

Postprocessed integrators for the high order integration of ergodic SDEs

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Abstract

The concept of effective order is a popular methodology in the deterministic literature for the construction of efficient and accurate integrators for differential equations over long times. The idea is to enhance the accuracy of a numerical method by using an appropriate change of variables called the processor. We show that this technique can be extended to the stochastic context for the construction of new high order integrators for the sampling of the invariant measure of ergodic systems. The approach is illustrated with modifications of the stochastic θ -method applied to Brownian dynamics, where postprocessors achieving order two are introduced. Numerical experiments, including stiff ergodic systems, illustrate the efficiency and versatility of the approach.

Keywords: stochastic differential equations, effective order, postprocessor, modified differential equations, invariant measure, ergodicity.

AMS subject classification (2010): 65C30, 60H35, 37M25

1 Introduction

A popular technique in the deterministic literature for the construction of efficient and high order integrators for differential equations is the notion of effective order of Butcher [10]. Inspired by this idea, we introduce in this paper a new methodology for the construction of high order integrators for the invariant measure of ergodic systems of stochastic differential equations (SDEs). Given a deterministic problem

$$\frac{dy(t)}{dt} = f(y(t)), \quad (1)$$

with a smooth vector field $f : \mathbb{R}^d \rightarrow \mathbb{R}^d$, the idea is to search for a computationally efficient integrator K_h for (1), named the kernel, and perturbations of the identity map χ_h and χ_h^{-1} , inverse of each other, and called respectively the postprocessor and preprocessors, such that the integrator $y_{n+1} = \Phi_h(y_n)$ defined by

$$\Phi_h = \chi_h \circ K_h \circ \chi_h^{-1}$$

has a higher order of accuracy than K_h . Considering a constant stepsize h yields

$$\Phi_h^N = \chi_h \circ K_h^N \circ \chi_h^{-1}, \quad (2)$$

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which means that N compositions of Φ_h can be efficiently implemented by applying N steps of the kernel K_h and only once the processor maps χ_h^{-1}, χ_h , respectively at the beginning and the end of the integration. This approach is efficient if the computational cost of the kernel K_h is cheaper than the cost of Φ_h . It was first introduced in [10] as a mean to construct 5th order explicit Runge-Kutta methods with only 5 internal stages, corresponding to the number of function evaluations per time step. A renewed interest for this idea appeared in the context of deterministic geometric numerical integration [35, 23, 13], where the use of a constant stepsize is required in general, for the construction of high order integrators with a favourable long time behaviour (see e.g. [13, Sect. V.3.3] and references therein).

In this paper, we consider a system of (Itô) stochastic differential equations

$$dX(t) = f(X(t))dt + g(X(t))dW(t), \quad X(0) = X_0, \quad (3)$$

where $f : \mathbb{R}^d \rightarrow \mathbb{R}^d$ and $g : \mathbb{R}^d \rightarrow \mathbb{R}^{d \times m}$ are smooth fields assumed globally Lipschitz for simplicity, and $W(t) = (W_1(t), \dots, W_m(t))^T$ is a standard m -dimensional Wiener process. Under appropriate smoothness and growth assumptions on the fields f, g , one can show that (9) has ergodic dynamics, i.e. for an arbitrary initial condition $X_0 = x$, assumed deterministic for simplicity, the time average of the trajectory satisfies with probability 1,

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \phi(X(t)) dt = \int_{\mathbb{R}^d} \phi(y) d\mu(y).$$

for all smooth test functions ϕ with derivatives at all orders with polynomial growth. In addition, in many situations, one can show the following exponential ergodicity property for all $t \geq 0$,

$$\left| \mathbb{E}(\phi(X(t))) - \int_{\mathbb{R}^d} \phi(y) d\mu(y) \right| \leq K(x) e^{-\lambda t} \quad (4)$$

where $\lambda > 0$ is independent of x, t and $K(x)$ depends on ϕ and the initial condition $X_0 = x$ (assume deterministic for simplicity), but is independent of t .

Consider a one-step numerical integrator for (3),

$$X_{n+1} = \Psi(X_n, h, \xi_n). \quad (5)$$

We say that numerical method X_n for the approximation of (9) at time $t_n = nh$ is ergodic if it has a unique invariant probability law μ^h with finite moments of any order and with probability 1,

$$\lim_{N \rightarrow \infty} \frac{1}{N+1} \sum_{n=0}^N \phi(X_n) = \int_{\mathbb{R}^d} \phi(y) d\mu^h(y), \quad (6)$$

for all initial condition $X_0 = x$ and all test functions ϕ . We say that the scheme has order $r \geq 1$ with respect to the invariant measure if

$$|e(\phi, h)| \leq Ch^r \quad \text{with} \quad e(\phi, h) := \lim_{N \rightarrow \infty} \frac{1}{N+1} \sum_{n=0}^N \phi(X_n) - \int_{\mathbb{R}^d} \phi(y) d\mu(y), \quad (7)$$

where C is independent of h small enough and X_0 . Analogously to (4), in many situations, one can show for all $t_n = nh$ and all initial condition $X_0 = x$, the estimate

$$\left| \mathbb{E}(\phi(X_n)) - \int_{\mathbb{R}^d} \phi(y) d\mu(y) \right| \leq K(x) e^{-\lambda t_n} + Ch^r \quad (8)$$

where $C, K(x)$ are independent of n, h .

A standard approach for the construction of integrators with high order for the invariant measure is to design methods with high weak order of accuracy. This is known for large classes of ergodic SDEs in particular for a degenerate noise and locally Lipschitz fields in [25]. This can be combined with extrapolation techniques from Talay [37]. It is known, however, that high order can still be achieved using low weak order methods, as shown in particular for certain classes of splitting methods for nonlinear Langevin dynamics [20, 21, 5, 4]. We also mention the exact schemes based on Markov Chain Monte-Carlo methods, see e.g. the survey [34]. An approach proposed in [3, 4] permits to design methods with a high order for the invariant measure despite a low deterministic order of accuracy. It relies on recent developments in the stochastic context [1, 39, 11, 18, 19] of the theory of backward error analysis and modified differential equations, a fundamental tool in the field of deterministic geometric numerical integration [35, 23, 13]. In the same spirit, the proposed approach of postprocessed integrators, based on Butcher's effective order [10], relies on many ideas from [3].

We shall illustrate our approach at the example of Brownian dynamics generated by the overdamped Langevin equation

$$dX(t) = -\nabla V(X(t))dt + \sigma dW(t), \quad (9)$$

where $V : \mathbb{R}^d \rightarrow \mathbb{R}$ is a smooth potential, $\sigma > 0$ is a constant, and $W = (W_1, \dots, W_d)^T$ is a standard d -dimensional Wiener process. This model describes the motion of a particle in a potential subject to thermal noise [31, 12]. Under appropriate assumptions on the potential V , the system is ergodic and has a unique invariant measure μ which is characterized by the Gibbs density function (sometimes called the Boltzmann density function)

$$\rho(x) = Ze^{-\frac{2}{\sigma^2}V(x)}, \quad (10)$$

where Z is a renormalization constant such that $\int_{\mathbb{R}^d} \rho(y)dy = 1$. We show that our approach is closely related to an efficient non-Markovian method of order two proposed in [20] for (9), with convergence properties first analyzed in [22]. It was obtained considering the large friction limit in a particular splitting method for Langevin dynamics. We show in this paper that this scheme can be interpreted as Markovian up to a change of variable, which is precisely the postprocessor map.

This paper is organized as follows. In Section 2, we introduce our new methodology to extend Butcher's effective order technique to the stochastic context and we provide examples of postprocessed integrators. In Section 3, we recall standard assumptions that guaranty the ergodicity of the system and we state the assumptions on the numerical methods needed for our analysis. In Section 4, we state our main results and derive conditions on a postprocessor to achieve high order for the invariant measure of a given integrator with emphasis on the case of Brownian dynamics. Finally, the Section 5 is devoted to the numerical experiments, and shows the efficiency and versatility of the approach for various stiff and nonstiff Brownian dynamics models.

