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Random time step probabilistic methods for uncertainty quantification in chaotic and geometric numerical integration

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Abstract
A novel probabilistic numerical method for quantifying the uncertainty induced by the time integration of ordinary differential equations (ODEs) is introduced. Departing from the classical strategy to randomise ODE solvers by adding a random forcing term, we show that a probability measure over the numerical solution of ODEs can be obtained by introducing suitable random time steps in a classical time integrator. This intrinsic randomisation allows for the conservation of geometric properties of the underlying deterministic integrator such as mass conservation, symplecticity or conservation of first integrals. Weak and mean square convergence analysis is derived. We also analyse the convergence of the Monte Carlo estimator for the proposed random time step method and show that the measure obtained with repeated sampling converges in the mean square sense independently of the number of samples. Numerical examples including chaotic Hamiltonian systems, chemical reactions and Bayesian inferential problems illustrate the accuracy, robustness and versatility of our probabilistic numerical method.

Keywords Probabilistic methods for ODEs · Random time steps · Uncertainty quantification · Chaotic systems · Geometric integration · Inverse problems

Mathematics Subject Classification 65C30 · 65F15 · 65L09

1 Introduction

A variety of methods for integrating ordinary differential equations (ODEs) has been studied in the last decades (Hairer et al. 2006, 1993; Hairer and Wanner 1996), with an emphasis on building accurate and stable deterministic approximations of the exact solution. In general, these methods are based on a time discretisation on which the solution of the ODE is approximated via an iterative deterministic algorithm. Given a time step h, which indicates the refinement of the discretisation, all these methods provide a point value for the approximation of the solution and guarantee that in the asymptotic limit of $h \to 0$ the numerical approximation will coincide with the exact solution. However, for some problems such as chaotic systems or inference problems having a distributional solution can help to quantify the uncertainty introduced by the numerical discretisation without invoking the asymptotic limit $h \to 0$.

In recent years, probabilistic numerical methods for differential equations have been proposed (Chkrebtii et al. 2016; Conrad et al. 2017; Schober et al. 2014) in order to quantify the uncertainty introduced by the time discretisation in a statistical manner. A review summarising the recent advancements in the field of probabilistic numerical can be found in Cockayne et al. (2019) and Oates and Sullivan (2019). In general, these methods proceed iteratively to establish a probability measure over the numerical solution, thus providing a richer information than a single point value. In particular, probabilistic solvers offer a quantitative characterisation of late time errors by tuning the noise introduced by the method according to the accuracy of the solver. In this way, it is possible to obtain a reliable approach for capturing the sensitivity of the solution to numerical error, while transferring the convergence properties of classical deterministic integrators to the introduced probability measure in a consistent manner.

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In the following, we will first show two examples motivating the probabilistic approach and then present the main contributions of this work.

1.1 Motivating examples

Probabilistic integrators for ODEs do not provide more accurate solutions than classical deterministic methods nor are they computationally cheaper. Nevertheless, they can be useful in a variety of different problems, among which we identified the integration of chaotic dynamical systems and the solution of Bayesian inverse problems, which are briefly presented here.

Chaotic differential equations

Let us consider the Lorenz system (Lorenz 1963), which is defined by the following ODE

$$\begin{aligned} y_1' &= \eta(y_2 - y_1), & y_1(0) &= -10, \\ y_2' &= y_1(\rho - y_3) - y_2, & y_2(0) &= -1, \\ y_3' &= y_1 y_2 - \beta y_3, & y_3(0) &= 40. \end{aligned} \tag{1}$$

It is well known that for $\rho = 28$, $\eta = 10$, $\beta = 8/3$, this equation has a chaotic behaviour, i.e. a small perturbation forces the trajectories to deviate from the true solution. Integrating numerically (1) the error which is introduced at each time step is indeed a perturbation, and thus, any numerical solution cannot be considered reliable. In order to explore the state space of this chaotic dynamical system, we introduce a random perturbation on the initial condition, implemented as a scalar Gaussian random variable $\varepsilon \sim \mathcal{N}(0, \sigma^2)$ and artificially added to the first component $y_1(t)$ at time $t = 0$. In Fig. 1, we show $M = 20$ numerical trajectories given by a second-order Runge–Kutta method for three different scales of the noise. It is possible to remark that in all the three cases, the numerical solutions almost coincide up to some time $\bar{t}$, thus diverging and showing the chaotic nature of the Lorenz system. It could be argued that up to time $\bar{t}$, the numerical solution offers a reliable approximation of the true solution as the dynamics have not yet switched to the chaotic regime. Nevertheless, it is unclear how to choose σ^2 so that the amount of noise that is introduced is balanced with the numerical error. Probabilistic methods for differential equations such as the one presented in this work and the one introduced by Conrad et al. (2017) provide a rigorous analysis that suggests how to introduce a source of artificial noise in a consistent manner.

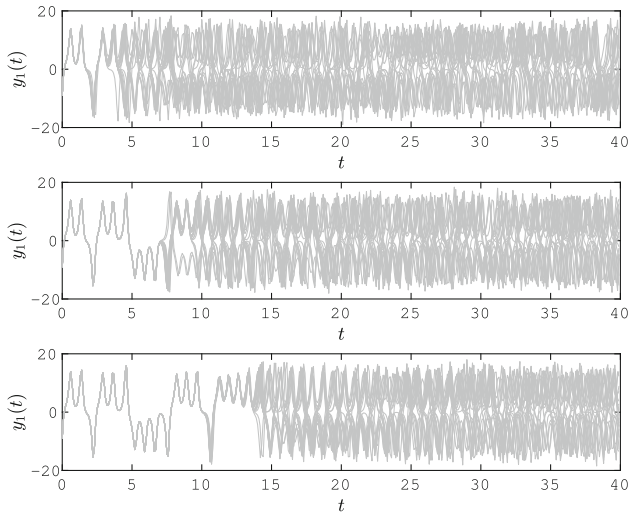

Fig. 1 First component $y_1(t)$ of the solution of (1) with decreasing Gaussian perturbations on the initial condition from top to bottom ($\sigma = 10^{-1}, 10^{-3}, 10^{-5}$, respectively)

Bayesian inference

Problems of Bayesian inference are most often used to justify the usefulness of probabilistic methods for differential equations. The impact of a probabilistic component in the numerical approximation of inverse problems involving ODEs has already been presented in several works (e.g. Chkrebtii et al. 2016; Cockayne et al. 2017; Conrad et al. 2017). In particular, the common underlying idea of these works is that if a deterministic integrator with a fixed finite time step is employed to approximate the solution of the ODE appearing in an inverse problem, the numerical error introduced by deterministic solvers can lead to inappropriate and non-predictive posterior concentrations. In the limit of an infinitely refined time discretisation, the posterior distributions obtained with a classical numerical method will indeed tend to the true distribution, but for a fixed time step (i.e. for a fixed computational budget) numerical error can lead to posterior concentrations away from the true value of the parameter of interest. These inappropriate solutions to inverse problems can be corrected by employing a probabilistic integrator to solve the ODE, thus obtaining posterior distributions that reflect the uncertainty given by the numerical solver (see Fig. 3 for an example).

1.2 Contributions

The method we analyse in this paper is inspired from the work of Conrad et al. (2017), where a probabilistic method for ODEs is presented. This method consists of perturbing a deterministic numerical solution (e.g. arising from a Runge–Kutta discretisation) with an additive source of noise at each time step. By appropriately scaling the random term, they

manage to obtain a probabilistic solution without altering the convergence of the underlying deterministic scheme.

An additive noise contribution could nonetheless produce disruptive effects on favourable geometric features of deterministic schemes. A direct example of this non-robust behaviour is given by ODEs for which the solution is supposed to stay positive and small. In this case, the addition of a random contribution could force the solution in the negative plane; hence, the numerical solution could be physically meaningless. Chemical reactions with small population size for one species at some time of the evolution are typical physical examples. In particular, an additive random term could force the solution on the negative plane with a non-zero probability, and this probability could become non-negligibly big in case the magnitude of one component of the solution is small. Other geometric properties of an underlying ODE are also destroyed when perturbing the flow by a noisy forcing term.

Motivated by these issues, we present in this work a new probabilistic method for ODEs based on a random selection of the time steps. Hence, the randomness of the scheme becomes intrinsic in contrast to the additive noise method. For this new robust probabilistic integrator, we are able to prove strong and weak convergence towards the exact solution of the underlying ODE. Precisely, setting the variance of the random time steps to be proportional to some power of a deterministic time step allows to retrieve the rates of the underlying Runge–Kutta integrator.

It has been pointed out by Kersting and Hennig (2016) that probabilistic methods based on sampling should be equipped with a criterion to choose the number of samples, so that computational effort is not wasted or, conversely, the sample size is not insufficient to describe the dynamics in a probabilistic fashion. In order to address this issue, in this work we show that Monte Carlo estimators drawn from our probabilistic solver converge with respect to the time step in the mean square sense independently of the sample size. We are able to prove a similar property for the scheme proposed in Conrad et al. (2017).

A large variety of dynamical systems is characterised by geometrical properties of their flow map (Hairer et al. 2006). Most notably, Hamiltonian systems, which are employed for modelling a variety of physical phenomena, are endowed with the property of symplecticity. It is possible to obtain good approximations of the solutions of Hamiltonian systems via mimicking numerically the geometric properties of the exact flow, i.e. by employing symplectic integrators. In particular, for symplectic integrators the energy function conserved by the exact flow is approximately conserved by numerical trajectories over long time spans, which in turn guarantees high-quality numerical solutions at the price of a rather low computational effort. While geometric properties of Runge–Kutta schemes have been analysed extensively in the deterministic case, they have not been considered yet for probabilistic numerical methods. The method we present in this work, being only an intrinsic modification of a Runge–Kutta integrator, is endowed with the geometric properties of its deterministic counterpart. In particular, we first show that our probabilistic scheme inherits the property of exact conservation of first integrals of the considered dynamics. Then, we show that in Hamiltonian systems the good approximation of the energy function given by symplectic schemes is preserved by our randomisation procedure over polynomially long times.

1.3 Outline

The paper is organised as follows. In Sect. 2, we introduce the setting for probabilistic numerics and present our novel numerical scheme. We then show in Sects. 3 and 4 the properties of weak and mean square convergence of the numerical solution towards the exact solution of the ODE. In Sect. 5, we analyse the accuracy of Monte Carlo estimators drawn from the numerical solution. The geometric properties of the numerical scheme are presented in Sects. 6 and 7, while in Sect. 8 we introduce Bayesian inverse problems in the ODE setting and show how our method can be integrated in existing sampling strategies. Finally, we show a variety of numerical experiments confirming our theoretical results in Sect. 9.

