 - h), \end{aligned} \quad (26)$$

which has weak order two for the system of SDEs (1).

Remark 3.1 *In principle one should also replace g by $g_{h,1}$ in the last term of (26), but omitting hg_1 for this term does not affect the weak order two of accuracy. Indeed,*

$$g'_{h,1}(X_n)g_{h,1}(X_n) = g'(X_n)g(X_n) + C(X_n)h + \mathcal{O}(h^2),$$

where $C(x)$ is a smooth function. Using $\mathbb{E}(C(X_n)h((\Delta W_n)^2 - h)) = 0$, we deduce

$$\mathbb{E}(g'_{h,1}(X_n)g_{h,1}(X_n)((\Delta W_n)^2 - h)) = \mathbb{E}(g'(X_n)g(X_n)((\Delta W_n)^2 - h)) + \mathcal{O}(h^3),$$

and thus it does not influence the accuracy of the method because it induces a $\mathcal{O}(h^3)$ perturbation of $\mathbb{E}(\phi(X_{n+1}))$.

Notice that the integrator (26) belongs to a sub-class of a general family of second order weak method introduced by Milstein [26]. For $\theta = 0$ it has also been considered by Talay who proved its order of convergence [39]. For $\theta = 1/2$ the method was considered by Milstein who showed its good stability behavior for scalar SDEs with additive noise. For $\theta = 1$, the method does not seem to have appeared explicitly in the literature. We will show below that it has favorable stability properties for scalar SDEs with multiplicative noise (mean-square stability).

Remark 3.2 *Notice that \mathcal{L}_0^2 is a differential operator of order four in general. Thus, the difference $\frac{1}{2}\mathcal{L}_0^2 - \mathcal{A}_1$ is a differential operator of order two of the same form as \mathcal{L}_0 only if \mathcal{A}_1 contains the same third and fourth order derivative of ϕ as $\frac{1}{2}\mathcal{L}_0^2$. As explained further, this is true for the Milstein method. However, this would not be the case for the Euler-Maruyama method where the term $\frac{1}{2}g'(x)g(x)^3\phi^{(3)}(x)$ involving the third derivative of ϕ in $\frac{1}{2}\mathcal{L}_0^2\phi$ is not cancelled in general (unless $g' = 0$, i.e. for additive noise). Therefore, as observed in [42], a modified SDE cannot be constructed for the Euler-Maruyama method.*

3.1.2 Multi-dimensional case

The formula derived for the one-dimensional case can easily be extended to the multi-dimensional case. Consider the multi-dimensional SDE (1), where f is a column vector of size d and g is a $d \times m$ matrix (below, we denote by $\cdot_{[i]}$ the i th component of a vector in \mathbb{R}^d and by $\cdot_{[i,j]}$ the coefficients of a $d \times m$ matrix). For a fixed parameter θ , consider the θ -M method

$$X_{n+1} = X_n + (1 - \theta)hf(X_n) + \theta hf(X_{n+1}) + g(X_n)\Delta W_n + M(X_n, W), \quad (27)$$

where the Milstein term $M(X_n, W)$ is defined for $i = 1, \dots, d$ by

$$M_{[i]} = \Xi_i(X_n) : I = \sum_{j_1, j_2=1}^m \Xi_{i[j_1, j_2]} I_{[j_1, j_2]}.$$

The coefficient of the $m \times m$ matrix Ξ_i are defined for $i = 1, \dots, d$ by

$$\Xi_{i[j_1, j_2]} = \sum_{k=1}^d \frac{\partial g_{[i, j_2]}}{\partial x_k} g_{[k, j_1]},$$

and the coefficients of the $m \times m$ matrix I of multiple integrals given by

$$I_{[j_1, j_2]} = \int_{t_n}^{t_{n+1}} \left(\int_{t_n}^s dW_{j_1}(t) \right) dW_{j_2}(s). \quad (28)$$

Following the procedure for the one-dimensional case, we obtain the modified θ -M method of weak order two

$$X_{n+1} = X_n + (1 - \theta)hf_{h,1}(X_n) + \theta hf_{h,1}(X_{n+1}) + g_{h,1}\Delta W_n + M(X_n, W), \quad (29)$$

where $f_{h,1} = f + hf_1$, $g_{h,1} = g + hg_1$, and f_1, g_1 are given (componentwise) by

$$\begin{aligned} f_{1,[i]} &= \left(\frac{1}{2} - \theta \right) (f'f)_{[i]} + \frac{1}{2} \left(\frac{1}{2} - \theta \right) gg^T : f''_{[i]}, \\ g_{1,[i,j]} &= \left(\frac{1}{2} - \theta \right) (f'g)_{[i,j]} + \frac{1}{2} g'_{[i,j]}f + \frac{1}{4} gg^T : g''_{[i,j]}, \end{aligned} \quad (30)$$

for all $i = 1, \dots, d$ and $j = 1, \dots, m$.

Remark 3.3 *The multiple integral matrix I in (28) is difficult to evaluate in general and needs to be approximated. One can use for instance the following weak approximation for the matrix I in the definition (28) (see for instance [19, eq. (5.12.9)])*

$$J = \frac{1}{2}(\Delta W_n \Delta W_n^T + E_n),$$

where E_n is a random skew-symmetric matrix whose coefficients $E_{n,[j_1, j_2]}$ are independent two-point distributed random variables,

$$\mathbb{P}(E_{n,[j_1, j_2]} = \pm h) = 1/2, \quad \text{for all } 1 \leq j_1 < j_2 \leq d$$

and $E_{n,[j_1, j_2]} = -E_{n,[j_2, j_1]}$ for all $j_1, j_2 = 1, \dots, m$. Using J instead of I does not alter the weak order two of accuracy of the method (29) (it does however decrease the strong order of the method from 1 to 1/2). The independent Gaussian variables ΔW_{n_j} can also be replaced by independent three point random variables with

$$\mathbb{P}(\Delta W_{n_j} = \pm \sqrt{3h}) = \frac{1}{6}, \quad \mathbb{P}(\Delta W_{n_j} = 0) = \frac{2}{3}, \quad (31)$$

without decreasing the weak order two of the method.