2 Postprocessed integrators

In this section, we describe the idea of postprocessed integrators for an ergodic system of SDEs (3). Given a smooth test function ϕ , we recall that there are two standard strategies

when computing ergodic averages $\int_{\mathbb{R}^d} \phi(y) d\mu(y)$ using a one step integrator (5) to compute numerical realizations of (3).

1. Given an initial condition X_0 , one can consider a single numerical trajectory X_0, X_1, X_2, \dots over a long time interval of size $T = Nh$, and then compute the approximation

$$\frac{1}{N+1} \sum_{k=0}^N \phi(X_k) \simeq \int_{\mathbb{R}^d} \phi(y) d\mu(y),$$

taking advantage of the estimate (7).

2. Alternatively, one can compute a large number M of independent numerical trajectories $\{X_0^i, X_1^i, X_2^i, \dots, X_N^i\}$, $i = 1 \dots, M$ on a relatively shorter time interval $T = Nh$ and use the approximation

$$\frac{1}{M} \sum_{i=1}^M \phi(X_N^i) \simeq \int_{\mathbb{R}^d} \phi(y) d\mu(y),$$

based on the exponential estimate (8). The advantage of this second approach, as shown in [28] in the context of ergodic SDEs, is that it permits to treat easily the case of non-globally Lipschitz vector fields using standard integrators (in particular explicit ones) by using *the concept of rejecting exploding trajectories*, a rigorous methodology introduced in [29]. This procedure is often preceded by an equilibration period to make the law of X_0^i close to the invariant measure μ , see e.g. [28] for details.

The idea of postprocessed integrators is to consider an integrator (5) with order r for the invariant measure in (7) and (8), and to search for a postprocessor $\bar{X}_n = G_n(X_n)$, which can be a deterministic or a stochastic perturbation of X_n , such that \bar{X}_n has a higher order of accuracy $\bar{r} > r$ for the invariant measure. Precisely, for all h assumed small enough, and all $t_n = nh$,

$$\left| \lim_{N \rightarrow \infty} \frac{1}{N+1} \sum_{k=0}^N \phi(\bar{X}_k) - \int_{\mathbb{R}^d} \phi(y) d\mu(y) \right| \leq Ch^{\bar{r}} \quad (11)$$

$$\left| \mathbb{E}(\phi(\bar{X}_n)) - \int_{\mathbb{R}^d} \phi(y) d\mu(y) \right| \leq K(x) e^{-\lambda t_n} + Ch^{\bar{r}}, \quad (12)$$

where C, λ are independent of h, n and the initial condition $X_0 = x$, and $K(x)$ is independent of h, n .

If ergodic averages are computed using the estimate (11), then the postprocessor $\bar{X}_k = G_k(X_k)$ is applied at every time step k , but it has a negligible overcost in some situations where no additional function evaluations are needed as shown below. In addition \bar{X}_k can always be computed in parallel with X_{k+1} , independently. If alternatively, ergodic averages are approximated based on the exponential estimate (12), then the postprocessor $\bar{X}_N = G_N(X_N)$ is applied only once at the end time $t_N = Nh$ of each numerical trajectory, resulting in a negligible overhead.

Remark 2.1. Compared to the deterministic setting (2), G_n plays the role of the post-processor map χ_h . In contrast, notice however that no preprocessor χ_h^{-1} is involved in the stochastic setting. This is not surprising because the limit $\mathbb{E}(\phi(\bar{X}(t))) \rightarrow \int_{\mathbb{R}^d} \phi(y) \mu(y) dy$ for

$t \rightarrow \infty$ is independent of the initial condition $X_0 = x$. In other words, the ergodic systems “forgets” the initial condition. The advantage compared to the deterministic case is that the postprocessor map G_n needs not to be reversible, it can be in particular the flow of a stiff deterministic problem, or even a stochastic problem.

To illustrate our new approach, we focus on the problem of Brownian dynamics (9), and we consider the standard stochastic θ -method

$$X_{n+1} = X_n + h(1 - \theta)f(X_n) + h\theta f(X_{n+1}) + \sigma\sqrt{h}\xi_n, \quad (13)$$

where $f = -\nabla V$ and $\xi_n \sim \mathcal{N}(0, I)$ are independent Gaussian random vectors with dimension d . For $\theta = 0$, it reduces to the Euler-Maruyama method, while for $\theta \neq 0$, the method is implicit and requires in general the resolution of a non-linear system at each timestep. For $\theta \geq 1/2$, it is shown in [17] that the θ -method is mean-square A -stable, a property which makes it well-suited for stiff mean-square stable stochastic problems. This scheme has weak order one of accuracy, except in the special case $\theta = 1/2$ for which the weak order of the method is two. It was shown in [36] that the θ -method preserves exactly the invariant measure in the linear case if and only if $\theta = 1/2$ (i.e. for $V(x)$ a quadratic function in (9), which corresponds to an Ornstein-Uhlenbeck process). This result was extended in [8] for linear second order problems with additive noise, where it was shown that the $\theta = 1/2$ -method is in fact the only measure exact scheme in a certain class of stochastic Runge-Kutta methods involving only one Wiener increment per step.

For multi-dimensional nonlinear problems of the form (9), we introduce the following postprocessed methods of order 2 for the invariant measure based on modifications of the θ -method (13). Precisely, we prove in Section 4 that for each method below, \bar{X}_n has order $\bar{\tau} = 2$ for the invariant measure in (11),(12). For $\theta = 0$, we obtain the following modification of the Euler-Maruyama method, which is equivalent to a method first proposed in [20] (see (18) below)

$$X_{n+1} = X_n + hf\left(X_n + \frac{1}{2}\sigma\sqrt{h}\xi_n\right) + \sigma\sqrt{h}\xi_n, \quad \bar{X}_n = X_n + \frac{1}{2}\sigma\sqrt{h}\xi_n. \quad (14)$$

For $\theta = 1$, we derive the new scheme

$$X_{n+1} = X_n + hf(X_{n+1} + a\sigma\sqrt{h}\xi_n) + \sigma\sqrt{h}\xi_n, \quad a = -\frac{1}{2} + \frac{\sqrt{2}}{2}, \quad (15)$$

together with two possible postprocessors

$$\bar{X}_n = X_n + c\sigma\sqrt{h}J_n^{-1}\xi_n, \quad c = \frac{\sqrt{2\sqrt{2}-1}}{2} \quad (16)$$

and alternatively,

$$\bar{X}_n = X_n + hbf(\bar{X}_n) + c\sigma\sqrt{h}\xi_n, \quad b = \frac{\sqrt{2}}{2}, \quad c = \frac{\sqrt{4\sqrt{2}-1}}{2}. \quad (17)$$

The matrix J_n^{-1} in (16) is defined as the inverse of the $d \times d$ Jacobian matrix

$$J_n = I - hf'(X_n + a\sigma\sqrt{h}\xi_{n-1}).$$

Remark 2.2. The matrix J_n is involved in standard Newton iterations needed to solve the nonlinear system (15). For an efficient implementation, it is known that one should never compute the inverse J_n^{-1} itself but rather solve the appropriate linear systems. Using a precomputed LU decomposition of this matrix, the evaluation of $J_n^{-1}\xi_n$ in (16) therefore has a negligible cost. This term is introduced only to improve the numerical stability and does not influence the order 2 of accuracy of the postprocessed method (15),(16), as discussed in Section 4 (Theorem 4.6). The use of Jacobian matrices such as J_n for stabilization is classical for stiff deterministic problems [14, Sect. IV.8], and reveals efficient also in the context of mean-square stable stiff SDEs in [2].