2 Random time step Runge–Kutta method

Let us consider a Lipschitz function $f\colon \mathbb{R}^d \to \mathbb{R}^d$ and the ODE

$$y' = f(y), \quad y(0) = y_0 \in \mathbb{R}^d. \tag{2}$$

In the following, we will write for simplicity the solution $y(t)$ of (2) in terms of the flow of the ODE. In particular, we consider the family $\{\varphi_t\}_{t\geq 0}$ of functions $\varphi_t\colon \mathbb{R}^d \to \mathbb{R}^d$ such that

$$y(t) = \varphi_t(y_0).$$

Given a time step h, let us consider a Runge–Kutta method which deterministically approximates the solution $\varphi_t(y_0)$ of (2). In particular, we can write the numerical solution y_k approximating $\varphi_{t_k}(y_0)$, with $t_k = kh$ in terms of the numerical flow $\{\Psi_t\}_{t\geq 0}$, with $\Psi_t\colon \mathbb{R}^d \to \mathbb{R}^d$, which is uniquely determined by the coefficients of the method, as

$$y_{k+1} = \Psi_h(y_k), \quad k = 0, 1, \ldots.$$

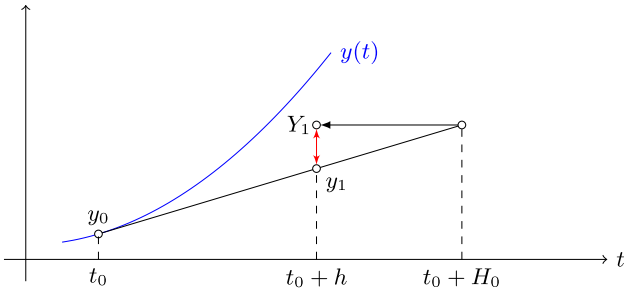

Fig. 2 Graphical representation of one step of the RTS-RK method with $\Psi_h(y) = y + hf(y)$. The red arrow is the stochastic contribution due to random time stepping. (Color figure online)

In order to provide a probabilistic interpretation of the numerical solution rather than a series of point values, Conrad et al. propose the scheme defined by

$$Y_{k+1} = \Psi_h(Y_k) + \xi_k(h), \quad k = 0, 1, \ldots, \tag{3}$$

where Y_k is a random variable approximating $y(t_k)$ with $Y_0 = y_0$ and $\xi_k(h)$ are appropriately scaled independent and identically distributed (i.i.d.) random variables with values in $\mathbb{R}^d$. Maintaining the same notation as in (3), in this work we propose a random time-stepping Runge–Kutta method (RTS-RK), i.e. the scheme defined by the recurrence relation

$$Y_{k+1} = \Psi_{H_k}(Y_k), \quad k = 0, 1, \ldots, \tag{4}$$

where Y_k is still a random variable approximating $y(t_k)$ and the time steps H_k are locally given by a sequence of i.i.d. random variables with values in $\mathbb{R}^+$. A graphical representation of one step of the RTS-RK method is given in Fig. 2. Let us finally remark that the sequence Y_k, $k = 0, 1, \ldots$, form a homogeneous Markov chain, as the transition probability is independent of the index k.

Remark 1 We note that in terms of computational cost simulating the two methods (3) and (4) is equivalent.

2.1 Assumptions and notation

We now present the main assumptions and notations which are used throughout the rest of this work. Firstly, we have to consider the possible values taken by the random step sizes, which have to satisfy restrictions that are necessary not to spoil the properties of deterministic methods.

Assumption 1 The i.i.d. random variables H_k satisfy for all $k = 0, 1, \ldots$

(i) $H_k > 0$ a.s.,
(ii) there exists $h > 0$ such that $\mathbb{E}H_k = h$,
(iii) there exist $p \geq 1/2$ and $C > 0$ independent of k such that the scaled random variables $Z_k := H_k - h$ satisfy

$$\mathbb{E}Z_k^2 = Ch^{2p+1}.$$

The class of random variables satisfying the hypotheses above is general. However, it is practical for an implementation point of view to have examples of these variables.

Example 1 Let us consider the random variables $\{H_k\}_{k\geq 0}$ such that

$$H_k \overset{\text{i.i.d.}}{\sim} \mathcal{U}(h - h^{p+1/2}, h + h^{p+1/2}),$$
$$0 < h < 1, \quad p \geq 1/2.$$

We easily verify that the assumptions (i) and (ii) are verified as $h < 1$ and that (iii) is verified with $C = 1/3$. Another choice of random variables could simply be

$$H_k \overset{\text{i.i.d.}}{\sim} \log\mathcal{N}\big(\log h - \log\sqrt{1 + h^{2p}}, \log(1 + h^{2p})\big), \tag{5}$$

for which the properties above are trivially verified (with $C = 1$), provided $p > 1/2$.

We secondly introduce an assumption on the deterministic method underlying the RTS-RK scheme, identified by its numerical flow Ψ_h.

Assumption 2 The Runge–Kutta method defined by the numerical flow $\{\Psi_t\}_{t\geq 0}$ is of order q, i.e. for h small enough, there exists a constant $C > 0$ such that

$$\|\Psi_h(y) - \varphi_h(y)\| \leq Ch^{q+1}, \quad \forall y \in \mathbb{R}^d.$$

Remark 2 Depending on the domain of definition of the vector field f, the choice of an unbounded distribution for the time step could give rise to two critical issues. In particular,

(i) if $f : D \to \mathbb{R}^d$, where $D \in \mathbb{R}^d$ is a bounded open subset of $\mathbb{R}^d$, allowing the time step to assume unbounded values as, for example, in case of the log-normal distribution (5), may force the solution outside D,
(ii) if Ψ_h is the numerical flow of an implicit method, the solution could be ill-posed.

In both the two cases above, we suggest to employ uniform time steps as in Example 1, which allow the time steps to be small enough almost surely. For the first issue, more sophisticated techniques of path rejection could be employed (Milstein and Tretyakov 2005), but the mean square convergence properties which will be examined in Sect. 4 would not hold.

In order to tackle the second issue presented in Remark above, we introduce a further assumption.

Assumption 3 If the map Ψ_t is implicit, the time steps H_k satisfy $H_k \leq M < \infty$ almost surely, where M is small enough to allow the scheme to be well-posed.

Let us finally remark that the choice of the distribution of the time steps is artificial and therefore arbitrary. Hence, choosing a bounded distribution does not represent a limitation to the numerical scheme.

3 Weak convergence analysis

The first property of the RTS-RK method we wish to analyse is its weak convergence, which gives an indication about the behaviour of the numerical solution (4) in the mean sense. In the following, we denote by $\mathcal{C}_b^l(\mathbb{R}^d, \mathbb{R})$ the functions in $\mathcal{C}^l(\mathbb{R}^d, \mathbb{R})$ with all derivatives up to order l bounded uniformly in $\mathbb{R}^d$. Moreover, we consider the integration of (2) over the finite length domain $[0, T]$, where $T > 0$ is the final time. Let us define the weak order of convergence.

Definition 1 The numerical method (4) has weak order r for (2) if for any sufficiently smooth function $\Phi\colon \mathbb{R}^d \to \mathbb{R}$ there exists a constant $C > 0$ independent of h such that

$$|\mathbb{E}\Phi(Y_k) - \Phi(y(kh))| \leq Ch^r,$$

for all $k = 1, 2, \ldots, N$ and $T = Nh$.

Let us introduce the Lie derivative of the flow $\mathcal{L} = f \cdot \nabla$, which allows us to adopt the semi-group notation for the exact solution of (2) (see e.g. Hairer et al. 2006, Section III.5.1) or Pavliotis and Stuart 2008, Section 4.3) and write for any smooth function Φ

$$\Phi(\varphi_h(y)) = \mathrm{e}^{h\mathcal{L}}\Phi(y). \tag{6}$$

Moreover, let us recall that the probabilistic numerical solution $\{Y_k\}_{k\geq 0}$ forms a homogeneous Markov chain. Therefore, given $h > 0$ there exists an operator $\mathcal{P}_h$, the generator (Pavliotis 2014, Section 2.3), such that

$$\mathbb{E}\big(\Phi(Y_{k+1}) \mid Y_k = y\big) = (\mathcal{P}_h\Phi)(y).$$

In order to have an analogy with notation (6), we adopt the exponential form of the infinitesimal generator and denote in the following $\mathcal{P}_h = \mathrm{e}^{h\mathcal{L}_h}$, where we explicitly write the dependence of the Markov generator on the step size h. Furthermore, due to the homogeneity of the Markov chain, we can write

$$\mathbb{E}\big(\Phi(Y_{k+1}) \mid Y_0 = y\big) = \mathrm{e}^{h\mathcal{L}_h}\mathbb{E}\big(\Phi(Y_k) \mid Y_0 = y\big). \tag{7}$$

We can now state a result of local weak convergence of the probabilistic numerical solution.

Lemma 1 (Weak local order) *Let Assumptions 1, 2 and 3 hold and let f in (2) be sufficiently smooth. If $\mathbb{E}|H_0^4| < \infty$, there exists a constant $C > 0$ independent of h and y such that for any function $\Phi \in \mathcal{C}_b^l(\mathbb{R}^d, \mathbb{R})$, with $l = \max\{q, 3\}$*

$$|\mathbb{E}(\Phi(Y_1) \mid Y_0 = y) - \Phi(\varphi_h(y))| \leq Ch^{\min\{2p+1, q+1\}}.$$

Proof Since f is sufficiently smooth, the map $t \mapsto \Psi_t(y)$ is of class $C^2(\mathbb{R}^+, \mathbb{R}^d)$ and Lipschitz continuous with constant L_Ψ independent of y. Let us expand the functional Φ computed on the numerical solution as

$$\begin{aligned}
\Phi(Y_1) &= \Phi(\Psi_{H_0}(Y_0)) \\
&= \Phi\Big(\Psi_h(Y_0) + (H_0 - h)\partial_t\Psi_h(Y_0) \\
&\quad + \frac{1}{2}(H_0 - h)^2\partial_{tt}\Psi_h(Y_0) + \mathcal{O}(|H_0 - h|^3)\Big) \\
&= \Phi(\Psi_h(Y_0)) + \Big((H_0 - h)\partial_t\Psi_h(Y_0) \\
&\quad + \frac{1}{2}(H_0 - h)^2\partial_{tt}\Psi_h(Y_0)\Big) \cdot \nabla\Phi(\Psi_h(Y_0)) \\
&\quad + \frac{1}{2}(H_0 - h)^2\partial_t\Psi_h(Y_0)\partial_t\Psi_h(Y_0)^\top : \nabla^2\Phi(\Psi_h(Y_0)) \\
&\quad + \mathcal{O}(|H_0 - h|^3),
\end{aligned} \tag{8}$$

where we denote by $\nabla^2\Phi$ the Hessian matrix of Φ and by $:$ the inner product on matrices induced by the Frobenius norm on $\mathbb{R}^d$, i.e. $A : B = \mathrm{tr}(A^\top B)$. Taking the conditional expectation with respect to $Y_0 = y$ and applying Assumption 1, we get

$$\begin{aligned}
\mathrm{e}^{h\mathcal{L}_h}\Phi(y) - \Phi(\Psi_h(y)) &= \frac{1}{2}Ch^{2p+1}\partial_{tt}\Psi_h(y) \cdot \nabla\Phi(\Psi_h(y)) \\
&\quad + \frac{1}{2}Ch^{2p+1}\partial_t\Psi_h(y)\partial_t\Psi_h(y)^\top : \nabla^2\Phi(\Psi_h(y)) \\
&\quad + \mathcal{O}(h^{3p+3/2}),
\end{aligned} \tag{9}$$

where we exploited Hölder's inequality for the last term. Moreover, expanding Φ in y we get

$$\begin{aligned}
\Phi(\Psi_h(y)) &= \Phi\left(\Psi_0(y) + h\partial_t\Psi_0(y) + \mathcal{O}(h^2)\right) \\
&= \Phi(y) + \mathcal{O}(h),
\end{aligned}$$

which implies

$$\begin{aligned}
\mathrm{e}^{h\mathcal{L}_h}\Phi(y) - \Phi(\Psi_h(y)) &= \frac{1}{2}Ch^{2p+1}\partial_{tt}\Psi_h(y) \cdot \nabla\Phi(y) \\
&\quad + \frac{1}{2}Ch^{2p+1}\partial_t\Psi_h(y)\partial_t\Psi_h(y)^\top : \nabla^2\Phi(y) + \mathcal{O}(h^{2p+1}).
\end{aligned} \tag{10}$$

Let us remark that due to the smoothness of the flow we have

$$\mathrm{e}^{h\mathcal{L}}\Phi(y) - \Phi(\Psi_h(y)) = \mathcal{O}(h^{q+1}). \tag{11}$$

Combining (11) and (10), we have the one-step weak error of the probabilistic method on the original ODE, i.e.

$$e^{h\mathcal{L}}\Phi(y) - e^{h\mathcal{L}_h}\Phi(y) = \mathcal{O}(h^{\min\{2p+1,q+1\}}),$$

which proves the desired result. □

Remark 3 Let us remark that rigorously if $\partial_{tt}\Psi_h(y)$ is bounded independently of y, then equality (8) holds. In fact, as it can be noticed in (9), a sufficient requirement is that $h^{p+1/2}\partial_{tt}\Psi_h(y)$ is bounded independently of h.