Notice that derivative free versions of the modified θ -M methods (29), of weak order two, could be obtained following [35] by approximating all the derivatives by finite differences.

3.1.3 A mean-square stable modified θ -M method

In this section we show that we can construct a second order modified θ -M method with favorable mean-square stability. To study the stability in the mean-square sense of numerical integrators, a widely used test equation introduced in [36] for SDEs is the following scalar SDE with multiplicative noise

$$dX = \lambda X dt + \mu X dW(t), \quad (32)$$

where the parameters $\lambda, \mu \in \mathbb{C}$. We notice that other test equations have been considered recently in [5] to better account for the stability behavior of numerical integrators when applied to systems of SDEs. The mean-square stability domain of (32) is given by

$$\mathcal{S} = \{(\lambda, \mu) \in \mathbb{C}^2 ; \Re \lambda + \frac{1}{2} |\mu|^2 < 0\}. \quad (33)$$

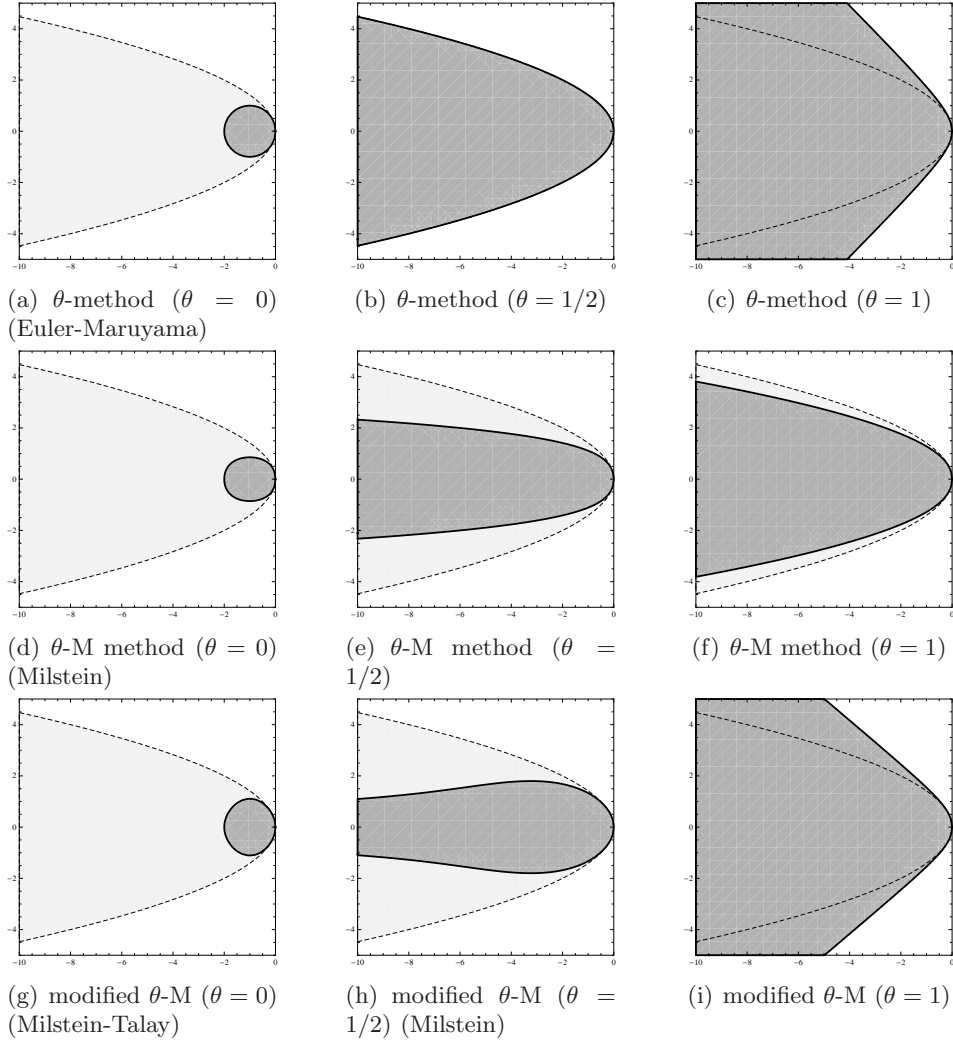


Figure 1: Comparison of mean-square stability domains (dark gray area) of the θ -methods, the θ -M methods, and the modified θ -M methods. The modified θ -M methods with $\theta = 0, 1/2$ have been proposed by Milstein and Talay. Horizontal axis: p , vertical axis: q .

The set of (λ, μ) that fulfill condition (33) can be visualized, for $\lambda, \mu \in \mathbb{R}$, as the shaded area with a boundary given by the dotted parabolas in Figure 1. The θ -M method applied to the linear test equation (32) yields

$$X_{n+1} = \frac{(1 + p(1 - \theta) + qV_n + \frac{1}{2}q^2(V_n^2 - 1))}{1 - \theta p} X_n,$$

where V_n are independent Gaussian variables with a $\mathcal{N}(0, 1)$ distribution and $p = \lambda h$ and $q = \mu\sqrt{h}$. Squaring the result and taking the expectation, we obtain the relation $\mathbb{E}(|X_{n+1}|^2) = R_{\theta, M}(p, q)\mathbb{E}(|X_n|^2)$, where

$$R_{\theta, M}(p, q) = \frac{|1 + p(1 - \theta)|^2 + |q|^2 + |q|^4/2}{|1 - \theta p|^2}. \quad (34)$$

We next define the set

$$\mathcal{S}_{\theta, M} = \{(p, q) \in \mathbb{C}^2 ; R_{\theta, M}(p, q) < 1\}.$$

The method is called mean-square (MS) stable if

$$R_{\theta, M}(p, q) \leq 1, \quad \text{for all } (p, q) \in \mathcal{S},$$

or alternatively if $\mathcal{S} \subset \mathcal{S}_{\theta, M}$. It is readily seen that there does not exist a value of $\theta \in [0, 1]$ such that the θ -M method is MS stable. Furthermore, MS stability is recovered for $\theta = 3/2$ [15].