Substituting $X_n = \bar{X}_n - \frac{1}{2}\sigma\sqrt{h}\xi_n$ in (14), a calculation shows that the scheme (14) is equivalent to the method

$$\bar{X}_{n+1} = \bar{X}_n + hf(\bar{X}_n) + \frac{1}{2}\sigma\sqrt{h}(\xi_n + \xi_{n+1}). \quad (18)$$

The scheme (18) of order two, which has the same cost as the standard Euler-Maruyama method of order one, was first introduced in [20] as a non-Markovian method. A rigorous analysis of its order two of convergence for the numerical invariant measure of (9) was first proposed in [22]. Notice that the point of view of postprocessed integrators provides here an alternative proof of the order two of accuracy of the scheme (18). Analogously, notice that a non-Markovian formulation of the postprocessed method (15),(16) can also be written,

$$\bar{X}_{n+1} = \bar{X}_n + hf(\bar{X}_{n+1} + \sigma\sqrt{h}(a\xi_n - c\xi_{n+1})) + \sigma\sqrt{h}((1-c)\xi_n + c\xi_{n+1}),$$

where a, c are defined in (15),(16), and we omit for simplicity the stabilization term J_n .

3 Background

We recall in this section standard results and assumptions that will be useful for the analysis of postprocessed integrators in Section 4. We assume that f, g in (3) are smooth fields and we focus for simplicity on the case of globally Lipchitz vector fields.

We denote $\mathcal{C}_P^\infty(\mathbb{R}^d, \mathbb{R})$ the set of \mathcal{C}^∞ functions whose derivatives up to any order have a polynomial growth of the form

$$|\phi(x)| \leq C(1 + |x|^s) \quad (19)$$

for some constants s and C independent of x . A classical fundamental tool for the analysis of (3) is the backward Kolmogorov equation [27, Chap. 2]. Given $\phi \in \mathcal{C}_P^\infty(\mathbb{R}^d, \mathbb{R})$ and setting $u(t, x) = \mathbb{E}(\phi(X(t)) | X_0 = x)$, it yields that $u(x, t)$ is the solution of the deterministic parabolic PDE

$$\frac{\partial u}{\partial t} = \mathcal{L}u, \quad u(x, 0) = \phi(x), \quad x \in \mathbb{R}^d, t > 0, \quad (20)$$

where the generator \mathcal{L} is defined by

$$\mathcal{L}\phi := f \cdot \nabla\phi + \frac{1}{2}gg^T : \nabla^2\phi, \quad (21)$$

where $\nabla\phi$ and $\nabla^2\phi$ are the gradient vector and the Hessian matrix of ϕ , and $A : B = \text{trace}(A^T B)$ is a scalar product on matrices.

Assumption 3.1. *We assume the following.*

1. f, g are of class C^∞ , with bounded derivatives of any order, and g is bounded;
2. the generator \mathcal{L} in (21) is a uniformly elliptic operator, i.e. there exists $\alpha > 0$ such that for all $x, \xi \in \mathbb{R}^d$, $x^T g(\xi) g(\xi)^T x \geq \alpha x^T x$;
3. there exist $C, \beta > 0$ such that for all $x \in \mathbb{R}^d$, $x^T f(x) \leq -\beta x^T x + C$.

Assumption 3.1 implies automatically that (3) is ergodic with a unique invariant measure (see e.g. [15]) and satisfies the exponential ergodicity property (4). Notice that hypo-elliptic generators \mathcal{L} could also be considered, to include the case of Langevin dynamics. We obtain for all $\phi \in \mathcal{C}_P^\infty(\mathbb{R}^d, \mathbb{R})$ the identity

$$\lim_{t \rightarrow \infty} u(x, t) = \phi(x) + \int_0^\infty \mathcal{L}u(t, x) dt = \int_{\mathbb{R}^d} \phi(y) \rho(y) dy. \quad (22)$$

Considering L^2 -adjoint of the generator \mathcal{L} , given by

$$\mathcal{L}^* \phi = -\operatorname{div}(f\phi) + \frac{1}{2} g g^T : \nabla^2 \phi, \quad (23)$$

we recall that the density ρ of the invariant measure μ of (3) is the unique solution of

$$\mathcal{L}^* \rho = 0. \quad (24)$$

We make the following assumptions on the one step integrator (5). For $\phi \in \mathcal{C}_P^\infty(\mathbb{R}^d, \mathbb{R})$, consider the quantity

$$U(x, h) = \mathbb{E}(\phi(X_1) | X_0 = x). \quad (25)$$

We assume that the scheme has local weak order p i.e. it satisfies for all initial condition $X_0 = x$,

$$|\mathbb{E}(\phi(X_1)) - \mathbb{E}(\phi(X(h)))| \leq C(x) h^{p+1}, \quad (26)$$

for all h sufficiently small, where $C(x)$ is independent of h but depends on x, ϕ .

Assumption 3.2. *We assume that (25) has a weak Taylor series expansion of the form,*

$$U(x, h) = \phi(x) + h A_0 \phi(x) + h^2 A_1 \phi(x) + \dots, \quad (27)$$

for all $\phi \in \mathcal{C}_P^\infty(\mathbb{R}^d, \mathbb{R})$, where A_i , $i = 0, 1, 2, \dots$ are linear differential operators with coefficients depending smoothly on the drift and diffusion functions f, g , and their derivatives (and depending on the choice of the integrator). In addition, we assume that A_0 coincides with the generator \mathcal{L} given in (21), which means that the method has (at least) local order one in the weak sense,

$$A_0(f, g) = \mathcal{L}. \quad (28)$$

For instance, for the θ -method (13) applied to (9), a calculation shows

$$\begin{aligned} A_1 \phi &= \frac{1}{2} \phi''(f, f) + \frac{\sigma^2}{2} \sum_{i=1}^d \phi'''(e_i, e_i, f) + \frac{\sigma^4}{8} \sum_{i,j=1}^d \phi^{(4)}(e_i, e_i, e_j, e_j) + \theta \phi' f' f \\ &+ \theta \frac{\sigma^2}{2} \phi' \sum_{i=1}^d f''(e_i, e_i) + \theta \sigma^2 \sum_{i=1}^d \phi''(f' e_i, e_i), \end{aligned} \quad (29)$$

where e_1, \dots, e_d is the canonical basis of \mathbb{R}^d , and $\phi'(x), \phi''(x), \phi'''(x), \dots$ are the derivatives of ϕ , which are linear, bilinear, trilinear, \dots , forms, respectively (and analogously for f). We refer to [39, 1] for examples of similar calculations. We shall also use the following assumption [26] (see [27, Chap. 2.2]) which permits to guaranty that the numerical moments $\mathbb{E}(|X_n|^k)$ up to any order k are bounded along time. This also permits to infer automatically “a global weak order p ” from the local weak error (26) of a given integrator, see [27, Chap. 2.2].

Assumption 3.3. *We assume that the numerical integrator (3) satisfies for all $x \in \mathbb{R}^d$ that*

$$|\mathbb{E}(X_1 - X_0 | X_0 = x)| \leq C(1 + |x|)h, \quad |X_1 - X_0| \leq M(1 + |X_0|)\sqrt{h}, \quad (30)$$

where C is independent of h small enough and M is a random variable that has bounded moments of all orders independent of h and X_0 .

Theorem 3.4 below is standard and combines results derived by Talay and Milstein. Precisely, it has been proved in [37] for specific methods (the Euler-Maruyama and the Milstein methods), while the general procedure to infer the global weak order from the local weak order is due to Milstein [26] and can be found in [27, Chap. 2.2, 2.3]. The proof of Theorem 3.4 is thus omitted.