In order to obtain a result on the global order of convergence, we need a further stability assumption, which is the same as Assumption 3 in Conrad et al. (2017).

Assumption 4 The function f and the distribution of the random time steps H_k, $k = 0, 1, \ldots$, are such that the operator $e^{h\mathcal{L}_h}$ satisfies for all functions $\psi \in \mathcal{C}_b^q(\mathbb{R}^d, \mathbb{R})$ and a positive constant L,

$$\sup_{u\in\mathbb{R}^d} |e^{h\mathcal{L}_h}\psi(u)| \leq (1 + Lh) \sup_{u\in\mathbb{R}^d} |\psi(u)|, \tag{12}$$

where L may depend on f and on the distribution of the random time steps, but not on ψ or h.

Remark 4 Let us remark that in order for Ψ_h to satisfy Assumption 2, i.e. for Ψ_h to be of order q, the right-hand side f must be of class $\mathcal{C}_b^q(\mathbb{R}^d, \mathbb{R}^d)$ (see e.g. Hairer et al. 1993, Theorem II.3.1). Therefore, in order to apply bound (12) to composite functions $\Phi \circ \varphi_h \colon \mathbb{R}^d \to \mathbb{R}$ where $\Phi \in \mathcal{C}_b^\infty(\mathbb{R}^d, \mathbb{R})$, by the chain rule we need Assumption 4 to hold for functions in $C_b^q(\mathbb{R}^d, \mathbb{R})$. This fact will be exploited in the proof of Theorem 1.

We now give a lemma useful for bounding discrete sequences, which is taken from Milstein and Tretyakov (2004, Lemma 1.6).

Lemma 2 *Suppose that for arbitrary N and $k = 0, \ldots, N$ we have*

$$e_k \leq (1 + Ah)e_{k-1} + Bh^r,$$

where $h = T/N$, $A > 0$, $B \geq 0$, $r \geq 1$ and $e_k \geq 0$, $k = 0, \ldots, N$. Then

$$e_k \leq e^{AT}e_0 + \frac{B}{A}(e^{AT} - 1)h^{r-1}.$$

The proof of Lemma 2 follows from the discrete Grönwall inequality. We can now state the main result on weak convergence.

Theorem 1 (Weak order) *Let the assumptions of Lemma 1 and Assumption 4 hold. Then, there exists a constant $C > 0$ independent of h and of the initial condition such that for all functions $\Phi \in \mathcal{C}_b^l(\mathbb{R}^d, \mathbb{R})$, with $l = \max\{q, 3\}$*

$$|\mathbb{E}\Phi(Y_k) - \Phi(y(kh)))| \leq Ch^{\min\{2p,q\}}, \tag{13}$$

for all $k = 1, 2, \ldots, N$ and $T = Nh$.

Proof Let us introduce the following notation

$$w_k(u) = \Phi(\varphi_{t_k}(u)),$$
$$W_k(u) = \mathbb{E}(\Phi(Y_k) \mid Y_0 = u).$$

By the triangle inequality and the Markov property (7), we have

$$\sup_{u\in\mathbb{R}^d} |W_k(u) - w_k(u)| \leq \sup_{u\in\mathbb{R}^d} |e^{h\mathcal{L}}w_{k-1}(u) - e^{h\mathcal{L}_h}w_{k-1}(u)| + \sup_{u\in\mathbb{R}^d} |e^{h\mathcal{L}_h}w_{k-1}(u) - e^{h\mathcal{L}_h}W_{k-1}(u)|.$$

We then apply Lemma 1 to the first term and Assumption 4 to the second and denote $e_k := \sup_{u\in\mathbb{R}^d} |W_k(u) - w_k(u)|$, thus obtaining

$$e_k \leq Ch^{\min\{2p+1,q+1\}} + (1 + Lh)e_{k-1}.$$

We can therefore apply Lemma 2 with $A = L$ and $r = \min\{2p + 1, q + 1\}$ and therefore get for a constant $C > 0$

$$\sup_{u\in\mathbb{R}^d} |w_k(u) - W_k(u)| \leq Ch^{\min\{2p,q\}},$$

which is the desired result. □

Remark 5 In Conrad et al. (2017), the authors define ordinary and stochastic modified equations in order to prove a result of weak convergence applying techniques of backward error analysis. In particular, they show that their probabilistic solver approximates in the weak sense a stochastic differential equation (SDE) where the deterministic part is given by the original ODE. For our probabilistic solver, it is possible to prove that the numerical solutions approximates in the weak sense the solution of an SDE which depends on the derivative of the map $t \mapsto \Psi_t(y)$. Such a construction is shown in the Appendix.

Remark 6 Let us recall that the random variable Y_k given by RTS-RK is thought of as an approximation of $y(kh)$ regardless of the value of the sum of the random time steps. Hence, the comparison in (13) is legitimate and does not induce time misalignment between true and numerical solutions. This basic property applies to all results in the following.

4 Mean square convergence analysis

The second property of (4) we analyse is its mean square order of convergence, which gives an indication on the pathwise distance between each realisation of the numerical solution and the exact solution of (2). Let us define the mean square order of convergence.

Definition 2 The numerical method (4) has mean square order of convergence r for (2) if there exists a constant $C > 0$ independent of h and of the initial condition y_0 such that

$$\left(\mathbb{E}\|Y_k - y(kh)\|^2\right)^{1/2} \leq Ch^r$$

for all $k = 1, 2, \ldots, N$ and $T = Nh$.

Remark 7 Let us remark that the mean square convergence is stronger than the traditional strong convergence, since, by Jensen's inequality

$$\mathbb{E}\|Y_k - y(kh)\| \leq \left(\mathbb{E}\|Y_k - y(kh)\|^2\right)^{1/2} \leq Ch^r.$$

We start by analysing how the method converges with respect to the mean step size h in the local sense, i.e. after one step of the numerical integration.

Lemma 3 (Local mean square convergence) *Under Assumptions 1, 2 and 3 the numerical solution Y_1 given by one step of the RTS-RK method (4) satisfies*

$$\left(\mathbb{E}\|Y_1 - y(h)\|^2\right)^{1/2} \leq Ch^{\min\{p+1/2, q+1\}}, \tag{14}$$

where C is a real positive constant independent of h and of the initial condition y_0 and the coefficients p, q are given in the assumptions.

Proof By triangular and Young's inequalities, we have for all $y \in \mathbb{R}^d$

$$\begin{aligned}\mathbb{E}\|\Psi_{H_0}(y) - \varphi_h(y)\|^2 &\leq 2\mathbb{E}\|\Psi_{H_0}(y) - \Psi_h(y)\|^2 \\ &\quad + 2\|\Psi_h(y) - \varphi_h(y)\|^2.\end{aligned}$$

We now consider Assumptions 1 and 2, thus getting

$$\begin{aligned}\mathbb{E}\|\Psi_{H_0}(y) - \varphi_h(y)\|^2 &\leq 2L_\Psi^2 \mathbb{E}|H_0 - h|^2 + 2C_1 h^{2(q+1)} \\ &= 2L_\Psi^2 C_2 h^{2p+1} + 2C_1 h^{2(q+1)} \\ &\leq C^2 h^{2\min\{p+1/2, q+1\}},\end{aligned}$$

where C_1 and C_2 are the constants given in Assumptions 1 and 2, respectively. This is the desired result with $C = \max\{2L_\Psi^2 C_2, 2C_1\}^{1/2}$. □

As a consequence of the one-step convergence, we can prove a result of global mean square convergence.

Theorem 2 (Global mean square convergence) *Let f be globally Lipschitz and $t_k = kh$ for $k = 1, 2, \ldots, N$, where $Nh = T$. Then, under the assumptions of Theorem 3 the numerical solution given by (4) satisfies*

$$\sup_{k=1,2,\ldots,N} \left(\mathbb{E}\|Y_k - y(t_k)\|^2\right)^{1/2} \leq Ch^{\min\{p,q\}}, \tag{15}$$

where C is a real positive constant independent of h and of the initial condition.

In order to prove this result, let us introduce the following lemma.

Lemma 4 *Given ODE (2) with f globally Lipschitz, then for any y and w in $\mathbb{R}^d$ and $0 < h < 1$ we have*

$$\|\varphi_h(y) - \varphi_h(w)\| \leq (1 + Ch)\|y - w\|, \tag{16}$$

$$\|\varphi_h(y) - \varphi_h(w) - (y - w)\| \leq Ch\|y - w\|, \tag{17}$$

where C is a positive constant independent of h and of the initial condition y_0.

The proof of Lemma 4 follows from the global Lipschitz continuity of f and the Grönwall inequality. We can now prove the main result on mean square convergence.

Proof of Theorem 2 In the following, we denote by C a constant that does not depend on h and on the initial condition y_0 whose value may change from line to line. Let us define $e_k^2 := \mathbb{E}\|Y_k - y(t_k)\|^2$. Adding and subtracting the exact flow applied to the numerical solution, we obtain

$$\begin{aligned}e_{k+1}^2 &= \mathbb{E}\|\Psi_{H_k}(Y_k) - \varphi_h(Y_k)\|^2 + \mathbb{E}\|\varphi_h(Y_k) - \varphi_h(y(t_k))\|^2 \\ &\quad + 2\mathbb{E}\Big(\big(\varphi_h(Y_k) - \varphi_h(y(t_k))\big)^\top \big(\Psi_{H_k}(Y_k) - \varphi_h(Y_k)\big)\Big).\end{aligned} \tag{18}$$

Let us consider the three terms in (18) separately. For the first term, we have by Theorem 3

$$\mathbb{E}\|\Psi_{H_k}(Y_k) - \varphi_h(Y_k)\|^2 \leq Ch^{\min\{2p+1, 2(q+1)\}}. \tag{19}$$

For the second term, due to (16), we have

$$\mathbb{E}\|\varphi_h(Y_k) - \varphi_h(y(t_k))\|^2 \leq (1 + Ch)^2 e_k^2. \tag{20}$$

Let us now define $Z = \varphi_h(Y_k) - \varphi_h(y(t_k)) - (Y_k - y(t_k))$. Then we can rewrite the inner product as

$$\begin{aligned}&\mathbb{E}\Big(\big(\varphi_h(Y_k) - \varphi_h(y(t_k))\big)^\top \big(\Psi_{H_k}(Y_k) - \varphi_h(Y_k)\big)\Big) \\ &\quad = \mathbb{E}\Big(\big(Y_k - y(t_k)\big)^\top \big(\Psi_{H_k}(Y_k) - \varphi_h(Y_k)\big)\Big) \\ &\qquad + \mathbb{E}\Big(Z^\top \big(\Psi_{H_k}(Y_k) - \varphi_h(Y_k)\big)\Big).\end{aligned} \tag{21}$$