Remark 3.4 *In contrast, the θ -methods (the methods (27) with $M \equiv 0$), whose stability function reads*

$$R_{\theta}(p, q) = \frac{|1 + p(1 - \theta)|^2 + |q|^2}{|1 - \theta p|^2},$$

can be shown to be MS stable if and only if $\theta \geq 1/2$ as reported in [16].

We come now to study the stability properties of the modified θ -M methods (26) whose stability functions can be easily deduced from (34) and read

$$\tilde{R}_{\theta, M}(p, q) = \frac{|1 + \tilde{p}(1 - \theta)|^2 + |\tilde{q}|^2 + |q|^4/2}{|1 - \theta \tilde{p}|^2},$$

where $\tilde{p} = p + (\frac{1}{2} - \theta)p^2$, $\tilde{q} = q + (1 - \theta)pq$. A simple calculation shows that this method is MS stable if and only if $\theta = 1$. Thus, for $\theta = 1$ we have constructed the second order weak method (26) which is MS stable. This method is thus suitable for the numerical integration of stiff systems of SDEs as illustrated in the numerical example below.

In Figure 1 we plot the mean-square stability domain for the standard θ -methods, the standard θ -M methods and the modified θ -M methods (the light-dark region which lies inside the dotted parabola is the stability domain \mathcal{S} of the exact solution of the test problem). For $\theta \in [0, 1]$, it can be seen that the θ -M methods are never MS stable, and that only for $\theta = 1$ is the modified θ -M method MS stable.

Numerical experiments. We illustrate the numerical behavior of the modified θ -M methods previously constructed. We consider an economy model for asset prices proposed in [18], see also [17]. It is an Itô system of SDEs in dimension $d = 3$, with $m = 2$ non-commutative noises, given by

$$\begin{aligned} dX_1 &= \beta_1 X_1 X_2 dW_1, \\ dX_2 &= -(X_2 - X_3)dt + \beta_2 X_2 dW_2, \\ dX_3 &= \alpha(X_2 - X_3)dt, \end{aligned} \tag{35}$$

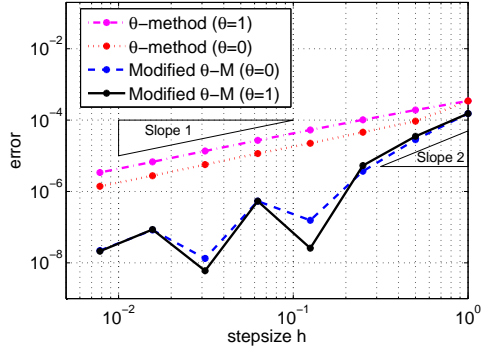
where $X_1(t)$, $X_2(t)$ and $X_3(t)$ represent the asset price, the instantaneous volatility and the average volatility, respectively. We take the parameters $\beta_1 = 1, \beta_2 = 0.3$, the initial value $X(0) = (1, 0.1, 0.1)^T$, and we consider the time interval $[0, 1]$ as in [17]. We shall consider various values of the volatility parameter α .

Since the drift vector field in (35) is linear, the modified θ -M methods (36) for (35) are linearly implicit and using the formulas (29) and (30), it can be written as

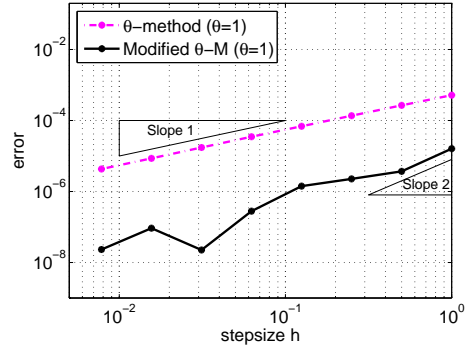
$$(Id - \theta hA)X_{n+1} = (Id + (1 - \theta)hA)X_n + g_{h,1}(X_n)\Delta W_n + M(X_n, \Delta W_n), \tag{36}$$

where A denotes the matrix

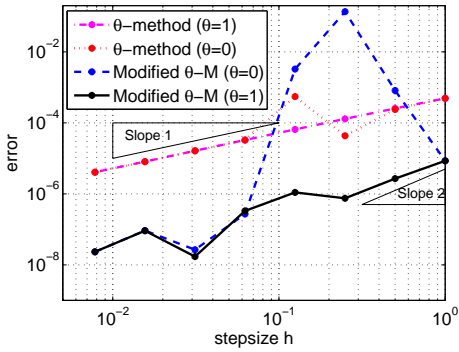
$$A = \left[1 - h \left(\frac{1}{2} - \theta \right) (1 + \alpha) \right] \begin{pmatrix} 0 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & \alpha & -\alpha \end{pmatrix},$$



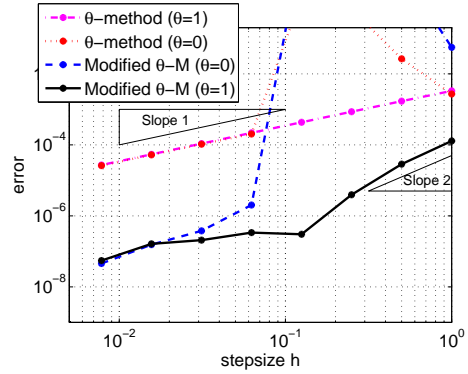
(a) Error for $\mathbb{E}(X_1^2)$. Nonstiff case $\alpha = 1$.