Theorem 3.4. [37, 26] *Let X_N be an ergodic numerical solution of (3) on $[0, T]$ and assume Assumption 3.1, Assumption 3.2, Assumption 3.3. Assume further the local weak order p estimate (26) where $C(x)$ has a polynomial growth of the form (19). Then, the invariant measure error in (7) satisfies for all $\phi \in \mathcal{C}_p^\infty(\mathbb{R}^d, \mathbb{R})$ and $h \rightarrow 0$,*

$$e(\phi, h) = \lambda_p h^p + \mathcal{O}(h^{p+1}) \quad (31)$$

for any deterministic initial condition, with λ_p defined as

$$\lambda_p = \int_0^{+\infty} \int_{\mathbb{R}^d} \left(A_p - \frac{1}{(p+1)!} \mathcal{L}^{p+1} \right) u(y, t) \rho(y) dy dt \quad (32)$$

where $u(x, t)$ is the solution of (20). In addition, there exists constants $\lambda, C, K(x) > 0$ such that for all $n \geq 0$,

$$\left| \mathbb{E}(\phi(X_n)) - \int_{\mathbb{R}^d} \phi(y) d\mu(y) - \lambda_p h^p \right| \leq K(x) e^{-\lambda t_n} + C h^{p+1} \quad (33)$$

where $t_n = nh$, the constants $C, K(x), \lambda$ are independent of n, h , and h is assumed small enough ($C, K(x)$ depend on ϕ and $K(x)$ depends on x).

In fact, the assumption that the integrator has weak order p in Theorem 3.4 can be relaxed, as explain in the following remark.

Remark 3.5. *Using $\mathcal{L}^* \rho = 0$ and considering the L^2 -adjoint¹ A_p^* of the linear differential operator A_p , we deduce that λ_p in (32) satisfies*

$$\lambda_p = \int_0^{+\infty} \int_{\mathbb{R}^d} u(y, t) A_p^* \rho(y) dy dt.$$

¹For instance, for the Euler-Maruyama method, setting $\theta = 0$ in (29) and using the notation Δ for the Laplace operator, we obtain $A_1 \phi = \frac{1}{2} \phi''(f, f) + \frac{\sigma^2}{2} (\Delta \phi)' f + \frac{\sigma^4}{8} \Delta^2 \phi$ and

$$A_1^* \phi = \frac{1}{2} \operatorname{div} (\phi(f' f + \operatorname{div}(f) f) + \|f\|^2 \nabla \phi - \sigma^2 f \Delta \phi) + \frac{\sigma^4}{8} \Delta^2 \phi.$$

We see that if $A_p^* \rho = 0$, then the scheme has order $p + 1$ for the invariant measure. More generally, it is shown in [3] based on backward error analysis results in [11] on the torus and generalizations [18, 19] in \mathbb{R}^d that the (local) weak order p assumption (26) in Theorem 3.4 (equivalent to $A_{j+1} = \mathcal{L}^j/j!$ for all $j < p$ in Assumption 3.2) can be replaced by the more general condition

$$A_j^* \rho = 0, \quad \text{for } j = 1, \dots, p-1. \quad (34)$$

This permits to derive in [3] new high order integrators based on modified differential equations while it serves in [4] as a tool for the analysis of the order of convergence of Lie-Trotter splitting methods applied to Langevin dynamics.

4 Analysis of postprocessed integrators

This section is devoted to the analysis of postprocessed integrators. To illustrate our approach, we first study the simplest linear case of the Orstein-Uhlenbeck process in dimension one. We then focus on the analysis for nonlinear problems, with special emphasis on the case of Brownian dynamics.

4.1 Accuracy and stability analysis in the linear case

We consider for simplicity the Orstein-Uhlenbeck process in dimensions $d = m = 1$,

$$dX = -\gamma X dt + \sigma dW(t), \quad (35)$$

where $\gamma, \sigma > 0$ are fixed constants. It corresponds to Brownian dynamics (9) with $V(x) = \frac{\gamma}{2}x^2$. For all initial condition $X_0 = x$, the exact solution $X(t)$ is a Gaussian random variable with $\lim_{t \rightarrow \infty} \mathbb{E}(X(t)^2) = \frac{\sigma^2}{2\gamma}$. Indeed, this system is ergodic and its invariant measure is Gaussian, with density

$$\rho(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{\gamma}{2\sigma^2}x^2}.$$

Since the invariant measure is Gaussian, the error is obtained simply by comparing the exact and numerical variances. Applying a one step numerical method to (35), in particular a Runge-Kutta method, yields in general a recursion of the form

$$X_{n+1} = A(z)X_n + B(z)\sqrt{h}\sigma\xi_n, \quad (36)$$

where $z = -\gamma h$ and $A(z) = 1 + z + \mathcal{O}(z^2)$ and $B(z) = 1 + \mathcal{O}(z)$ are analytic functions depending on the choice of the method and $\xi_n \sim \mathcal{N}(0, 1)$ are independent Gaussian random variables. Then, a calculation using the recursion $\mathbb{E}(X_{n+1}^2) = \mathbb{E}(X_n^2)A(z)^2 + B(z)^2\sigma^2h$ yields

$$\lim_{n \rightarrow \infty} \mathbb{E}(X_n^2) = \frac{\sigma^2}{2\gamma} |R(z)|, \quad \text{where } R(z) = \frac{2zB(z)^2}{A(z)^2 - 1}, \quad z = -\gamma h, \quad (37)$$

for all h small enough such that $|A(z)| < 1$ (stable stepsize), and $\lim_{n \rightarrow \infty} \mathbb{E}(X_n^2) = \infty$ if $|A(z)| > 1$ and $\mathbb{E}(X_0^2) \neq 0$ (unstable stepsize).

Stability for linear problems We recall here useful standard stability results. The scalar linear SDE (35) can be considered as a test equation which gives insight on the behavior for nonlinear problem with additive noise. Notice that other test equations are used in the literature in the case of multiplicative noise, see [32, 17, 33, 7, 38, 30, 6].

We see from the above discussion that $\mathbb{E}(X_n^2)$ remains bounded as $n \rightarrow \infty$ (mean-square stability) if $|A(z)| < 1$. For the θ method, it can be checked [17, 16] that this is satisfied for all stepsize $h > 0$ if and only if $\theta \geq 1/2$, while for the Euler-Maruyama method ($\theta = 0$), we have the stepsize restriction $h\gamma < 2$ which can be a severe restriction for large values of γ . This stability property for all complex γ with positive real part, unconditionally on the stepsize h , is called A -stability in the framework of deterministic Runge-Kutta methods [14]. This makes the θ -method with $\theta \geq 1/2$ well suited for stiff stochastic problems, in contrast to the Euler-Maruyama method. We have the additional feature $\lim_{\gamma \rightarrow +\infty} \mathbb{E}(X_1^2) = 0$ for all $X_0 = x$ if and only if $\theta = 1$, a property called L -stability in the setting of deterministic Runge-Kutta-methods ($\sigma = 0$), and that is also important in the context of mean-square stable stiff SDEs [2]. The L -stability property is desirable for severely stiff problems with very large eigenvalues on the negative real axis, because it permits to damp the higher modes. We emphasize that the L -stability property $\lim_{\gamma \rightarrow +\infty} \mathbb{E}(\bar{X}_1^2) = 0$ is also satisfied for the postprocessed methods (15),(16) and (15),(17).

Accuracy analysis We see from (37) that the method (without postprocessor) has order p for the Gaussian invariant measure if and only if $R(z) = 1 + \mathcal{O}(z^p)$ for $z \rightarrow 0$. Applying a corrector $\bar{X}_n = G_n(X_n)$ of the form

$$G_n(x) = C(z)x + D(z)\sqrt{h}\sigma\xi_n, \quad z = -\gamma h,$$

where $C(z) = 1 + \mathcal{O}(z)$ does not affect the mean-square stability of \bar{X}_n , we obtain

$$\lim_{n \rightarrow \infty} \mathbb{E}(\bar{X}_n^2) = \frac{\sigma^2}{2\gamma} C(z)^2 |R(z)| + h\sigma^2 D(z)^2, \quad z = -\gamma h.$$

Comparing with the exact solution for which $\lim_{t \rightarrow \infty} \mathbb{E}(X(t)^2) = \frac{\sigma^2}{2\gamma}$, we deduce that the method has order p for the invariant measure of the Orstein-Uhlenbeck process if and only if the above limit is $\frac{\sigma^2}{2\gamma} + \mathcal{O}(h^p)$, equivalently

$$R(z)C(z)^2 - 2zD(z)^2 = 1 + \mathcal{O}(z^p), \quad z \rightarrow 0. \quad (38)$$

It turns out that the above identity holds exactly for the postprocessed scheme (14) for which $A(z) = 1 + z$, $B(z) = 1 + z/2$, $C(z) = 1$, $D(z) = 1/2$. This yields the following remark which states that the explicit postprocessed scheme (14) (equivalently (18) from [20]) has no bias in sampling the invariant measure for all stepsize h , a feature in the linear case shared with the implicit $\theta = 1/2$ -method [36].