We bound the two terms in (21) separately. For the first term, by the law of total expectation, we have

$$\begin{aligned}&\mathbb{E}\Big(\big(Y_k - y(t_k)\big)^\top\big(\Psi_{H_k}(Y_k) - \varphi_h(Y_k)\big)\Big)\\&\quad= \mathbb{E}\mathbb{E}\Big(\big(Y_k - y(t_k)\big)^\top\big(\Psi_{H_k}(Y_k) - \varphi_h(Y_k)\big) \mid Y_k\Big)\\&\quad= \mathbb{E}\Big(\big(Y_k - y(t_k)\big)^\top\mathbb{E}\big(\Psi_{H_k}(Y_k) - \varphi_h(Y_k) \mid Y_k\big)\Big).\end{aligned}$$

Applying Cauchy–Schwarz inequality to the outer expectation, we get

$$\begin{aligned}&\mathbb{E}\Big(\big(Y_k - y(t_k)\big)^\top\big(\Psi_{H_k}(Y_k) - \varphi_h(Y_k)\big)\Big)\\&\quad\le \Big(\mathbb{E}\|\mathbb{E}\big(\Psi_{H_k}(Y_k) - \varphi_h(Y_k) \mid Y_k\big)\|^2\Big)^{1/2} e_k\\&\quad\le Ch^{\min\{2p+1,q+1\}}e_k,\end{aligned}$$

where we applied Lemma 1. We now consider the second term in (21). By the Cauchy–Schwarz inequality, we have

$$\begin{aligned}&\mathbb{E}\Big(Z^\top\big(\Psi_{H_k}(Y_k) - \varphi_h(Y_k)\big)\Big)\\&\quad\le \big(\mathbb{E}\|Z\|^2\big)^{1/2}\big(\mathbb{E}\|\Psi_{H_k}(Y_k) - \varphi_h(Y_k)\|^2\big)^{1/2}.\end{aligned}$$

We now apply (17) and Theorem 3 to obtain

$$\mathbb{E}\Big(Z^\top\big(\Psi_{H_k}(Y_k) - \varphi_h(Y_k)\big)\Big) \le Ch^{\min\{p+3/2,q+2\}}e_k.$$

We can hence bound the scalar product in (21) with Young's inequality and assuming $h < 1$ as

$$\begin{aligned}&\mathbb{E}\Big(\big(\varphi_h(Y_k) - \varphi_h(y(t_k))\big)^\top\big(\Psi_{H_k}(Y_k) - \varphi_h(Y_k)\big)\Big)\\&\quad\le Ch^{\min\{p+3/2,q+1\}}e_k\\&\quad\le \frac{he_k^2}{2} + C\frac{h^{\min\{2p+2,2q+1\}}}{2}.\end{aligned}\tag{22}$$

Combining (19), (20) and (22), we have

$$e_{k+1}^2 \le Ch^{\min\{2p+1,2q+1\}} + (1+Ch)e_k^2,$$

which implies the desired result by Lemma 2 and since $e_0 = 0$. □

Remark 8 Let us remark that the difference between global and local orders of convergence, i.e. between (14) and (15), is not exactly one, as it usually is in the purely deterministic case. In fact, due to the independence of the random variables there is only a $1/2$ loss in the random part of the exponent, while the natural loss of one order is verified in the deterministic component.

Remark 9 As for the additive noise method proposed in Conrad et al. (2017), the result of mean square convergence suggests that a reasonable choice for the noise scale p is to fix $p = q$, where q is the order of the Runge–Kutta method Ψ_h. In this way, the properties of convergence of the underlying deterministic method are preserved, while yielding a probabilistic interpretation of the numerical solution.

5 Mean square convergence of Monte Carlo estimators

The third property we analyse is the mean square convergence of Monte Carlo estimators drawn from the random time-stepping Runge–Kutta method. Let us consider a function $\Phi \in \mathcal{C}_b^\infty(\mathbb{R}^d, \mathbb{R})$ with Lipschitz constant L_Φ and a final time $T > 0$. Moreover, let us introduce the notation $Z = \Phi(y(T))$ and $Z_N = \mathbb{E}\Phi(Y_N)$, where N is such that $T = Nh$. In general, the quantity Z_N is not accessible, and we have to replace it by its Monte Carlo estimator

$$\widehat{Z}_{N,M} = M^{-1}\textstyle\sum_{i=1}^M \Phi(Y_N^{(i)}).\tag{23}$$

where M is the number of realisations of the numerical solution and we denote by $\{Y_N^{(i)}\}_{i=1}^M$ a set of i.i.d. realisations of the numerical solution. Hence, we are interested in studying the mean square error of the Monte Carlo estimator, which is defined as

$$\mathrm{MSE}(\widehat{Z}_{N,M}) = \mathbb{E}(Z - \widehat{Z}_{N,M})^2.$$

In the following result, we prove that this quantity converges to zero independently of the number of trajectories M, in the limit $h \to 0$.

Theorem 3 *Under Assumptions 1, 2 and 3, the Monte Carlo estimator $\widehat{Z}_{N,M}$ satisfies*

$$\mathrm{MSE}(\widehat{Z}_{N,M}) \le C\Big(h^{2\min\{2p,q\}} + \frac{h^{2\min\{p,q\}}}{M}\Big),\tag{24}$$

where C is a positive constant independent of h and M.

Proof Thanks to the classic decomposition of the MSE, we have

$$\mathrm{MSE}(\widehat{Z}_{N,M}) = \mathrm{Var}\,\widehat{Z}_{N,M} + \big(\mathbb{E}(\widehat{Z}_{N,M} - Z)\big)^2.$$

Due to the unbiasedness of the Monte Carlo estimator $\widehat{Z}_{N,M}$ and applying Theorem 1 to the second term, we have

$$\mathrm{MSE}(\widehat{Z}_{N,M}) \le \mathrm{Var}\,\widehat{Z}_{N,M} + Ch^{2\min\{2p,q\}}.$$

The variance of the estimator can be trivially bounded by exploiting the Lipschitz continuity of Φ and the independence of the samples as

$$\begin{aligned}\operatorname{Var}\widehat{Z}_{N,M} &= M^{-1}\operatorname{Var}\big(\Phi(Y_N)\big)\\ &\leq M^{-1}\mathbb{E}\big(\Phi(Y_N)-\Phi(y(T))\big)^2\\ &\leq M^{-1}L_\Phi^2\mathbb{E}\|Y_N-y(T)\|^2.\end{aligned}$$

Applying Theorem 2, we get

$$\operatorname{Var}\widehat{Z}_{N,M} \leq M^{-1}L_\Phi^2 C h^{2\min\{p,q\}},$$

which proves the desired result. □

Let us remark that with the choice $p=q$, which is the minimum p for which the order of convergence of the underlying deterministic method is not affected by the probabilistic setting, we have $\mathrm{MSE}(\widehat{Z}_{N,M}) \leq Ch^{2q}$ with $M=1$. Hence, the Monte Carlo estimators drawn from (4) converge in the mean square sense independently of the number of samples M in (23). In the sub-optimal case $p<q$, one should carefully select the number of trajectories M so that the two terms in (24) are balanced. In particular, this would lead to

$$M=\begin{cases}\mathcal{O}(1), & \text{if} \quad p\geq q,\\ \mathcal{O}(h^{2(p-q)}), & \text{if} \quad p<q\leq 2p,\\ \mathcal{O}(h^{-2p}), & \text{if} \quad 2p<q,\end{cases}$$

where the notation $M=\mathcal{O}(h^r)$ for a real number r means that there exist constants C_1 and C_2 such that $C_1h^r \leq M \leq C_2h^r$.

Remark 10 Let us remark that in order to have uncertainty quantification for a fixed value $h>0$ it is necessary to draw a sample with $M>1$, since otherwise the probability distribution over the numerical solution would be a Dirac delta. Theorem 3 does not provide an indication of how the value of M should be chosen in order to have a good empirical description of the probability measure induced by the RTS-RK method, but still ensures quantitatively that the Monte Carlo estimators drawn from this distribution have a good quality.

6 Conservation of first integrals

Numerical methods for ODEs are often studied in terms of their geometric properties (Hairer et al. 2006). In particular, we investigate here whether the random choice of time steps in (4) spoils the properties of the underlying deterministic Runge–Kutta method. Let us recall the definition of first integral for an ODE.

Definition 3 Given a function $I:\mathbb{R}^d\to\mathbb{R}$, then $I(y)$ is a first integral of (2) if $I'(y)f(y)=0$ for all $y\in\mathbb{R}^d$.

If this property of the ODE is conserved by a numerical integrator, i.e. if for the any $y\in\mathbb{R}^d$ it is true that $I(\Psi_h(y))=I(y)$, then we say that the numerical method conserves the first integral. In particular, this implies that the first integral I is conserved along the trajectory of the numerical solution, i.e. $I(y_k)=I(y_0)$ for all $k\geq 0$.

Example 2 To illustrate this concept, we first discuss the case of linear first integrals, which can be seen as a general case of the conservation of mass in physical systems. Let us consider a linear first integral $I(y)=v^\top y$ and any Runge–Kutta method with coefficients $\{b_i\}_{i=1}^s$, $\{a_{ij}\}_{i,j=1}^s$. Then, we have for a time step $H_0>0$

$$I(Y_1)=v^\top y_0+H_0\textstyle\sum_{i=1}^s b_i v^\top f(y_0+H_0\sum_{j=1}^s a_{ij}K_j),$$

where $\{K_i\}_{i=1}^s$ are the internal stages of the Runge–Kutta method. Since $I(y)$ is a first integral, $v^\top f(y)=0$ for any $y\in\mathbb{R}^d$. Hence $I(Y_1)=I(y_0)$ and iteratively $I(Y_k)=I(y_0)$ for all $k\geq 0$ along the numerical trajectory. The equality above shows that any RTS-RK method conserves linear first integrals path-wise, or in the strong sense.

It is known that no Runge–Kutta method can conserve any polynomial invariant of order $n\geq 3$ (Hairer et al. 2006, Theorem IV.3.3). Nonetheless, for some particular problems there exist tailored Runge–Kutta methods which can conserve polynomial invariants of higher order. We therefore can state the following general result.

Theorem 4 *Let $I(y)$ be a first integral for (2) and Ψ_h be the numerical flow of a Runge–Kutta scheme for (2). If the scheme defined by Ψ_h conserves $I(y)$ for any $h>0$, then the numerical method (4) conserves $I(y)$ almost surely.*

Proof If $I(\Psi_h(y))=I(y)$ for any h, then $I(\Psi_{H_0}(y))=I(y)$ almost surely for any value that H_0 can assume. □

We now consider quadratic first integrals, i.e. first integrals of the form $I(y)=y^\top Sy$ with S a symmetric matrix, which are conserved by Runge–Kutta methods that satisfy the hypotheses of Cooper's theorem (Hairer et al. 2006, Theorem IV.2.2). The conservation of quadratic first invariants is of the utmost importance, for example, for Hamiltonian systems, as it implies the symplecticity of the scheme. It is known (Hairer et al. 2006, Theorem IV.2.1) that all Gauss methods conserve quadratic first integrals. The simplest member of this class of methods is the implicit midpoint rule, which is a one-stage method defined by coefficients $b_1=1$ and $a_{11}=1/2$.