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



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



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

Figure 2: Finance model (35). Comparison of weak convergence rates for the modified θ -M with $\theta = 1$ (solid lines), the θ -method with $\theta = 1$ (dashed-dotted lines), the θ -method with $\theta = 0$ (Euler-Maruyama method, dotted line), and the modified θ -M with $\theta = 0$ (Milstein-Talay method, dashed line).

and where

$$g_{h,1}(X)\Delta W = \begin{pmatrix} \beta_1 X_1 (X_2 + \frac{h}{2}(X_3 - X_2))\Delta W_1 \\ \beta_2 \left((1 - h(\frac{1}{2} - \theta))X_2 + \frac{h}{2}(X_3 - X_2) \right)\Delta W_2 \\ \alpha\beta_2 h(\frac{1}{2} - \theta)X_2\Delta W_2 \end{pmatrix},$$

$$M(X, \Delta W) = \begin{pmatrix} \frac{1}{2}\beta_1^2 X_1 X_2^2 (\Delta W_1^2 - h) + \beta_1\beta_2 X_1 X_2 I_{[2,1]} \\ \frac{1}{2}\beta_2^2 X_2 (\Delta W_2^2 - h) \\ 0 \end{pmatrix}.$$

We take for the random variables $\Delta W_n = (\Delta W_{n_1}, \Delta W_{n_2})^T$ independent Gaussian variables with mean zero and variance h^2 . Notice that similar results have been obtained when considering instead discrete random variables satisfying (31). The above multiple integral $I_{[2,1]}$ in the Milstein term $M(X, \Delta W)$ is approximated by $I_{[2,1]} \approx (\Delta W_1 \Delta W_2 + \xi_n h)/2$, where ξ_n are independent random variables satisfying $\mathbb{P}(\xi_n = \pm 1) = 1/2$ as detailed in Remark 3.3.

To confirm the weak order two of convergence of the modified θ -M method (29), we compute the relative errors in the quantities $\mathbb{E}[X_1^2]$ in Figures 2(a)-(c) and $\mathbb{E}[X_2^2]$ in Figure 2(d) at the final time $t = 1$ for the stepsizes $h = 2^{-i}$, $i = 0, \dots, 7$. The reference solutions are computed using the small timestep $h = 2^{-14}$. To check carefully the accuracy of the methods, the errors are approximated using the averages over several millions of trajectories computed

in FORTRAN, using the random generator [31]. For a fair comparison, notice that we use the same set of random numbers for each numerical integrator. We observe in Figure 2 the expected lines of slope two (solid lines) both in the nonstiff case ($\alpha = 1$) and the stiff cases ($\alpha = 25$ and $\alpha = 100$). Notice that for small timesteps ($h < 0.25$) the zigzag that we observe is due to the Monte-Carlo error, which could be further reduced by increasing the number of samples. For comparison, we also plot the results for the classical implicit θ -method ($\theta = 1$) (weak order one), obtained from (36) by removing the Milstein term $M(X_n, \Delta W_n)$ and setting $h = 0$ in the definitions of A and $g_{h,1}(X)\Delta W$. We also compare with two classical explicit integrators, the Euler-Maruyama method (weak order one) and the Talay method (weak order two), obtained by taking $\theta = 0$ in (36). Notice these two explicit methods are not (unconditionally) mean-square stable. Indeed, since for large α , the largest eigenvalue in the drift function of (35) has size α , the mean-square stability constraint for these explicit methods has the form $\alpha h \leq C$, where C is a constant of moderate size, independent of h and α . We observe in Figures 2(c)-(d) that these methods are indeed unstable for $h > 2^{-4}$ for the (moderately) stiff case $\alpha = 25$. For the very stiff case $\alpha = 100$ (Figure 2(b)), these methods show too much instability to fit in the scales of the figure and are thus omitted.

This numerical experiment shows that the modified θ -M method with $\theta = 1$ has the same (unconditional) mean-square stability as the standard θ -method ($\theta \geq 1/2$), but with an improved accuracy by several orders of magnitude due to the improved weak order two of convergence.

3.2 High weak order integrators preserving quadratic invariants

In this section, we construct numerical integrators for Stratonovich SDEs of high weak order which exactly conserve all quadratic first integrals (up to machine precision). We consider the SDE (1) in Stratonovich form with a one-dimensional noise

$$dX = f(X)dt + g(X) \circ dW(t), \quad X(0) = X_0, \quad (37)$$

where the notation $\circ dW(t)$ emphasizes that the Stratonovich stochastic integrals are considered for (37). As a basic numerical integrator to apply our methodology of modified equation, we choose the fully implicit midpoint rule, as first introduced in [27],

$$X_{n+1} = X_n + hf \left(\frac{X_n + X_{n+1}}{2} \right) + g \left(\frac{X_n + X_{n+1}}{2} \right) \Delta W_n, \quad (38)$$

where ΔW_n is a scalar random variable. It is shown in [27] that (38) has weak order one in the case of a one-dimensional or commutative multi-dimensional noise. Notice however that for general SDEs with multi-dimensional noise, the weak order is $1/2$.

Remark 3.5 *The method (38) is implicit with respect to both the drift and the noise terms. In the case where ΔW_n is a standard Gaussian variable, the unboundedness of ΔW_n for arbitrarily small h leads to non-uniqueness of solutions to the non-linear system (38) and the integrator is not well defined. One way to address this problem, is to replace ΔW_n , with a suitable chosen bounded random variable [27] (see also [28, Sect. 1.3]). Here we shall simply consider discrete random variable, e.g. (31), as in Remark 3.3, which are obviously bounded.*

First integral conservation A quantity $C(x)$ is called a first integral of the system (37) if it is exactly conserved along time for all realizations of the Wiener process $W(t)$, i.e. $C(X(t)) = C(X_0)$ for all time t and all initial condition $X(0) = X_0$. Given a smooth function

$C(x)$, the identity⁵ $dC(X) = \nabla C(X) \cdot f(X)dt + \nabla C(X) \cdot g(X) \circ dW(t)$ shows that $C(X)$ is a first integral of (37) if and only if

$$\nabla C(x) \cdot f(x) = \nabla C(x) \cdot g(x) = 0 \quad \text{for all } x \in \mathbb{R}^d. \quad (39)$$

Proposition 3.6 *The implicit midpoint rule (38) exactly preserves all quadratic first integrals $C(x)$ of (37), i.e. $C(x_{n+1}) = C(x_n)$ for all h and all realizations of ΔW_n .*