Remark 4.1. *The postprocessed scheme (14) applied to Brownian dynamics (9) samples exactly the invariant measure in the case of a linear drift (i.e. if $V(x)$ is a quadratic function on \mathbb{R}^d).*

In [9], in the context of linear second order problems, new s -stage explicit Runge-Kutta methods are introduced with high order in the velocity correlation matrix with accuracy $\mathcal{O}(h^s)$ for $s = 3, 4, 5$, respectively. In the same spirit, we make the following remark which

states using (38) that there always exist postprocessors achieving arbitrarily high order for sampling the invariant measure for all consistent integrators applied to the Orstein-Uhlenbeck process.

Remark 4.2. *Given a consistent method of the form (36) for (35), for arbitrary integer s , there exists a deterministic postprocessor of the form $\bar{X}_n = C(-\gamma h)X_n$ where $C(z) = R(z)^{-1/2} + \mathcal{O}(z^s)$ is a polynomial of degree strictly less than s (corresponding in particular to an $(s-1)$ -stage explicit Runge-Kutta method) such that the corresponding postprocessed scheme has order s for the invariant measure. For instance, for the Euler-Maruyama method (see (13) with $\theta = 0$), we obtain $C(z) = \sqrt{1+z/2} = 1 + z/4 - z^2/32 + \dots$*

4.2 Postprocessed integrators for nonlinear ergodic SDEs

We may now state the main result of this paper for the analysis of postprocessed integrators. We shall use the commutator notation $[A, B] = AB - BA$ on linear differential operators.

Theorem 4.3. *Assume the hypotheses of Theorem 3.4 and consider a numerical method $\{X_n\}_{n \geq 0}$ with weak order p . Let G_n denote independent and identically distributed random maps in \mathbb{R}^d , independent of $\{X_j\}_{j \leq n}$ and satisfying (30) with X_1 replaced by $G_1(X_0)$ and a weak Taylor expansion of the form*

$$\mathbb{E}(\phi(G_n(x))) = \phi(x) + h^p \bar{A}_p \phi(x) + \mathcal{O}(h^{p+1}), \quad (39)$$

for all $\phi \in \mathcal{C}_P^\infty(\mathbb{R}^d, \mathbb{R})$, where the constant in \mathcal{O} has a polynomial growth with respect to x of the form (19). Assuming further

$$(A_p + [\mathcal{L}, \bar{A}_p])^* \rho = 0, \quad (40)$$

then $\bar{X}_n = G_n(X_n)$ yields an approximation of order $p+1$ for the invariant measure, precisely

$$\left| \lim_{N \rightarrow \infty} \frac{1}{N+1} \sum_{k=0}^N \phi(\bar{X}_k) - \int_{\mathbb{R}^d} \phi(y) d\mu(y) \right| \leq Ch^{p+1} \quad (41)$$

$$\left| \mathbb{E}(\phi(\bar{X}_n)) - \int_{\mathbb{R}^d} \phi(y) d\mu(y) \right| \leq K(x) e^{-\lambda t_n} + Ch^{p+1}, \quad (42)$$

for all $\phi \in \mathcal{C}_P^\infty(\mathbb{R}^d, \mathbb{R})$ with $t_n = nh$, where $C, K(x)$ are independent of n and h assumed small enough but depend of ϕ (and $K(x)$ depends on the initial condition $X_0 = x$).

Proof. Using (39) yields

$$\mathbb{E} \left(\int_{\mathbb{R}^d} \phi(G_n(y)) \rho(y) dy \right) = \int_{\mathbb{R}^d} \phi(y) \rho(y) dy + h^p \int_{\mathbb{R}^d} \phi(y) \bar{A}_p^* \rho(y) dy + \mathcal{O}(h^{p+1}),$$

and we obtain from (22),

$$\begin{aligned} \int_{\mathbb{R}^d} \phi(y) \bar{A}_p^* \rho(y) dy &= - \int_0^\infty \int_{\mathbb{R}^d} \mathcal{L} u(t, y) \bar{A}_p^* \rho(y) dy dt = \int_0^\infty \int_{\mathbb{R}^d} [\mathcal{L}, \bar{A}_p] u(t, y) \rho(y) dy dt \\ &= - \int_{\mathbb{R}^d} A_p \phi(y) \rho(y) dy = -\lambda_p \end{aligned}$$

where λ_p is defined in (32), and we used assumption (40) and $\mathcal{L}^*\rho = 0$ (see (24)). We deduce

$$\mathbb{E} \left(\int_{\mathbb{R}^d} \phi(G_n(y)) \rho(y) dy \right) = \int_{\mathbb{R}^d} \phi(y) \rho(y) dy - h^p \lambda_p + \mathcal{O}(h^{p+1}), \quad (43)$$

We now apply Theorem 3.4 where ϕ is replaced by $\phi \circ G_n = \phi + \mathcal{O}(h)$. We deduce using (33) and properties of conditional expectations that $\bar{X}_n = G_n(X_n)$ satisfies

$$\left| \mathbb{E}(\phi(\bar{X}_n)) - \mathbb{E} \left(\int_{\mathbb{R}^d} \phi(G_n(y)) \rho(y) dy \right) - h^p \lambda_p \right| \leq K(x) e^{-\lambda t_n} + Ch^{p+1}.$$

This combined with (43) concludes the proof of (42) and analogously (41). \square

Remark 4.4. Similarly to Remark 3.5, observe in Theorem 4.3 that the (local) weak order p assumption (26) on the scheme X_n can be replaced by the more general condition (34).

Remark 4.5. Notice that in the assumptions of Theorem 4.3, the postprocessor map G_n needs not neither to involve the same random variables as $X_n \mapsto X_{n+1}$ nor to be independent from these random variables. In particular, the postprocessors \bar{X}_n in (14), (16), (17) could be defined using other independent Gaussian random variables with law $\mathcal{N}(0, I)$ instead of ξ_n . Our numerical investigations indicate that there is no benefit to generate additional random variables.

4.3 Application to Brownian dynamics

To illustrate the proposed approach, we focus on the Brownian dynamics model (9) where $f = -\nabla V$ is the gradient of a smooth potential. We assume² Assumption 3.1, which guaranties the ergodicity of the system and the exponential estimate (4).

We now consider the following modification with negligible overhead of the θ -method,

$$X_{n+1} = X_n + h(1 - \theta)f(X_n + a\sigma\sqrt{h}\xi_n) + h\theta f(X_{n+1} + a\sigma\sqrt{h}\xi_n) + \sigma\sqrt{h}\xi_n, \quad (44)$$

where a is a fixed scalar parameter, together with the postprocessor

$$\bar{X}_n = X_n + bh((1 - \theta)f(X_n) + \theta f(\bar{X}_n)) + c\sigma\sqrt{h}\xi_n, \quad (45)$$

where $\xi_n \sim \mathcal{N}(0, I)$ are independent Gaussian random vectors with dimension d , and b, c are fixed parameters. Notice that for all a , the modified θ -method (44) with $\theta \neq 1/2$ has the same order one of accuracy for the invariant measure as the standard version (13). For $a = b = c = 0$, we recover the standard θ -method (13) and $\bar{X}_n = X_n$. The following Theorem provides order conditions on a, b, c for \bar{X}_n to achieve second order of accuracy for the invariant measure.