Corollary 1 *If the Runge–Kutta scheme defined by Ψ_h conserves quadratic first integrals, then the numerical method (4) conserves quadratic first integrals almost surely.*

Proof This result is a direct consequence of Theorem 4. □

The properties above for the RTS-RK method are not satisfied by the additive noise method presented in Conrad et al. (2017). In particular, let us remark that the conservation of first integrals is exact for any trajectory of the RTS-RK method and is not an average property. In other words, we can say that (4) conserves linear first integrals in the strong sense. For the additive noise numerical method (3), we have

$$\begin{aligned} I(Y_1) &= v^\top y_0 + h\textstyle\sum_{i=1}^s b_i v^\top f(y_0 + h\sum_{j=1}^s a_{ij} K_j) \\ &\quad + v^\top \xi_0(h), \\ &= v^\top (y_0 + \xi_0(h)). \end{aligned}$$

If the random variable ξ_0 is zero-mean, then $\mathbb{E}I(Y_1) = I(y_0)$ and iteratively along the solution $\mathbb{E}I(Y_k) = I(y_0)$. Linear first integrals are therefore conserved in average, but not in a path-wise fashion.

For quadratic first integrals, we have instead that the additive noise method does not conserve them neither path-wise nor in the weak sense, as we have

$$\begin{aligned} I(Y_1) &= (\Psi_h(y_0) + \xi_0(h))^\top S(\Psi_h(y_0) + \xi_0(h)) \\ &= I(y_0) + 2\xi_0(h)^\top S\Psi_h(y_0) + \xi_0(h)^\top S\xi_0(h). \end{aligned}$$

If the random variables are zero-mean and if there exists a matrix Q such that $\mathbb{E}\xi_0(h)\xi_0(h)^\top = Qh^{2p+1}$ for some $p \geq 1$ (Assumption 1 in Conrad et al. 2017), we then have

$$\mathbb{E}I(Y_1) = I(y_0) + Q : Sh^{2p+1}. \tag{25}$$

Hence, along the trajectories of the solution a bias is introduced in the first integral which persists even in the mean sense. In general, Theorem 4 is not valid for the additive noise method, as the random contribution drives the first integral far from its true value at each time step. In practice, this could produce large deviations of the numerical approximation from the true solution, especially in the long-time regime.

7 Hamiltonian systems

A class of dynamical systems of particular interest for their geometric properties is the class of Hamiltonian systems. Given a function $Q\colon \mathbb{R}^{2d} \to \mathbb{R}$, called the Hamiltonian, Hamiltonian systems can be written as

$$y' = J^{-1}\nabla Q(y), \quad y(0) = y_0 \in \mathbb{R}^{2d}, \tag{26}$$

where the matrix $J \in \mathbb{R}^{2d\times 2d}$ is defined as

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix},$$

and where I is the identity matrix in $\mathbb{R}^{d\times d}$. The Hamiltonian Q is a first integral for (26); hence, we require numerical integrators to conserve the energy, or at least not to deviate from its true value in an uncontrolled fashion. As it was shown in the previous section, when Q is a polynomial it is possible to obtain exact conservation with deterministic integrators and with their probabilistic counterparts obtained with the RTS-RK method. If Q is not a polynomial, exact conservation is in general not achievable, but a good approximation of the energy over long time spans is achievable through the notion of symplectic differentiable maps.

Definition 4 (Definition VI.2.2 in Hairer et al. 2006) Let $U \subset \mathbb{R}^{2d}$ be a non-empty open set. A differentiable map $g\colon U \to \mathbb{R}^{2d}$ is called symplectic if the Jacobian matrix g' is everywhere symplectic, i.e. if

$$(g')^\top J g' = J.$$

It is well known that the flow $\varphi_t : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ of any system of form (26) is symplectic. In a natural manner, a numerical integrator is called symplectic if its numerical flow Ψ_h is a symplectic map whenever it is applied to a smooth Hamiltonian system (Hairer et al. 2006, Definition VI.3.1). In the following, we will analyse both the local and global properties of the RTS-RK method built on symplectic integrators and applied to (26).

7.1 Symplecticity of the RTS-RK method

It has been pointed out (Hairer et al. 2006, Section VIII.1) that applying an adaptive step size technique to a symplectic method can destroy its symplecticity. Therefore, Skeel and Gear (1992) write any adaptive technique in terms of a map $\tau(y, h)$ such that the kth time step h_k is selected as $h_k = \tau(y_k, h)$, where h is a base value for the time step. Hence, in order to have again a symplectic method for variable time steps, the new condition to be satisfied is

$$\begin{aligned} V^\top J V = J, \quad V &= \partial_y \Psi_{\tau(y,h)}(y) \\ &\quad + \partial_t \Psi_{\tau(y,h)}(y) \partial_y \tau(y, h)^\top. \end{aligned}$$

Let us now consider the RTS-RK method based on a symplectic deterministic integrator. We have the following lemma.

Lemma 5 *If the flow Ψ_h of the deterministic integrator is symplectic, then the flow of the random time-stepping probabilistic method (4) is symplectic.*

Proof For the RTS-RK scheme, the kth time step H_k is generated by a random mapping as $H_k = \tau(y, h) = \tau(h) = h\Theta_k$, where Θ_k are appropriately scaled random variables such

that H_k satisfies Assumption 1. Hence, τ is independent of y, i.e. $\partial_y \tau(y,h) = 0$, and with the notation introduced above

$$V = \partial_y \Psi_{\tau(h)}(y).$$

Therefore, by the symplecticity of Ψ_t the condition $V^\top J V = J$ is satisfied and the flow map of the RTS-RK method is symplectic. □

Let us remark that the local symplecticity of the flow map is not sufficient for good conservation of the Hamiltonian for the numerical solution. Global properties of approximation of the energy are therefore presented below.

7.2 Long-time conservation of Hamiltonians

We now wish to study the mean conservation of the Hamiltonian along the trajectories of the RTS-RK method based on symplectic integrators. Our goal is obtaining a bound on the quantity $\mathbb{E}|Q(Y_n) - Q(y_0)|$ that holds over long times. Showing theoretically long-time conservation of the energy function in Hamiltonian systems requires backward error analysis. In the following, we will introduce the basis of this technique and show how they apply to our probabilistic integrator. For further details, a comprehensive treatment of backward error analysis ought to be found in Hairer et al. (2006, Chapter IX).

The first ingredient needed to perform a rigorous backward error analysis is a rather strong assumption on the regularity of the ODE, see e.g. Hairer et al. (2006, Section IX.7).

Assumption 5 The function f is analytic in a neighbourhood of the initial condition y_0 and there exist constants $C, R > 0$ such that $\|f(y)\| \leq C$ for $\|y - y_0\| \leq 2R$.

In general, backward error analysis is based on determining a modified equation $y' = \widetilde{f}(y)$ such that the numerical approximation is its exact solution. Hence, the function $\widetilde{f}$ will both depend on the original ODE and on the numerical flow map Ψ_h. In particular, for an integrator of order q the modified equation is given by a function $\widetilde{f}$ defined as

$$\widetilde{f}(y) = f(y) + h^q f_{q+1}(y) + h^{q+1} f_{q+2}(y) + \cdots,$$

where the functions $\{f_i\}_{i>q}$ are uniquely determined by f, its derivatives and by the coefficients of the Runge–Kutta method. The exactness of the numerical solution for the modified equation is nonetheless only formal, as the infinite sum defining $\widetilde{f}$ is not guaranteed to converge. Thus, it is necessary to truncate the sum in order to perform a rigorous analysis, i.e.

$$\widetilde{f}(y) = f(y) + h^q f_{q+1}(y) + h^{q+1} f_{q+2}(y) + \cdots + h^{N-1} f_N(y). \tag{27}$$

where $q < N < \infty$ is the truncation index. Let us remark that in the following we will always refer to the truncated function above when using the symbol $\widetilde{f}$. The truncation of the infinite sum implies that the numerical solution is not exact for the modified equation anymore. In particular, the error committed over one step on the modified equation is given by (see e.g. Hairer et al. 2006, Theorem IX.7.6)

$$\|\widetilde{\varphi}_h(y) - \Psi_h(y)\| \leq Che^{-\kappa/h}, \tag{28}$$

where $\widetilde{\varphi}$ is the exact flow of the modified equation and κ and C are constants depending on the coefficients of the method and on the regularity of f.

It is possible to prove (see e.g. Hairer et al. 2006, Section IX.8) that for a Hamiltonian system (26) and a symplectic integrator the modified equation is still a Hamiltonian system, i.e. there exists a modified Hamiltonian $\widetilde{Q}$ defined as

$$\widetilde{Q}(y) = Q(y) + h^q Q_{q+1}(y) + \cdots + h^{N-1} Q_N(y), \tag{29}$$

such that $\widetilde{f} = J^{-1}\nabla\widetilde{Q}$. Estimate (28) implies that the modified Hamiltonian is almost conserved by the symplectic integrator. In particular, if Q is Lipschitz, we have

$$|\widetilde{Q}(\Psi_h(y)) - \widetilde{Q}(y)| \leq Che^{-\kappa/h}. \tag{30}$$

The bound above guarantees that the modified Hamiltonian is well approximated for a long time, and as a consequence that the original Hamiltonian is almost conserved for the same time span. In particular, the following result is valid (see e.g. Hairer et al. (2006, Theorem IX.8.1.) or Benettin and Giorgilli (1994)).

Theorem 5 *Under Assumption 5 and for h sufficiently small, if the numerical solution y_n given by a symplectic method of order q applied to an Hamiltonian system is close enough to the initial condition y_0, then*

$$\widetilde{Q}(y_n) = \widetilde{Q}(y_0) + \mathcal{O}(e^{-\kappa/2h}),$$
$$Q(y_n) = Q(y_0) + \mathcal{O}(h^q).$$

over exponentially long time intervals $nh \leq e^{\kappa/2h}$.

The randomisation of the time steps implies that a general modified equation does not exist. Nonetheless, due to Lemma 5, it is possible to construct locally a random Hamiltonian modified equation at each time step. We thus define at each step the random modified Hamiltonian as

$$\widehat{Q}_j(y) = Q(y) + H_j^q Q_{q+1}(y) + \cdots + H_j^{N-1} Q_N(y). \tag{31}$$

As for the deterministic case, the random modified Hamiltonian $\widehat{Q}$ will be almost conserved by the numerical flow. In particular, we define the random local truncation error as

$$\eta_j := \widehat{Q}_j(\Psi_{H_j}(y)) - \widehat{Q}_j(y), \tag{32}$$

which, in the light of (30), satisfy

$$|\eta_j| \leq C H_j \mathrm{e}^{-\kappa/H_j}, \tag{33}$$

almost surely. In order to prove the conservation of the Hamiltonian over long time for the RTS-RK method, it is necessary to introduce a technical assumption on the higher moments of the random time steps.

Assumption 6 There exists $\bar{r} > 1$ such that for any $1 < r < \bar{r}$, the random time steps $\{H_j\}_{j\geq 0}$ satisfy

$$\mathbb{E}H_j^r = h^r + C_r h^{2p+r-1},$$

where p is defined in Assumption 1 and $C_r > 0$ satisfies $C_{2r} > 2C_r$ and is independent of h. Moreover, there exists $m, M > 0$ with $M > m$ such that $mh \leq H_j \leq Mh$ almost surely for all $j \geq 0$.