Proof. Since $C(x)$ is quadratic, we write $C(x) = x^T S x$, where S is a constant symmetric matrix. Using (39), with $X = (X_{n+1} + X_n)/2$ and $R(X) = hf(X) + g(X)\Delta W_n$, a short computation yields

$$C(X_{n+1}) - C(X_n) = X_n^T S R(X) + R(X)^T S X_{n+1} = 2X^T S R(X) = \nabla C(X) \cdot R(X) = 0.$$

□

3.2.1 New invariant preserving integrators of high weak order

Using the framework of integrators based on modified equations, we introduce the following new numerical integrator

$$X_{n+1} = X_n + hf_{h,1} \left(\frac{X_n + X_{n+1}}{2} \right) + gh_{,1} \left(\frac{X_n + X_{n+1}}{2} \right) \Delta W_n, \quad (40)$$

where $f_{h,1} = f + hf_1$ and $gh_{,1} = g + hg_1$ and show below that for

$$f_1 = \frac{1}{4} \left(\frac{1}{2} f''(g, g) - g' f' g \right) \quad g_1 = \frac{1}{4} \left(\frac{1}{2} g''(g, g) - g' g' g \right), \quad (41)$$

the numerical integrator is a second order weak method for the SDE (37) which preserves all quadratic first integrals. We notice that if we consider the modified Stratonovich SDE

$$dX = [f(X) + hf_1(X)] dt + [g(X) + hg_1(X)] \circ dW(t), \quad (42)$$

then (40) is equivalent to applying the original midpoint rule (38) to the modified Stratonovich SDE (42).

Proposition 3.7 *The integrator (40) for a system of Stratonovich SDEs (37) with $m = 1$ noise has weak order 2. It exactly conserves all quadratic first integrals of (37).*

Proof. The Stratonovich SDE (37) is equivalent to the Itô SDE

$$dX = \left(f(X) + \frac{1}{2} g'(X)g(X) \right) dt + g(X)dW(t), \quad (43)$$

where compared to the Itô system of SDEs (1), the vector field f is replaced by $f + \frac{1}{2}g'g$. This permits to deduce an expansion analogue to (10) associated to the Itô SDE (43). The weak expansion of (40) (applied to (37), equivalent to the Itô SDE (43)) is computed as follows. First we have (for $X_0 = x$) $X_1 = x + F = X_0 + hf(x + F/2) + g(x + F/2)\Delta W_0$, where

$$\begin{aligned} F &= hf + \frac{h}{2} f' F + \frac{h}{8} f''(F, F) + g\Delta W_0 + \frac{1}{2} g' F \Delta W_0 + \frac{1}{8} g''(F, F) \Delta W_0 \\ &+ \frac{1}{48} g'''(F, F, F) \Delta W_0 + \mathcal{O}(h^{5/2}). \end{aligned}$$

⁵Notice that Stratonovich calculus is used here.

For the computation of $\mathcal{A}_1\phi$ we consider the expansion

$$\begin{aligned}\phi(X_1) &= \phi(x + F) = \phi(X_0) + \sum_k F_{[k]} \partial_k \phi + \frac{1}{2} \sum_{kl} F_{[k]} F_{[l]} \partial_{kl} \phi + \frac{1}{6} \sum_{klm} F_{[k]} F_{[l]} F_{[m]} \partial_{klm} \phi \\ &+ \frac{1}{24} \sum_{klmi} F_{[k]} F_{[l]} F_{[m]} F_{[i]} \partial_{klmi} \phi + \dots\end{aligned}$$

We then compute $\mathbb{E}(\phi(X_1)|X_0 = x) = \mathbb{E}(\phi(x + F))$, identify the differential operator multiplying the term h^2 , and obtain after some tedious but straightforward computations,

$$\begin{aligned}\left(\frac{1}{2}\mathcal{L}^2\phi - \mathcal{A}_1\right)\phi &= \frac{1}{4} \left(\frac{1}{2}f''(g, g) - g'f'g + \frac{1}{4}g'''(g, g, g) - \frac{1}{4}g'g''(g, g) - g'g'g'g \right) \cdot \nabla_x \phi \\ &+ \frac{1}{8} \left(g \left(\frac{1}{2}g''(g, g) - g'g'g \right)^T + \left(\frac{1}{2}g''(g, g) - g'g'g \right) g^T \right) : \nabla_x^2 \phi \\ &= \left(f_1 + \frac{1}{2}(g'_1g + g'g_1) \right) \cdot \nabla_x \phi + \frac{1}{2}(gg_1^T + g_1g^T) : \nabla_x^2 \phi,\end{aligned}$$

where we define $f_1 = \frac{1}{4} \left(\frac{1}{2}f''(g, g) - g'f'g \right)$ and $g_1 = \frac{1}{4} \left(\frac{1}{2}g''(g, g) - g'g'g \right)$. The modified Itô SDE of Theorem 2.3 then reads

$$dX = \left(f_{h,1} + \frac{1}{2}g'g + \frac{h}{2}(g'_1g + g'g_1) \right) (X)dt + g_{h,1}(X)dW(t),$$

where $f_{h,1} = f + hf_1$ and $g_{h,1} = g + hg_1$. Using $g'_{h,1}g_{h,1} = g'g + h(g'_1g + g'g_1) + \mathcal{O}(h^2)$ and neglecting the $\mathcal{O}(h^2)$ terms, the above Itô SDE can be converted to the Stratonovich SDE (42). This proves that (40)-(41) is a second order weak method for the SDE (43). Finally, the conservation of quadratic first integrals by (40) is an immediate consequence of Proposition 3.6 and Lemma 3.8 below. \square

Lemma 3.8 *Any quadratic first integral $C(y)$ of (37) is a first integral of (42).*