Theorem 4.6. Assume Assumption 3.1 and consider the scheme (44) and the postprocessor (45) applied to Brownian dynamics (9). If

$$a^2 + 2\theta a + b - c^2 = 0, \quad a + b - c^2 - \frac{1}{4} + \frac{\theta}{2} = 0, \quad (46)$$

²Notice that the item 2. of Assumption 3.1 is automatically satisfied since $g(\xi)^T g(\xi) : \nabla^2 = \sigma^2 \Delta$ for the Brownian dynamics model (9), where Δ is the Laplacian operator.

then, assuming the ergodicity of $\{X_n\}$, we have

$$\begin{aligned} \left| \lim_{N \rightarrow \infty} \frac{1}{N+1} \sum_{k=0}^N \phi(\bar{X}_k) - \int_{\mathbb{R}^d} \phi(y) d\mu(y) \right| &\leq Ch^2 \\ \left| \mathbb{E}(\phi(\bar{X}_n)) - \int_{\mathbb{R}^d} \phi(y) d\mu(y) \right| &\leq K(x)e^{-\lambda t_n} + Ch^2, \end{aligned}$$

for all $\phi \in C^\infty(\mathbb{R}^d, \mathbb{R})$ with $t_n = nh$, where $C, K(x)$ are independent of n and h assumed small enough. In particular, assuming ergodicity, the postprocessed schemes (14), (15)-(16), and (15)-(17) satisfy the above estimates.

The proof of Theorem 4.6 is postponed to the Appendix. We explain here why it yields the order two of accuracy for the invariant measure of the postprocessed schemes (14), (15)-(16), and (15)-(17).

If $\theta = 0$ or $\theta \geq 1/2$, and for a given c , the order conditions (46) can be shown to have real solutions given by

$$a = \frac{1}{2} - \theta \pm \frac{\sqrt{2\theta(2\theta-1)}}{2}, \quad b = c^2 - \frac{1}{4} + \frac{\theta}{2} \mp \frac{\sqrt{2\theta(2\theta-1)}}{2}.$$

We now focus on special values of θ to construct various methods of order two for the invariant measure of (9).

- For $\theta = 0$ (Euler-Maruyama method), we obtain $a = \frac{1}{4}, b = c^2 - \frac{1}{4}$. Imposing respectively $b = 0$ and $c = 0$ yields the following postprocessed methods of order two: the method (14) from [20],

$$X_{n+1} = X_n + hf(X_n + \frac{1}{2}\sigma\sqrt{h}\xi_n) + \sigma\sqrt{h}\xi_n, \quad \bar{X}_n = X_n + \frac{1}{2}\sigma\sqrt{h}\xi_n.$$

and the variant

$$X_{n+1} = X_n + hf(X_n + \frac{1}{2}\sigma\sqrt{h}\xi_n) + \sigma\sqrt{h}\xi_n, \quad \bar{X}_n = X_n + \frac{h}{4}f(X_n).$$

- For $\theta = \frac{1}{2}$, we obtain $a = 0$ and $b = c^2$. This is not surprising because the standard θ -method (13) with $\theta = \frac{1}{2}$ is already exact for sampling the invariant measure as noted in [36], and it has weak order two when applied to SDEs with additive noise such as (9). Postprocessors for order two are therefore useless in this case.
- For $\theta = 1$, the assumption $b = 0$ yields the method (15),(16) (without the matrix J_n^{-1}) of the form

$$X_{n+1} = X_n + hf(X_{n+1} + a\sigma\sqrt{h}\xi_n) + \sigma\sqrt{h}\xi_n, \quad \bar{X}_n = X_n + c\sigma\sqrt{h}\xi_n.$$

Since the matrix J_n^{-1} in (16) is a $\mathcal{O}(h)$ perturbation of the identity, it does not change the order $p = 1$ weak expansion of the postprocessor in assumption (39) of Theorem 4.3. The method (15),(16) therefore has order two of accuracy for the invariant measure.

Imposing alternatively the condition of order 3 for linear problems (i.e. (38) with $p = 3$) yields the method (15),(17) of the form

$$X_{n+1} = X_n + hf(X_{n+1} + a\sigma\sqrt{h}\xi_n) + \sigma\sqrt{h}\xi_n, \quad \bar{X}_n = X_n + hb f(\bar{X}_n) + c\sigma\sqrt{h}\xi_n,$$

which has order two of accuracy for the invariant measure, and order three for linear problems (i.e. for a quadratic potential V).

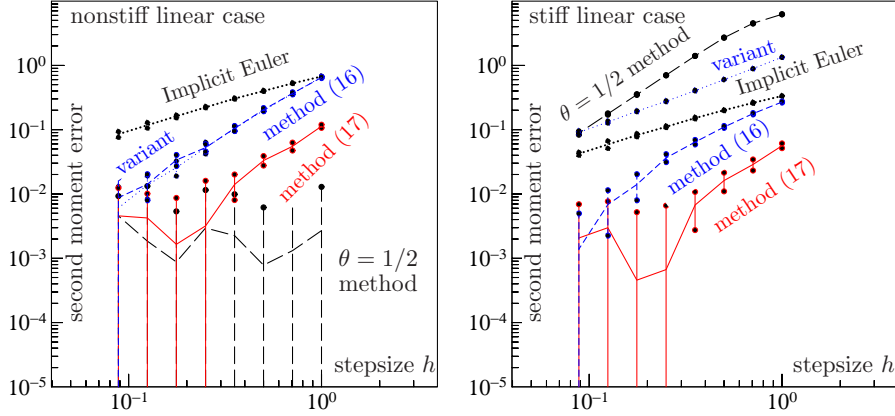


Figure 1: Linear problem with potential (47). Implicit Euler method ((13) with $\theta = 1$, order 1), $\theta = 1/2$ -method (order 2), and postprocessed versions ((15),(16) and (15),(17)) of order 2. The variant of the method (15),(16) without the stabilization term J_n^{-1} is also included. Error for the second moment $\int_{\mathbb{R}} (x_1^2 + x_2^2) \rho(x) dx$ versus time stepsize h obtained using 10 trajectories on a long time interval of length $T = 10^5$. The vertical bars indicate the standard deviation intervals due to the Monte-Carlo error.

5 Numerical experiments

In this section, we illustrate numerically the convergence properties of the new implicit schemes introduced in Section 2 for the high order sampling of the invariant measure of Brownian dynamics (9). Although our analysis applies only to globally Lipschitz vector fields, we shall consider numerical examples with non-globally Lipschitz fields, since such a regularity often arises in applications. We highlight once again that the use of the proposed schemes can still be made rigorous in this context, using the concept of rejecting exploding trajectories proposed in [29, 28].

We focus on stiff problems for which implicit methods are needed to avoid the severe step size restrictions of standard explicit integrators. We consider the standard implicit Euler method ((13) with $\theta = 1$), the standard $\theta = 1/2$ method (13), and the new postprocessed methods (15),(16) and (15),(17). We have implemented all methods in Fortran, using a Newton method with tolerance 10^{-13} to solve the nonlinear implicitness of the methods. The results for the explicit postprocessed scheme (14) from [20] are not included because a severe stepsize restriction $h \ll 1$ makes explicit methods unusable for such stiff problems (analogously to the deterministic case).

5.1 Linear test problem

We consider first the linear problem in 2D, with a quadratic potential defined by

$$V(x) = \frac{x_1^2}{2} + \frac{x_2^2}{2\varepsilon} + \frac{x_1 x_2}{4}. \quad (47)$$

For the arbitrary initial condition $x_1 = x_2 = -3$, we plot in Figure 1 the error for the second moment $\int_{\mathbb{R}} (x_1^2 + x_2^2) \rho(x) dx$ for many time stepsizes h , using the average over 10 long trajectories of length 10^5 . We compare in Figure 1 the nonstiff case ($\varepsilon = 1$) and the stiff case ($\varepsilon = 10^{-6}$).