This assumption guarantees that the higher moments of the random time steps are close to the corresponding powers of h in the mean and mean square sense. In particular, it is possible to verify that

$$\mathbb{E}(H_j^r - h^r) = C_r h^{2p+r-1},$$
$$\mathbb{E}(H_j^r - h^r)^2 = (C_{2r} - 2C_r) h^{2p+2r-1}.$$

Then, for any $r, s > 1$ such that $r + s < R$, it holds

$$\mathbb{E}(H_j^{r+s} - h^{r+s}) = \widehat{C}_{r,s} h^s \mathbb{E}(H_j^r - h^r),$$
$$\mathbb{E}(H_j^{r+s} - h^{r+s})^2 = \widetilde{C}_{r,s} h^{2s} \mathbb{E}(H_j^r - h^r)^2,$$

where $\widehat{C}_{r,s} = C_{r+s}/C_r$ and $\widetilde{C}_{r,s} = (C_{2(r+s)} - 2C_{r+s})/(C_{2r} - 2C_r)$. Finally, let us remark that Assumption 6 is satisfied for the uniform random time steps $H_j \overset{\text{i.i.d.}}{\sim} \mathcal{U}(h - h^{p+1/2}, h + h^{p+1/2})$ introduced in Example 1. Let us now prove a bound on the random variables η_j defined in (32).

Lemma 6 *Suppose that Assumptions 1, 3 and 6 hold true, and suppose that $0 < h \leq 1$. Then the random variables η_j satisfy*

$$\mathbb{E}|\eta_j|^r \leq C h^{\min\{r, p+r-3/2\}} \mathrm{e}^{-r\kappa/(Mh)},$$

where $C > 0$ is independent of h and for all $r \in \mathbb{N}$ with $r \geq 1$.

Proof The proof is given in the Appendix. □

Let us furthermore introduce two lemmas, which will be employed for proving long-time conservation of Hamiltonians. Let us remark that in Lemma 7 the values n, q, N indicate generic positive integers.

Lemma 7 *Let n, q, N be positive integers with $N > q$, and let us define the sets of real numbers $a = a_{n,q,N} := \{a_{jk},\ j = 0, \ldots, n-1,\ k = q, \ldots, N-1\}$ and $b = b_n := \{b_j,\ j = 0, \ldots, n-1\}$. Then*

$$\Big(\sum_{j=0}^{n-1}\Big(\sum_{k=q}^{N-1} a_{jk} + b_j\Big)\Big)^2 = \sum_{j=0}^{n-1} a_{jq}^2 + 2\sum_{j=1}^{n-1}\sum_{i=0}^{j-1} a_{jq}a_{iq} + R(a) + S(a,b),$$

where the remainder $R(a)$ can be written as $R = R_1 + R_2 + R_3$, with

$$R_1(a) = \sum_{j=0}^{n-1}\sum_{k=q+1}^{N-1} a_{jk}^2,$$
$$R_2(a) = 2\sum_{j=0}^{n-1}\sum_{k=q+1}^{N-1}\sum_{l=q}^{k-1} a_{jk}a_{jl},$$
$$R_3(a) = 2\sum_{j=1}^{n-1}\sum_{i=0}^{j-1}\sum_{k=q}^{N-1}\sum_{\substack{l=q \\ l+k>2q}}^{N-1} a_{jk}a_{il},$$

and the remainder $S(a,b)$ can be written as $S = S_1 + S_2 + S_3 + S_4$, with

$$S_1(a,b) = \sum_{j=0}^{n-1} b_j^2,$$
$$S_2(a,b) = 2\sum_{j=1}^{n-1}\sum_{i=0}^{j-1} b_i b_j,$$
$$S_3(a,b) = 2\sum_{j=1}^{n-1}\sum_{k=q}^{N-1} b_j a_{jk},$$
$$S_4(a,b) = 2\sum_{j=1}^{n-1}\sum_{i=0}^{n-1}\left(b_j\sum_{k=q}^{N-1} a_{ik} + b_i\sum_{k=q}^{N-1} a_{jk}\right).$$

Proof The proof is given in the Appendix. □

Lemma 8 *Let Assumption 1 hold with $p \geq 3/2$ and $h < 1$, and let Assumption 2, Assumption 5 and Assumption 6 hold. Moreover, let q be specified in Assumption 2 and N be the truncation index of the modified right-hand side (27). Let us consider the sets of real-valued random variables $\Delta := \{\Delta_{j,k}(H_j^k - h^k),\ j = 0, \ldots, n-1,\ k = q, \ldots, N-1\}$,*

where $\Delta_{j,k} := Q_{k+1}(Y_j) - Q_{k+1}(Y_{j+1})$ *and* $\eta := \{\eta_j, j = 0, \dots, n-1\}$. *Then, with the notation of Lemma 7, there exist positive constants* C_1, C_2 *independent of* h *and* n, *but possibly dependent on* q *and* N, *such that*

$$\mathbb{E}R(\Delta) \le C_1 \left(t_n h^{2(p+q+1/2)} + t_n^2 h^{2(2p+q-1/2)} \right),$$
$$\mathbb{E}S(\Delta, \eta) \le C_2 \left((t_n h + t_n^2) e^{-2\kappa/(Mh)} + (t_n h^{p+q+1/2} + t_n^2 h^{2p+q-1}) \mathrm{e}^{-\kappa/(Mh)} \right),$$

where $t_n = nh$.

Proof The proof is given in the Appendix. □

It is now possible to prove a result of long conservation of the Hamiltonian for symplectic RTS-RK methods.

Theorem 6 *Let* $0 < h \le 1$. *Suppose that Assumption 1 holds for* $p \ge 3/2$, *that Assumptions 3 and 5 hold and that Assumption 6 holds with* $\bar{r}$ *sufficiently large. Moreover, let* Y_n *be the solution given by the RTS-RK method built on a symplectic integrator of order* q *applied to a Hamiltonian system with Hamiltonian* Q. *If* $Y_0 = y_0$ *and the numerical solution* Y_n *is close enough to the initial condition* y_0 *almost surely, then there exist a constant* $C > 0$ *independent of* h *and* n *such that*

$$\mathbb{E}|Q(Y_n) - Q(y_0)| \le Ch^q,$$

for time intervals of length

$$t_n = \mathcal{O}\big(\min\{h^{1-2p}, \mathrm{e}^{\kappa/(4Mh)} h^{-(2p+2q-1)/4}, \mathrm{e}^{\kappa/(2Mh)}\} \big)$$

where p *is given in Assumption 1 and* M *in Assumption 6.*

Proof In the following proof, we denote by C a positive constant independent of h and n which can possibly change value from line to line. Let us first consider the modified Hamiltonian $\widetilde{Q}$ and expand the difference $\widetilde{Q}(Y_n) - \widetilde{Q}(y_0)$ in a telescopic sum as

$$\widetilde{Q}(Y_n) - \widetilde{Q}(y_0) = \sum_{j=0}^{n-1} \big(\widetilde{Q}(Y_{j+1}) - \widetilde{Q}(Y_j) \big). \tag{34}$$

We then consider each element of the sum, add and subtract the random modified Hamiltonian $\widehat{Q}_j$ computed in Y_{j+1} thus obtaining

$$\begin{aligned} \widetilde{Q}(Y_{j+1}) - \widetilde{Q}(Y_j) &= \widetilde{Q}(Y_{j+1}) - \widehat{Q}_j(Y_{j+1}) \\ &\quad + \widehat{Q}_j(Y_{j+1}) - \widetilde{Q}(Y_j) \\ &= \widetilde{Q}(Y_{j+1}) - \widehat{Q}_j(Y_{j+1}) \\ &\quad + \widehat{Q}_j(Y_j) - \widetilde{Q}(Y_j) + \eta_j. \end{aligned}$$

Hence, by applying definition (29) of $\widetilde{Q}$ and (31) of $\widehat{Q}_j$, we get

$$\widetilde{Q}(Y_{j+1}) - \widetilde{Q}(Y_j) = \sum_{k=q}^{N-1} (H_j^k - h^k) \Delta_{j,k} + \eta_j,$$

where $\Delta_{j,k}$ is defined in Lemma 8. Going back to (34), applying Jensen's inequality and Lemma 7 we obtain

$$\begin{aligned} \big(\mathbb{E}|\widetilde{Q}(Y_n) - \widetilde{Q}(y_0)|\big)^2 &\le \mathbb{E}\Big(\sum_{j=0}^{n-1} \Big(\sum_{k=q}^{N-1} (H_j^k - h^k) \Delta_{j,k} + \eta_j \Big) \Big)^2 \\ &= \sum_{j=0}^{n-1} \mathbb{E}\big((H_j^q - h^q)^2 \Delta_{j,q}^2 \big) \\ &\quad + 2 \sum_{j=1}^{n-1} \sum_{i=0}^{j-1} \mathbb{E}\big((H_j^q - h^q) \Delta_{j,q} (H_i^q - h^q) \Delta_{i,q} \big) \\ &\quad + \mathbb{E}R(\Delta) + \mathbb{E}S(\Delta, \eta). \end{aligned} \tag{35}$$

The first term in (35) satisfies

$$\left(\sum_{j=0}^{n-1} \mathbb{E}\big((H_j^q - h^q)^2 \Delta_{j,q}^2 \big) \right)^{1/2} \le C \sqrt{t_n} h^{p+q}, \tag{36}$$

due to (58). Now, considering (60), we obtain that the second term in (35) satisfies

$$\left(2 \sum_{j=1}^{n-1} \sum_{i=0}^{j-1} \mathbb{E}\left((H_j^q - h^q) \Delta_{j,q} (H_i^q - h^q) \Delta_{i,q} \right) \right)^{1/2} \le C t_n h^{2p+q-1}.$$

For the remainder term $\mathbb{E}R(\Delta)$, due to Lemma 8 we get

$$(\mathbb{E}R(\Delta))^{1/2} \le C \left(\sqrt{t_n} h^{p+q+1/2} + t_n h^{2p+q-1/2} \right).$$

For the remainder term $\mathbb{E}S(\Delta, \eta)$, due to Lemma 8 and since $h \le 1$ and $p \ge 3/2$ by assumption, we get

$$\begin{aligned} (\mathbb{E}S(\Delta, \eta))^{1/2} &\le C \Big(t_n^2 \big(\mathrm{e}^{-2\kappa/(Mh)} + h^{p+q+1/2} \mathrm{e}^{-\kappa/(Mh)} \big) \Big)^{1/2} \\ &\le C t_n \big(\mathrm{e}^{-\kappa/(Mh)} + h^{(2p+2q+1)/4} \mathrm{e}^{-\kappa/(2Mh)} \big). \end{aligned} \tag{37}$$

Finally, taking the square root of both sides of (35), replacing the expressions we obtained above and since $h \le 1$, we get that the modified Hamiltonian satisfies

$$\begin{aligned} \mathbb{E}|\widetilde{Q}(Y_n) - \widetilde{Q}(y_0)| &\le C \Big(\sqrt{t_n} h^{p+q} \\ &\quad + t_n h^{2p+q-1} + t_n \big(\mathrm{e}^{-\kappa/(Mh)} + h^{(2p+2q+1)/4} \mathrm{e}^{-\kappa/(2Mh)} \big) \Big). \end{aligned}$$

Hence, imposing for a constant $C > 0$

$$t_n \leq C \min\{h^{1-2p}, \mathrm{e}^{\kappa/(4Mh)} h^{-(2p+2q-1)/4}, \mathrm{e}^{\kappa/(2Mh)}\},$$

and since exponential terms are dominated by polynomial terms (see e.g. Hairer et al. 2006, Theorem IX.8.1), we obtain

$$\mathbb{E}|\widetilde{Q}(Y_n) - \widetilde{Q}(y_0)| \leq Ch^q. \tag{38}$$

Finally, applying the triangle inequality, since for all $y \in \mathbb{R}^d$ it holds $|Q(y) - \widetilde{Q}(y)| \leq Ch^q$ by definition of the modified Hamiltonian $\widetilde{Q}$ and due to (38), we get

$$\begin{aligned}\mathbb{E}|Q(Y_n) - Q(y_0)| &\leq \mathbb{E}|Q(Y_n) - \widetilde{Q}(Y_n)| + \mathbb{E}|Q(y_0) - \widetilde{Q}(y_0)| \\ &\quad + \mathbb{E}|\widetilde{Q}(Y_n) - \widetilde{Q}(y_0)| \\ &\leq Ch^q,\end{aligned}$$

which is the desired result. □

Remark 11 The result of Theorem 6 is consistent with the theory of deterministic symplectic integrators. In fact, in the limit $p \to \infty$, one can choose the coefficient M in Assumption 6 arbitrarily close to 1 and we have

$$\mathbb{E}|Q(Y_n) - Q(y_0)| = \mathcal{O}(h^q),$$

for exponentially long time spans $t_n = \mathcal{O}\big(\mathrm{e}^{\kappa/(2h)}\big)$, which is consistent with the theory of deterministic symplectic integrators summarised by Theorem 5.