Proof. Consider the original midpoint rule (38) applied to (37). Using Remark 2.4, we obtain that the modified SDE up to second order for backward error analysis associated to (38) is given by (42) with h replaced by $-h$,

$$d\hat{X} = \left[f(\hat{X}) - hf_1(\hat{X}) \right] dt + \left[g(\hat{X}) - hg_1(\hat{X}) \right] \circ dW(t), \quad \hat{X}(0) = X_0,$$

and we have from (21) with $p = 1, q = 0$, $\mathbb{E}(\phi(X_1)) - \mathbb{E}(\phi(\hat{X}(h))) = \mathcal{O}(h^2)$. Using Proposition 3.6, we have $C(X_1) = C(X_0)$. On the one hand, replacing $\phi(x)$ by $\phi(C(x))$, we obtain $\mathbb{E}(\phi(C(X_0))) - \mathbb{E}(\phi(C(\hat{X}(h)))) = \mathcal{O}(h^2)$. On the other hand, using (39), we have

$$d\phi(C(\hat{X})) = -h\phi'(C(x))(\nabla C(x) \cdot f_1(\hat{X}))dt + \nabla C(x) \cdot g_1(\hat{X}) \circ dW(t),$$

where $d\phi(C(\hat{X}))$ has size $\mathcal{O}(h)$. This yields $\mathbb{E}(\phi(C(X_0))) - \mathbb{E}(\phi(C(\hat{X}(h)))) = 0$ for all test functions ϕ , and thus $C(\hat{X}(h)) = C(X_0)$. We obtain $\nabla C(x) \cdot f_1(x) = \nabla C(x) \cdot g_1(x) = 0$. \square

We close this section by indicating that a further modification of the integrator (40) allows yet an even better accuracy. Consider

$$X_{n+1} = X_n + hf_{h,2} \left(\frac{X_n + X_{n+1}}{2} \right) + gh_1 \left(\frac{X_n + X_{n+1}}{2} \right) \Delta W_n, \quad (44)$$

where $f_{h,2} = f + hf_1 + h^2 f_2$ and $g = g + hg_1$ (as previously) with f_1, g_1 as defined in (41) and f_2 given by

$$f_2 = \frac{1}{12} \left(\frac{1}{2} f''(f, f) - f' f' f \right). \quad (45)$$

The above term f_2 corrects the deterministic error of size $\mathcal{O}(h^2)$, but the weak order of the integrator (44) remains 2, as detailed in the following proposition. Notice that it would be interesting to search for modified fields $f_{2,h}, g_{2,h}$ to achieve the weak order 3 (or more), if possible.

Proposition 3.9 *The integrator (44) for a system of Stratonovich SDEs (37) with $m = 1$ noise has weak order 2. It exactly conserves all quadratic first integrals of (37). In addition, if $g(x) = \mathcal{O}(\mu)$, then we have $\mathbb{E}(\phi(X_N)) - \mathbb{E}(\phi(X(t_N))) = \mathcal{O}(h^4 + \mu h^2)$ for all test functions ϕ .*

For comparison, we also consider the integrator of weak order one

$$X_{n+1} = X_n + hf_{h,2} \left(\frac{X_n + X_{n+1}}{2} \right) + g \left(\frac{X_n + X_{n+1}}{2} \right) \Delta W_n, \quad (46)$$

where $f_{h,2} = f + hf_1 + h^2 f_2$, with f_1, f_2 given in (41),(45). Notice that the integrators (44) and (46) are equivalent to the modifying implicit midpoint rule of order 4 for ODEs (deterministic case) introduced in [8] in the case where the noise function g is zero.

We summarize in the following table our theoretical findings in the case where the noise function g has size $\mathcal{O}(\mu)$ and the drift function f has size $\mathcal{O}(1)$.

Table 1: Comparison of four integrators conserving exactly all quadratic first integrals for the SDE system (37) (1-dimensional noise) with $f = \mathcal{O}(1)$ and $g = \mathcal{O}(\mu)$.

method	weak order of accuracy	order for ODEs (no noise: $g = 0$)	size of $\mathbb{E}(\phi(X_N)) - \mathbb{E}(\phi(X(t_N)))$
IMR, see (38)	1	2	$\mathcal{O}(h^2 + \mu^2 h)$
IMR2, see (40)	2	2	$\mathcal{O}(h^2)$
IMR(4), see (46)	1	4	$\mathcal{O}(h^4 + \mu^2 h)$
IMR2(4), see (44)	2	4	$\mathcal{O}(h^4 + \mu h^2)$

Example: a stochastic rigid body model To illustrate that the integrators previously introduced conserve quadratic first integrals and to compare the performance of the various methods proposed (see Table 1), we consider a randomly perturbed rigid body problem that is, the motion of a rigid body in \mathbb{R}^3 subject to a scalar white noise perturbation. The equations of motion of an asymmetric rigid body with Stratonovich noise in dimension $m = 1$ are given by ⁶

$$\begin{aligned} dX &= \widehat{X} \mathcal{I}^{-1} X dt + \mu \widehat{X} e_1 \circ dW(t), \\ dQ &= Q \widehat{\mathcal{I}^{-1} X} dt + \mu Q \widehat{e}_1 \circ dW(t), \end{aligned} \quad (47)$$

⁶We use the standard hat notation for the correspondence between 3×3 skew-symmetric matrices and size 3 vectors, $\widehat{X} = \begin{pmatrix} 0 & -X_3 & X_2 \\ X_3 & 0 & -X_1 \\ -X_2 & X_1 & 0 \end{pmatrix}$, for all $X = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix}$.

where $e_1 = (1, 0, 0)^T$, $\mu \geq 0$ is a parameter and $\mathcal{I} = \text{diag}(I_1, I_2, I_3)$. A generalization of equation (47) for a 3-dimensional noise is presented in [21, Eq. (6.9)-(6.10)], where one can also find a physical justification for these equations. This model is a variant of the model proposed in [22] with the additional feature that it preserves the spatial angular momentum QX , as detailed below. In the case where $\mu = 0$, we recover the standard deterministic equations of motion of an asymmetric rigid body. We refer to [14, Sect. VI.5] for a survey of geometric and invariant preserving integrators for the rigid body problem in the context of ODEs. The constants $I_1, I_2, I_3 > 0$ are the moments of inertia which characterize the rigid body. The function $X(t)$ represents the angular momentum in \mathbb{R}^3 in the body frame. The matrix $Q(t)$ is a rotation matrix in \mathbb{R}^3 which gives the orientation of the rigid body in a fixed frame. Notice that the first line in (47) can be rewritten simply as

$$\begin{aligned} dX_1 &= \left(\frac{1}{I_3} - \frac{1}{I_2} \right) X_2 X_3 dt, \\ dX_2 &= \left(\frac{1}{I_1} - \frac{1}{I_3} \right) X_3 X_1 dt + \mu X_3 \circ dW(t), \\ dX_3 &= \left(\frac{1}{I_2} - \frac{1}{I_1} \right) X_1 X_2 dt - \mu X_2 \circ dW(t). \end{aligned}$$