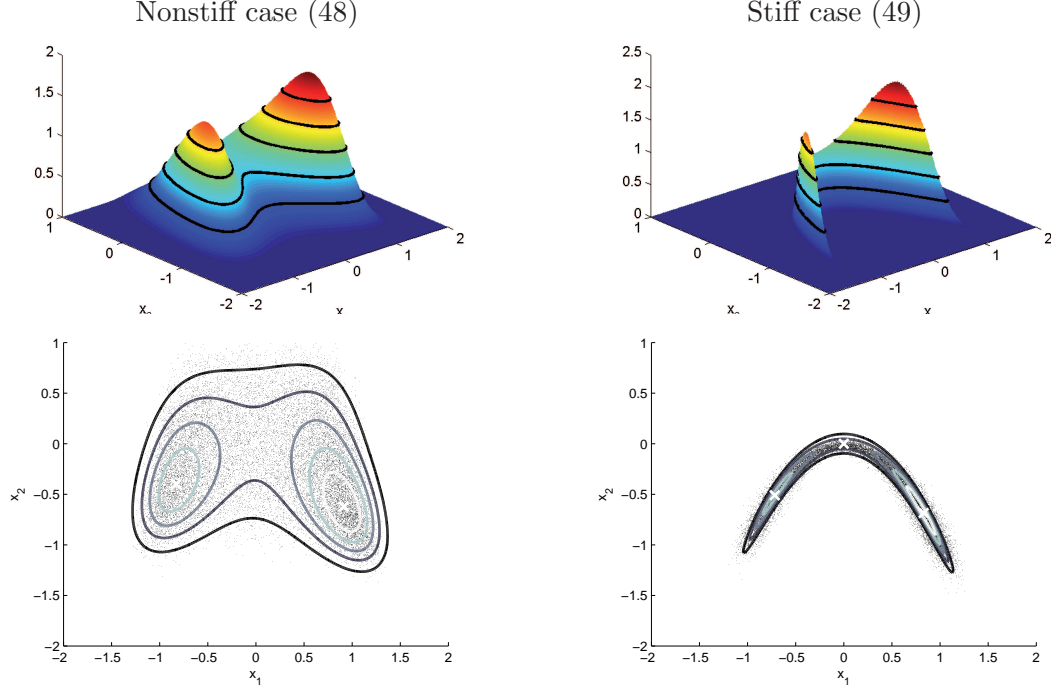


Figure 2: Plots of the Gibbs density (10) for the nonlinear problems with potential (48) (nonstiff case, left pictures) and (49) (stiff case, right pictures). Four level curves are represented in solid lines, the three extrema are represented with crosses. In the bottom pictures, a numerical trajectory of the method (15) is included, with length $T = 10^3$ and stepsize $h = 0.05$.

- In the nonstiff case (left picture of Figure 1), we observe the expected order 2 for the postprocessed method (15),(16) (we also include the variant without matrix J_n^{-1} in (16), which yields nearly identical results), while the postprocessed method (15),(17) has order 3 for linear problems and is significantly more accurate by a factor of about 10. A line of slope 1 can be observed for the standard implicit Euler method. The $\theta = 1/2$ method is exact for linear Brownian dynamics and the observed bias with magnitude 10^3 is due to the Monte-Carlo error (known [25] to decay as $\mathcal{O}(T^{-1/2})$).
- In the stiff case (right picture of Figure 1), the implicit Euler method and the postprocessed methods (15),(16) and (15),(17) do not lose their efficiency. In contrast, the $\theta = 1/2$ method becomes poorly accurate in the very stiff regime. This phenomena is well known already for severely stiff deterministic problems (the $\theta = 1/2$ method is not L -stable), and this is highlighted in the stochastic context in [24]. A loss of accuracy is also observed for the variant of the method (15),(16) where the term J_n^{-1} providing L -stability is omitted in (16).

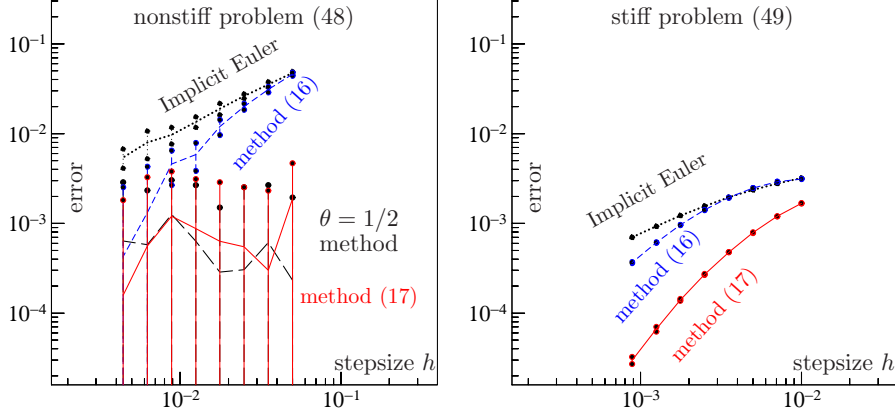


Figure 3: Nonlinear nonstiff problem (48) and stiff problem (49). Implicit Euler method ((13) with $\theta = 1$, order 1) and postprocessed versions (15),(16) and (15),(17) of order 2. The $\theta = 1/2$ -method (order 2) is also included in the nonstiff case (left picture). Error in $\int_{\mathbb{R}^d} (x_2 + x_1^2)^2 \rho(x) dx$ versus time stepsize h obtained using 10 trajectories on a long time interval of length $T = 10^5$. The vertical bars indicate the standard deviation intervals due to the Monte-Carlo error.

5.2 Nonlinear test problems

We next consider two nonlinear problems. On the one hand, we consider a nonstiff problem in dimension $d = 2$ with potential

$$V(x) = (1 - x_1^2)^2 + x_2^4 - x + x_1 \cos(x_2) + (x_2 + x_1^2)^2, \quad (48)$$

and on the other hand, we consider the stiff problem in dimension $d = 3$ with potential

$$V(x) = (1 - x_1^2)^2 + x_2^4 - x + x_3 \cos(x_2) + 100(x_2 + x_1^2)^2 + \frac{10^6}{2}(x_1 - x_3)^2. \quad (49)$$

In Figure 2, we plot the associated Gibbs density measure (10) together with five level curves for the components³ x_1, x_2 for the nonstiff problem (48) (left pictures) and the stiff problem (49) (right pictures). It can be seen that the distribution is much narrower in the stiff case and concentrated close to the curve $\{x_2 + x_1^2 = 0\}$, due to the stiff term $100(x_2 + x_1^2)^2$ in (49). In the bottom pictures of Figure 2, we also include one numerical trajectory of length $T = 10^3$ with stepsize $h = 0.05$ for the L -stable method (15). It fits well the invariant distribution for both the nonstiff and stiff cases.

For both problems, we take the initial conditions $x_i = i$ ($i = 1, 2, 3$) and consider ten long trajectories with length $T = 10^4$. Analogously to the linear case, we compare in Figure 3 the results in the nonstiff and stiff cases. We plot for many constant stepsizes h the errors for the evaluation of the quantity $\int_{\mathbb{R}^d} (x_2 + x_1^2)^2 \rho(x) dx$ (a reference value for this integral is computed using an accurate quadrature method).

- In the nonstiff case (left picture of Figure 3), we observe the expected convergence lines of slope 1 and 2 for the implicit Euler method and the variant postprocessed method

³Since (49) is in 3D, the right pictures of Figure 2 correspond to the Gibbs density measure for the marginal law of the components (x_1, x_2) .