Remark 12 It has been observed (see, for example, Hairer 1997; Hairer et al. 2006) that adopting variable step sizes in symplectic integration destroys the good properties of conservation of the Hamiltonian. In particular, the error on the Hamiltonian has a linear drift in time, i.e. the approximation has the same quality as the one given by a standard non-symplectic algorithm. Conversely, Theorem 6 proves that random step sizes do not spoil, under the assumptions specified above, the good long-time properties of symplectic integrators with fixed step size.

Remark 13 As it can be noticed in the proof of Lemma 8, we introduce the assumption $p \geq 3/2$ in order to simplify the terms composing the remainder $S(\Delta, \eta)$. In case $1 \leq p < 3/2$, e.g. when the symplectic Euler method is employed ($q = 1$) and the natural scaling $p = q$ is chosen, the $\mathcal{O}(h^q)$ approximation of the Hamiltonian still holds but with a slight reduction in the exponential terms appearing in the time span of validity.

Remark 14 Let us remark that in order for (37) to hold we implicitly assumed $t_n \geq 1$ to bound $\sqrt{t_n} \leq t_n$. If $t_n < 1$, we can bound every appearance of t_n from (36) to (37) as $t_n \leq 1$, and the desired result would still hold.

8 Bayesian inference

It has been recently shown (Chkrebtii et al. 2016; Conrad et al. 2017; Lie et al. 2018) that probabilistic methods for ordinary and partial differential equations guarantee robust results (with respect to the numerical discretisation error) in the context of Bayesian inverse problems. In this section, we briefly introduce a Bayesian inverse problem in the ODE setting and illustrate how the RTS-RK method can be employed in this framework.

Let us consider a function $f_\vartheta : \mathbb{R}^d \to \mathbb{R}^d$ which depends on a real parameter $\vartheta \in \Theta$, where Θ is an open subset of $\mathbb{R}^n$ and the ODE

$$y'_\vartheta = f_\vartheta(y), \quad y_\vartheta(0) = y_0 \in \mathbb{R}^d.$$

In order to simplify the notation, we consider y_0 to be a fixed initial condition. In general, y_0 could depend itself on ϑ. In the classical setting of numerical analysis, the main problem of interest is to determine the solution y_ϑ given the parameter ϑ. The inverse problem we consider is instead to determine ϑ through observations of the solution y_ϑ (or quantities derived from it). In the Bayesian setting, the inverse problem is recast in terms of probability distributions, and the goal is to establish a probability measure on ϑ, known as the posterior measure, given observed data and a probability measure, known as the prior, which captures all knowledge on the parameter available beforehand.

Let us denote by $z \in \mathbb{R}^m$ the observable and by $\mathcal{G} \colon \Theta \to \mathbb{R}^m$ the forward operator, which can be written as $\mathcal{G} = \mathcal{O} \circ \mathcal{S}$, where $\mathcal{S}$ is the solution operator and $\mathcal{O}$ is the observation operator. In this case, $\mathcal{S} \colon \mathbb{R}^n \to \mathcal{C}([0, T])$ is the operator mapping ϑ into the solution y_ϑ, and $\mathcal{O} \colon \mathcal{C}([0, T]) \to \mathbb{R}^m$ maps the solution into the observable. Observations are then given by evaluations of the forward model corrupted by noise. In particular, we model noise as a Gaussian random variable $\varepsilon \sim \mathcal{N}(0, \Sigma_\varepsilon)$ independent of ϑ, so that observations read

$$z = \mathcal{G}(\vartheta) + \varepsilon.$$

Under these assumptions, the likelihood of the observations can be written as

$$\pi(z \mid \vartheta) = \mathrm{e}^{-V_z(\vartheta)}, \tag{39}$$

where the function $V_z \colon \Theta \to \mathbb{R}$, called the potential or negative log-likelihood, is given by

$$V_z(\vartheta) = \frac{1}{2}\big(\mathcal{G}(\vartheta) - z\big)^\top \Sigma_\varepsilon^{-1}\big(\mathcal{G}(\vartheta) - z\big). \tag{40}$$

The second building block of Bayesian inverse problems is the prior distribution, which we denote by $\pi_0(\vartheta)$. The prior encodes all the knowledge on the parameter that is known

before observations are provided. In the following, we adopt a common abuse of notation, confounding measures and their probability density function.

Once the likelihood model and the prior distribution are established, it is possible to compute the posterior distribution $\pi(\vartheta \mid z)$ via Bayes' theorem, i.e.

$$\pi(\vartheta \mid z) = \frac{\pi(z \mid \vartheta)\pi_0(\vartheta)}{\mathcal{Z}(z)},$$

where $\mathcal{Z}(z)$ is the normalising constant given by

$$\mathcal{Z}(z) = \int_\Theta \pi(z \mid \vartheta)\pi_0(\vartheta)\, \mathrm{d}\vartheta.$$

Let us denote by $\mathcal{G}^h(\vartheta)$ the forward model where the solution operator is approximated by a Runge–Kutta method with time step h, and consequently with $V_z^h(\vartheta)$ and $\pi^h(z \mid \vartheta)$ the potential and the likelihood function obtained replacing $\mathcal{G}(\vartheta)$ with $\mathcal{G}^h(\vartheta)$. We can then define analogously the approximated posterior distribution $\pi^h(\vartheta \mid z)$ via Bayes' formula. In the following, we assume that the posteriors $\pi(\vartheta \mid z)$ and $\pi^h(\vartheta \mid z)$ are absolutely continuous with respect to the Lebesgue density. In Stuart (2010, Theorem 4.6), the author proves that the posterior distribution $\pi^h(\vartheta \mid z)$ converges to $\pi(\vartheta \mid z)$ with respect to h with the same rate as $V_z^h(\vartheta)$ converges to $V_z(\vartheta)$. There, convergence is shown with respect to the Hellinger distance for a Gaussian prior, which is defined for probability density functions which are absolutely continuous with respect to the Lebesgue density as

$$d_{\mathrm{Hell}}\big(\pi^h(\vartheta \mid z), \pi(\vartheta \mid z)\big)^2 = \frac{1}{2}\int_\Theta \left(\sqrt{\pi^h(\vartheta \mid z)} - \sqrt{\pi(\vartheta \mid z)}\right)^2 \mathrm{d}\vartheta.$$

Hence, when there is no restriction in computational resources and it is possible to choose h small, the approximated posterior distribution can be made arbitrarily close to the true posterior. The result is proved in Stuart (2010) under the hypothesis of a Gaussian prior, but can be extended to a wider class of thin-tailed priors as done in Dashti and Stuart (2016) and to heavy-tailed priors as done in Sullivan (2017).

In this work, we consider the case when h is fixed, and in particular, we are interested in the case where the numerical error dominates the noise contribution. It has been shown via examples in Cockayne et al. (2017) and Conrad et al. (2017) that in this small noise limit the approximated posterior distributions can be overly confident on the value of the parameter. In particular, the expectation of ϑ computed under the posterior distribution exhibits a bias with respect to the true value, which is not highlighted by the dispersion of the posterior itself. This undesirable phenomenon can be corrected by means of a probabilistic method, as the one presented in Conrad et al. (2017) or the RTS-RK method, to approximate the potential $V_z(\vartheta)$. Let us denote by $\xi \in \mathcal{X}$ the auxiliary random variable introduced by the probabilistic method. In the case of RTS-RK, we have $\xi = (H_0, H_1, \ldots, H_{N-1})^\top$ and $\mathcal{X} \subset \mathbb{R}_+^N$. The likelihood function, denoted as $\pi_{\mathrm{pr}}^h(z \mid \vartheta)$, is then defined by

$$\pi_{\mathrm{prob}}^h(z \mid \vartheta) = \mathbb{E}^\xi \mathrm{e}^{-V_z^{h,\xi}(\vartheta)}.$$

where $V_z^{h,\xi}$ is the approximation of the potential function given by the probabilistic method. The corresponding posterior distribution π_{pr}^h is then defined by

$$\pi_{\mathrm{prob}}^h(\vartheta \mid z) = \frac{\pi_{\mathrm{prob}}^h(z \mid \vartheta)\pi_0(\vartheta)}{\mathbb{E}^\xi\, \mathcal{Z}^{h,\xi}(z)}, \tag{41}$$

where the normalising constant is given by $\mathbb{E}^\xi\, \mathcal{Z}^{h,\xi}(z)$, where

$$\mathcal{Z}^{h,\xi}(z) = \int_\Theta \mathrm{e}_z^{-V^{h,\xi}}(\vartheta)\pi_0(\vartheta)\, \mathrm{d}\vartheta.$$

Modifying the posterior in this manner allows to obtain qualitatively better results, which account for the uncertainty introduced by the numerical solver. Moreover, this posterior distribution still converges to the true posterior for $h \to 0$ as proved in Lie et al. (2018), where (41) is called the marginal posterior.

In order to sample from the posteriors defined above, we employ Markov chain Monte Carlo (MCMC) algorithms. In particular, due to the manner in which the probabilistic posterior (41) is defined, the pseudo-marginal Metropolis–Hastings (PMMH) algorithm (Andrieu and Roberts 2009) is a suitable choice for sampling. We note that in case of a deterministic approximation of the forward model, the standard random walk Metropolis–Hastings can be employed.

8.1 Analytical posteriors in a linear problem

If the forward operator $\mathcal{G}$ is linear, the prior on the unknown parameter is Gaussian, and the negative log-likelihood is given by (40), then there is an explicit formula for the corresponding posterior distribution. Let us hence consider the following one-dimensional ODE

$$y'(t) = -y(t), \quad y(0) = \vartheta.$$

Given $h > 0$, we consider the inferential problem of determining the true initial condition ϑ^* from a single observation $z = \varphi_h(\vartheta^*) + \varepsilon$, where $\varphi_h(\vartheta^*) = \vartheta^* \mathrm{e}^{-h}$ is the true solution at time $t = h$ and $\varepsilon \sim \mathcal{N}(0, \sigma^2)$ is a source of noise. In this case, the parameter space is $\Theta = \mathbb{R}$ and the forward operator $\mathcal{G}$ is defined by $\mathcal{G}\colon \mathbb{R} \to \mathbb{R}$, $\mathcal{G}\colon \vartheta \mapsto \vartheta \mathrm{e}^{-h}$. In the following, we verify heuristically the convergence of the

posterior distributions obtained with deterministic and probabilistic integrators with respect to a vanishing noise scale. If a Gaussian prior $\pi_0 = \mathcal{N}(0, 1)$ is given for ϑ, the true posterior distribution is computable analytically and is given by

$$\pi(\vartheta \mid z) = \mathcal{N}\Big(\vartheta; \frac{z\mathrm{e}^{-h}}{\sigma^2 + \mathrm{e}^{-2h}}, \frac{\sigma^2}{\sigma^2 + \mathrm{e}^{-2h}}\Big), \tag{42}$$

where $\mathcal{N}(x; \mu, \alpha^2)$ is the density of a Gaussian random variable of mean μ and variance α^2 evaluated in x. Consistently, if $\sigma^2 \to 0$, we have that $z \to \vartheta^* \mathrm{e}^{-h}$ and therefore $\pi(\vartheta \mid z) \to \delta_{\vartheta^*}$.