The system of SDEs (47) has several first integrals, all of which are quadratic. It has QX as first integral, which represents the spatial momentum in \mathbb{R}^3 with respect to the body frame. It also has $Q^T Q = Id$ as first integral because Q is an orthogonal matrix. Since Q is orthogonal, the Casimir $C(X) = \frac{1}{2}(X_1^2 + X_2^2 + X_3^2)$ is also conserved. Considering the Hamiltonian $H(X) = \frac{1}{2}(X_1^2/I_1 + X_2^2/I_2 + X_3^2/I_3)$, we have

$$dH(X) = \mu \frac{X_2 X_3}{2} \left(\frac{1}{I_2} - \frac{1}{I_3} \right) \circ dW(t),$$

which shows that $H(X)$ is also a first integral if and only if $I_2 = I_3$ (symmetric body) or $\mu = 0$ (the noise is zero).

Using formulas (41) where the functions f and g correspond to the right-hand side of (47), a straightforward computation yields the modified SDE associated to (47),

$$\begin{aligned} dX &= \widehat{X}(\mathcal{I}^{-1} + \frac{h\mu^2}{4}\mathcal{J}^{-1})X dt + \mu \left(1 + \frac{h\mu^2}{4} \right) \widehat{X}e_1 \circ dW(t), \\ dQ &= Q(\widehat{\mathcal{I}^{-1}X} + \frac{h\mu^2}{4}\widehat{\mathcal{J}^{-1}X})dt + \mu \left(1 + \frac{h\mu^2}{4} \right) Q\widehat{e}_1 \circ dW(t), \end{aligned} \quad (48)$$

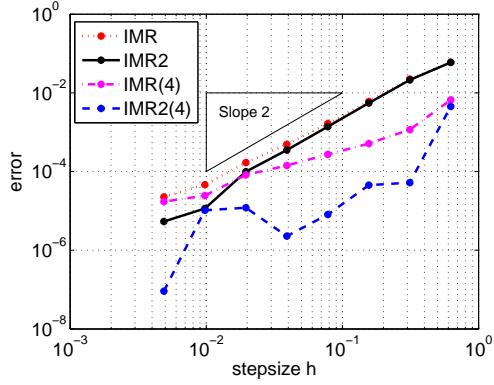
where we define $\mathcal{J} = \text{diag}(I_1, I_3, I_2)$. We obtain from Proposition 3.7 that applying the fully implicit midpoint rule (38) to the Statonovitch SDE (48) yields a weak order two approximation of the solution of (47) which exactly conserves all quadratic first integrals, i.e. $C(X_{n+1}) = C(X_n)$, $Q_{n+1}X_{n+1} = Q_nX_n$ and $Q_n^T Q_n = Id$ for all n , and in the case $I_2 = I_3$ (symmetric body), we have also $H(X_{n+1}) = H(X_n)$.

Remark 3.10 Notice that the modified SDE (48) is of the same form as the original rigid body equations (47) with modified data parameters. Indeed, replacing μ by

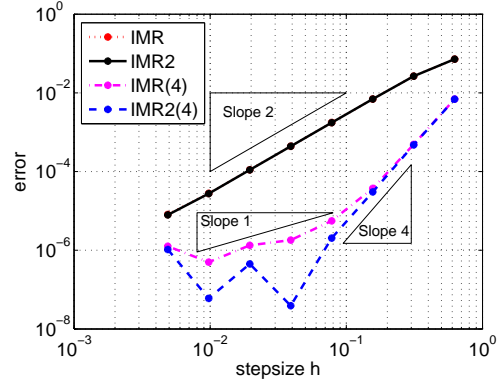
$$\tilde{\mu} = \mu(1 + h\mu^2/4),$$

and replacing $\mathcal{I} = \text{diag}(I_1, I_2, I_3)$ in the original SDE (47) by $\tilde{\mathcal{I}} = \text{diag}(\tilde{I}_1, \tilde{I}_2, \tilde{I}_3)$, where

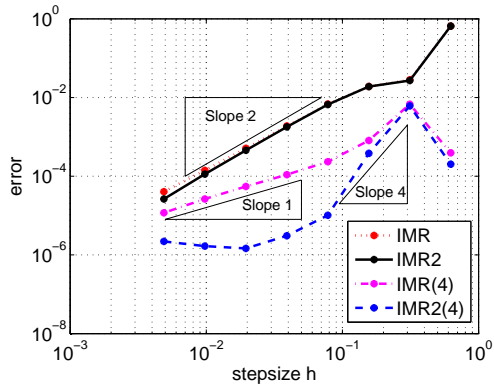
$$\frac{1}{\tilde{I}_1} = \frac{1}{I_1} \left(1 + \frac{h\mu^2}{4} \right), \quad \frac{1}{\tilde{I}_2} = \frac{1}{I_2} + \frac{h\mu^2}{4I_3}, \quad \frac{1}{\tilde{I}_3} = \frac{1}{I_3} + \frac{h\mu^2}{4I_2},$$



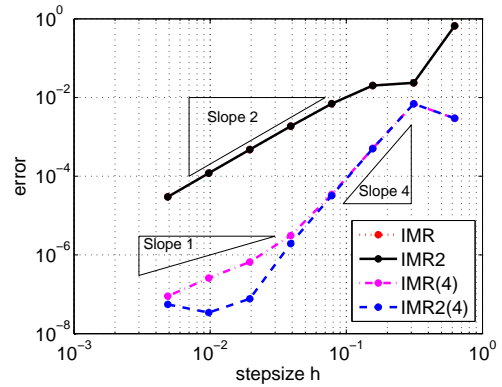
(a) Error for $\mathbb{E}(X_1^2)$. Noise size $\mu = 0.1$.