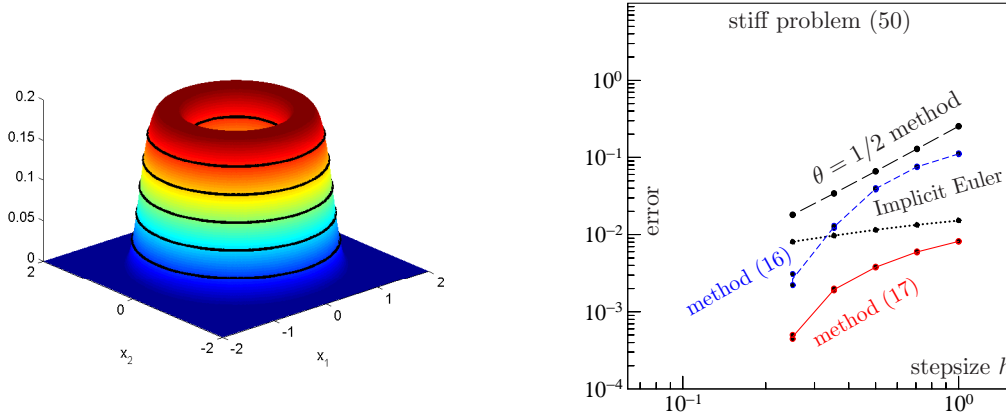


Figure 4: Nonlinear problem in dimension $d = 10$ with potential (50). Left picture: plot of the Gibbs density (10) in the case $d = 2$. Right picture: comparison of the implicit Euler method ((13) with $\theta = 1$, order 1) and postprocessed versions (new method (15),(17) and variant (15),(16)) of order 2. The $\theta = 1/2$ -method (order 2) is also included. Error for $\int_{\mathbb{R}^d} (|x| - 1)^2 \rho(x) dx$ versus time stepsize h obtained using 10 trajectories on a long time interval of length $T = 10^4$.

(15),(16), while the $\theta = 1/2$ method and the postprocessed method (15),(17) (order 2 for nonlinear problems, order 3 for linear problems) reveal much more accurate.

- In the stiff case (right picture of Figure 3), the Newton iterations of the $\theta = 1/2$ -method fail to converge for the considered stepsizes, a convergence curve is thus not included. The implicit Euler method still exhibits a convergence curve 1. The best accuracy is observed for the postprocessed method (15),(17) of order two.

Finally, as a more challenging problem, we consider the following potential in dimension $d = 10$,

$$V(x) = 25(1 - |x|)^4, \quad |x| = \sqrt{\sum_{i=1}^d x_i^2}. \quad (50)$$

This is a modification of a standard nonlinear model for the motion of a spring in d dimensions considered as an illustrative example in [34, Sect. 7]. We plot in Figure 4 (left picture) the Gibbs density measure (10) in dimension $d = 2$, and it can be seen that the distribution is concentrated close to the sphere $\{|x| = 1\}$ centred at the origin with radius 1. In Figure 4 (right picture), we plot the convergence curves for $\int_{\mathbb{R}^d} (|x| - 1)^2 \rho(x) dx$. Again, excellent performances of the postprocessed method (15),(17) can be observed. For the considered stepsizes, it is about 20 times more accurate than the standard $\theta = 1/2$ method, also of order two for the invariant measure. As a reference solution, we took the result of the $\theta = 1/2$ method with stepsize $h = 2^{-4.5} \simeq 4.4 \cdot 10^{-2}$.

6 Summary

In this paper, we extended to the stochastic context the methodology of effective order of Butcher. The approach of stochastic postprocessed integrators was illustrated in the

case of Brownian dynamics, for which new schemes of order two were constructed based on the θ -method, in particular implicit schemes with favourable stability properties for the sampling of the invariant measure of ergodic systems. We rediscovered the second order non-Markovian scheme from [20] and analyzed in [22] which can be interpreted as a postprocessed integrator. This new insight permitted us to construct new high order integrators based on the θ -method, and to provide a rigorous error analysis based on the standard theory of Markovian schemes. Our approach is in principle not restricted to Brownian dynamics and could apply to larger classes of SDEs (Theorem 4.3). This will be investigated in future works.

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7 Appendix

Proof of Theorem 4.6. For the scheme (44), a calculation analogous to (29) shows that (27) holds with

$$\begin{aligned} A_1\phi &= \frac{1}{2}\phi''(f, f) + \frac{\sigma^2}{2} \sum_{i=1}^d \phi'''(e_i, e_i, f) + \frac{\sigma^4}{8} \sum_{i,j=1}^d \phi^{(4)}(e_i, e_i, e_j, e_j) + \theta\phi'f'f \\ &+ \left((1-\theta)a^2 + \theta(a+1)^2 \right) \frac{\sigma^2}{2} \phi' \sum_{i=1}^d f''(e_i, e_i) + (a+\theta)\sigma^2 \sum_{i=1}^d \phi''(f'e_i, e_i). \end{aligned}$$

Using integration by parts, the following identities were proved in [3],

$$\begin{aligned} \langle \phi''(f, f) \rangle &= \langle -\phi'(f'f + \operatorname{div}(f)f + \frac{2}{\sigma^2}\|f\|^2 f) \rangle, \\ \langle \sigma^2 \sum_i \phi'''(f, e_i, e_i) \rangle &= \langle \phi'(\sigma^2 \sum_i f''(e_i, e_i) + 4f'f + 2\operatorname{div}(f)f + \frac{4}{\sigma^2}\|f\|^2 f) \rangle, \\ \langle \sigma^2 \sum_{ij} \phi^{(4)}(e_i, e_i, e_j, e_j) \rangle &= \langle -\sum_i 2\phi'''(f, e_i, e_i) \rangle, \\ \langle \sigma^2 \sum_i \phi''(f'e_i, e_i) \rangle &= \langle -\phi'(\sigma^2 \sum_i f''(e_i, e_i) + 2f'f) \rangle, \end{aligned} \tag{51}$$

where we use the notation $\langle u \rangle = \int_{\mathbb{R}^d} u(x)\rho(x)dx$ and the sums are for $i, j = 1, \dots, d$. For instance, to prove the first identity in (51), we integrate by parts and use $\partial_j \rho = \frac{2}{\sigma^2} f^j \rho$, where ∂_j denotes the derivative $\partial/(\partial x_j)$,

$$\begin{aligned} \langle \phi''(f, f) \rangle &= \int_{\mathbb{R}^d} \sum_{i,j=1}^d \partial_i \partial_j \phi f^i f^j \rho dy = - \int_{\mathbb{R}^d} \sum_{i,j=1}^d \partial_i \phi \partial_j (f^i f^j \rho) dy \\ &= - \left\langle \sum_{i,j=1}^d \partial_i \phi (f^i \partial_j f^j + \partial_j f^i f^j + f^i f^j \frac{2}{\sigma^2} f^j) \right\rangle \\ &= \left\langle -\phi'(f'f + \operatorname{div}(f)f + \frac{2}{\sigma^2}\|f\|^2 f) \right\rangle. \end{aligned}$$

The other identities in (51) can be proved analogously. We deduce

$$\langle A_1\phi \rangle = \left\langle \left(a^2 + 2\theta a \right) \frac{\sigma^2}{2} \phi' \sum_{i=1}^d f''(e_i, e_i) + \left(-\frac{1}{4} + a + \frac{1}{2}\theta \right) \sigma^2 \sum_{i=1}^d \phi''(f'e_i, e_i) \right\rangle$$

To improve the accuracy of the scheme (44), we now consider the postprocessor (45) where b and $c \geq 0$ are fixed parameters. Using $\bar{A}_1\phi = b\phi'f + \frac{c^2}{2}\sigma^2\Delta\phi$, we have

$$[\mathcal{L}, \bar{A}_1]\phi = \frac{(b-c^2)}{2}\sigma^2\phi' \sum_{i=1}^d f''(e_i, e_i) + (b-c^2)\sigma^2 \sum_{i=1}^d \phi''(f'e_i, e_i)$$

Summing up then yields the value of $\langle A_1\phi + [\mathcal{L}, \bar{A}_1]\phi \rangle$,

$$\left\langle \left(a^2 + 2\theta a + b - c^2 \right) \frac{\sigma^2}{2} \phi' \sum_{i=1}^d f''(e_i, e_i) + \left(-\frac{1}{4} + a + \frac{1}{2}\theta + b - c^2 \right) \sigma^2 \sum_{i=1}^d \phi''(f'e_i, e_i) \right\rangle$$

and this quantity is zero if (46) holds. We conclude the proof of Theorem 4.6 using Theorem 4.3. \square

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