(b) Error for $\mathbb{E}(X_1^2)$. Noise size $\mu = 0.01$.



(c) Error for $\mathbb{E}(\sin(e_1^T Q e_1))$. Noise size $\mu = 0.1$.



(d) Error for $\mathbb{E}(\sin(e_1^T Q e_1))$. Noise size $\mu = 0.01$.

Figure 3: Rigid body problem (47). Comparison of weak convergence rates for IMR, see (38) (dotted lines), IMR2, see (40) (solid lines), IMR2(4), see (44) (dashed lines), and IMR(4), see (46) (dashed-dotted lines).

yields the modified SDE (48). Thus, our modification to high weak order reduces to a perturbation of the parameters and has a negligible overcost.

Implementation We now detail the implementation of the standard implicit midpoint rule (38) for the stochastic rigid body problem (47). The implementation of the modified implicit midpoint rule (40) (and similarly for the method (44)) is deduced using Remark 3.10 by modifying the moments of inertia I_1, I_2, I_3 . We refer to [8] for the implementation of the corrector f_2 in (44) and (46).

It is a standard approach to use quaternions q_n to represent the orthogonal matrices Q_n (see [14] in the context of rigid body integrator implementations). The implicit midpoint rule (38) for the angular momentum $X(t)$ can be written as

$$X_{n+1} = X_n + h\widehat{X}I^{-1}X + \mu\widehat{X}e_1\Delta W_n,$$

where we denote $X = (X_{n+1} + X_n)/2$. This implicit system can be solved by a few fixed point iterations. Next, the configuration update

$$Q_{n+1} = Q_n + h\left(\frac{Q_n + Q_{n+1}}{2}\right)\widehat{I^{-1}X} + \mu\left(\frac{Q_n + Q_{n+1}}{2}\right)\widehat{e_1}\Delta W_n,$$

is equivalent to $Q_{n+1} = Q_n \Omega$, where Ω is the orthogonal matrix defined by the Cayley transform $\Omega = (Id + \widehat{Z})(Id - \widehat{Z})^{-1}$ with $Z = \frac{h}{2}\mathcal{I}^{-1}X + \frac{\Delta W_n \mu}{2}e_1$. Thus, the configuration update for the rotation matrix Q_n reduces to a multiplication of quaternions⁷

$$q_{n+1} = q_n \cdot \frac{\omega}{\|\omega\|}, \quad \text{with } \omega = 1 + \frac{h}{2} \left(i \frac{X_1}{I_1} + j \frac{X_2}{I_2} + k \frac{X_3}{I_3} \right) + i \frac{\Delta W_n}{2} \mu,$$

where the matrices Q_n, Q_{n+1} are represented by the quaternions q_{n+1}, q_n , respectively.

Convergence rates We consider the system (47) on the time interval $[0, 10]$. We take the moments of inertia $I_1 = 0.345$, $I_2 = 0.653$, $I_3 = 1.0$, which correspond to the water molecule (nearly flat body). Initial values are $X(0) = (0.8, 0.6, 0)^T$ and $Q(0)$ is the identity matrix. We have carefully implemented the above integrators in FORTRAN, using quaternions for the rotation matrices. In Figure 3, we plot the errors for $\mathbb{E}(X_1^2)$, $\mathbb{E}(\sin(e_1^T Q e_1))$ at final time $t = 10$ versus the timestep $h = 2^{-i}$, $i = 1, \dots, 8$. The reference solution is computed using the small timestep $h = 2^{-14}$. To check carefully the accuracy of the methods, we compute numerically the expectancies using the averages over several millions of trajectories. We consider two values of the noise parameter: $\mu = 0.1$ and $\mu = 0.01$. We observe in all cases lines of slope two for the modified midpoint rule IMR2 (40) which confirms its weak order two of accuracy. For the standard midpoint rule IMR in (38) and the modified version IMR(4) in (46) which both have weak order one, we observe for large stepsizes h , lines of slope four and two respectively in the case where the deterministic error (h^2 or h^4) is dominant compared to $\mu^2 h$. For smaller timesteps, we retrieve lines of slope one, the weak order of these two methods. Similarly, for the improved modified midpoint rule IMR2(4) in (44), we observe lines of slope four for large timesteps and only two for small timestep. This corroborates the theoretical results collected in Table 1.

4 Conclusion

In this paper, we introduced a new framework for increasing the weak order of accuracy of a given numerical method for SDE by considering the numerical integration of a suitably modified problem. Our methodology, that uses tools developed for backward error analysis for stochastic problems [42, 11], generalizes to SDEs the framework of numerical integrators based on modified equations introduced in [8] for deterministic problems. This approach permits to fulfill automatically the numerous order conditions for high order weak schemes. We illustrated our approach at the example of the Milstein-Talay θ -method, and obtained for $\theta = 1$ a mean-square stable integrator of weak order two. The numerical experiments conducted for a stiff problem in economy show the improved accuracy by several magnitudes compared to the classical θ -method of weak order one. In the spirit of backward error analysis for the study of geometric integrators for ODEs, where the modified equations inherit the geometric properties of the integrators, we also derived new high weak order integrators based on the implicit midpoint rule, that automatically conserve all quadratic first integrals. The efficiency of the approach is illustrated at the example of a stochastic rigid body model which possesses several quadratic first integrals. A natural extension of this work would be to search for modified equations to construct new integrators of weak order three or more with good stability or geometric properties.

We note that this new approach also allows to construct higher order Chebyshev methods for stiff SDEs. An attempt to generalize such methods, introduced in [1, 2], to higher order has been proposed in [7]. This generalization involves the solution of a large number of order

⁷Notice that $\|\omega\|$ denotes the norm of the quaternion ω , thus $\omega/\|\omega\|$ is a quaternion of norm 1.

conditions and the resulting methods appear to have less favorable stability properties than the method proposed in [1, 2]. In [3], we show that using techniques based on modifying equations as proposed in this paper, it is possible to construct high weak order Chebyshev method in an efficient way with better stability properties than the method given in [7].

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