If we approximate $\varphi_h(\vartheta)$ for a given initial condition ϑ with a single step of the explicit Euler method (i.e. with step size h), we get $\Psi_h(\vartheta) = (1-h)\vartheta$. Computing the posterior distribution obtained with this approximation leads to

$$\pi^h(\vartheta \mid z) = \mathcal{N}\left(\vartheta; \frac{(1-h)z}{\sigma^2 + (1-h)^2}, \frac{\sigma^2}{\sigma^2 + (1-h)^2}\right). \tag{43}$$

In the limit of $\sigma^2 \to 0$, we get in this case that the posterior distribution tends to $\pi^h(\vartheta \mid z) \to \delta_{\bar{\vartheta}}$, where $\bar{\vartheta} = \mathrm{e}^{-h}\vartheta^*/(1-h)$. The posterior distribution is hence tending to a biased Dirac delta with respect to the true value.

Let us consider the additive noise method (3) applied to the explicit Euler method, i.e. the random approximation $y(h) \approx Y_1$, where $Y_1 = (1-h)\vartheta + \xi$ and where $\xi \sim \mathcal{N}(0, h^3)$, so that the method converges consistently with the deterministic method. In this case, the posterior distribution that we denote by $\pi^h_{\mathrm{prob,AN}}$ is given by

$$\pi^h_{\mathrm{prob,AN}}(\vartheta \mid z) = \mathcal{N}\Big(\vartheta; \frac{(1-h)z}{\widetilde{\sigma}^2 + (1-h)^2}, \frac{\widetilde{\sigma}^2}{\widetilde{\sigma}^2 + (1-h)^2}\Big).$$

where $\widetilde{\sigma}^2 = \sigma^2 + h^3$. Hence, taking the limit $\sigma^2 \to 0$ gives

$$\pi^h_{\mathrm{prob,AN}}(\vartheta \mid z) \to \mathcal{N}\Big(\vartheta; \frac{(1-h)\mathrm{e}^{-h}\vartheta^*}{h^3 + (1-h)^2}, \frac{h^3}{h^3 + (1-h)^2}\Big), \tag{44}$$

which shows that while the asymptotic mean is still biased with respect to the true value, the uncertainty in the forward model is reflected by a positive variance. Let us now consider the random time step explicit Euler with step size distribution $H \sim \mathcal{U}(h - h^{p+1/2}, h + h^{p+1/2})$. In this case, the forward model is given by

$$Y_1 = \vartheta - H\vartheta = (1-h)\vartheta + U\vartheta, \quad U \sim \mathcal{U}(-h^{p+1/2}, h^{p+1/2}).$$

Hence, disregarding all multiplicative constants that are independent of ϑ and setting $p = q = 1$, we get the posterior

$$\pi^h_{\mathrm{prob,RTS}}(\vartheta \mid z) \propto \exp\Big(-\frac{\vartheta^2}{2}\Big) \frac{1}{\vartheta}\Big(\Phi\Big(\frac{((1-h) + h^{3/2})\vartheta - z}{\sigma}\Big) - \Phi\Big(\frac{((1-h) - h^{3/2})\vartheta - z}{\sigma}\Big)\Big), \tag{45}$$

where Φ denotes the cumulative distribution function of a standard Gaussian random variable. Since we require in Assumption 1(i) that $H > 0$ almost surely, the time step H cannot be Gaussian and the closed-form expression of the posterior is not as neatly defined as in the additive noise case. In the limit for $\sigma \to 0$, we get the limiting distribution

$$\pi^h_{\mathrm{prob,RTS}}(\vartheta \mid z) \propto \exp\Big(-\frac{\vartheta^2}{2}\Big) \frac{1}{\vartheta} \chi_{\{y_{\min} \le \vartheta \le y_{\max}\}},$$

where $y_{\min}$ and $y_{\max}$ are given by

$$y_{\min} = \frac{\mathrm{e}^{-h}\vartheta^*}{((1-h) + h^{3/2})}, \quad y_{\max} = \frac{\mathrm{e}^{-h}\vartheta^*}{((1-h) - h^{3/2})}.$$

It is hence possible to remark that for the RTS-RK method the variance of the posterior distribution is not collapsing to zero for $\sigma \to 0$ as in the deterministic case.

We fix $h = 0.5$ and consider $\sigma = \{0.1, 0.05, 0.025, 0.0125\}$, thus generating four observational noises η_i as $\eta_i = \sigma_i Z$ for a random variable $Z \sim \mathcal{N}(0, 1)$. In Fig. 3, we show posteriors (42), (43), (44) and (45), which confirm our claim, i.e. that probabilistic methods take into account the variability in the forward model caused by the numerical approximation and transfer it to the posterior belief.

9 Numerical experiments

In this section, we present a series of numerical experiments that illustrate the versatility and usefulness of our new random time-stepping method. These experiments also corroborate the theoretical results presented in the previous sections.

9.1 Weak order of convergence

In order to verify the result predicted in Theorem 2, we consider the FitzHugh–Nagumo equation, which is defined as

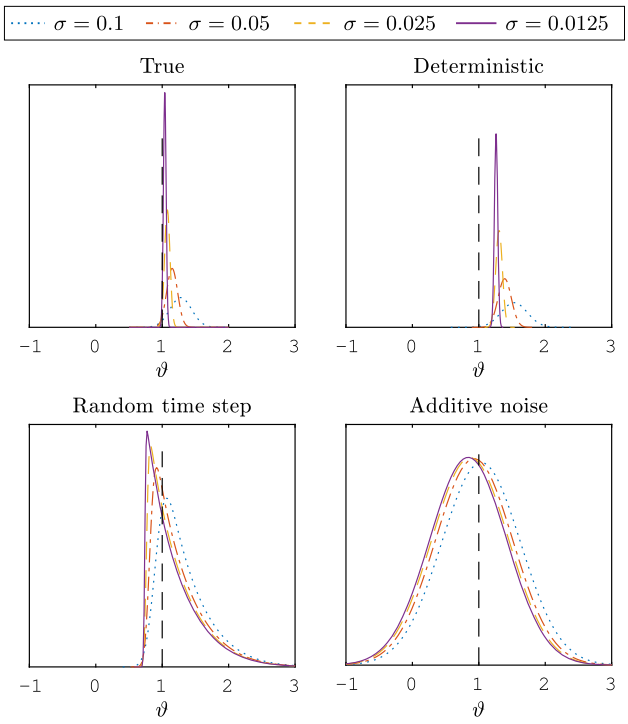

Fig. 3 Analytical posterior distributions in the linear case of Sect. 8.1 for the true solution and its approximations with the deterministic explicit Euler method and the two probabilistic versions with additive noise (3) and with random time steps (4). In this case, $h = 0.5$ and the variance σ^2 of the observation error is reduced progressively. The true value of the initial condition $\vartheta^* = 1$ is shown with a vertical black dashed line

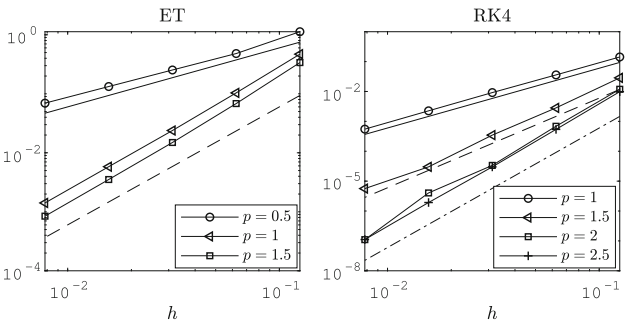

Fig. 4 Weak order of convergence for the random time-stepping explicit trapezoidal (ET) and fourth-order Runge–Kutta (RK4) as a function of the value of p of Assumption 1. In the left figure, reference slopes 1 and 2 are displayed (solid and dashed lines), while in the right figure reference slopes 2, 3 and 4 are displayed (solid, dashed and dash-dotted lines)

$$\begin{aligned} y_1' &= c\left(y_1 - \frac{y_1^3}{3} + y_2\right), \quad y_1(0) = -1, \\ y_2' &= -\frac{1}{c}(y_1 - a + by_2), \quad y_2(0) = 1, \end{aligned} \tag{46}$$

where a, b, c are real parameters with values $a = 0.2$, $b = 0.2$, $c = 3$. We integrate the equation from time $t_0 = 0$ to final time $T = 1$. The reference solution is generated with a high-order method on a fine time scale. The deterministic integrators we choose in this experiment are the explicit trapezoidal rule and the classic fourth-order Runge–Kutta method. The random steps are uniform as in Example 1. We vary their mean in the range $h_i = 0.125 \cdot 2^{-i}$ with $i = 0, 1, \ldots, 4$, and we vary the value of p in Assumption 1 in order to verify the theoretical result of Theorem 1. In particular, we consider $p \in \{0.5, 1, 1.5\}$ for the explicit trapezoidal rule and $p \in \{1, 1.5, 2, 2.5\}$ for the classic fourth-order Runge–Kutta method. The function $\Phi : \mathbb{R}^d \to \mathbb{R}$ of the solution we consider is defined as $\Phi(x) := x^\top x$. Finally, we consider 10^6 trajectories of the numerical solution in order to approximate the expectation with a Monte Carlo sum. Results (Fig. 4) show that the order of convergence predicted theoretically is confirmed by numerical experiments.

9.2 Mean square order of convergence

We now verify the weak order of convergence predicted in Theorem 1. For this experiment, we consider ODE (46) as well, with the same time scale T and parameters as in Sect. 9.1. The reference solution at final time is generated in this case as well with a high-order method on a fine time scale. We consider as deterministic solvers the explicit trapezoidal rule and the classic fourth-order Runge–Kutta method, which verify Assumption 2 with $q = 2$ and $q = 4$, respectively. Moreover, we consider uniform random time steps as in Example 1, where we vary the value of p in Assumption 1 in order to verify the order of convergence predicted in Theorem 2. In particular, we consider $p \in \{1, 2, 3\}$ for the explicit trapezoidal rule and $p \in \{2, 3, 4, 5\}$ for the classic fourth-order Runge–Kutta method. We vary the mean time step h taken by the random time steps H_n in the range $h_i = 0.125 \cdot 2^{-i}$, with $i = 0, 1, \ldots, 4$. Then, we simulate 10^3 realisations of the numerical solution Y_{N_i}, with $N_i = T/h_i$ for $i = 0, 1, \ldots, 4$, and compute the approximate mean square order of convergence for each value of h with a Monte Carlo mean. Results (Fig. 5) show that the orders predicted theoretically by Theorem 2 are confirmed numerically.

9.3 Mean square convergence of Monte Carlo estimators

We shall now verify numerically the validity of Theorem 3. We consider ODE (46), with final time $T = 1$ and the same parameters as above. In this case as well, we consider the explicit trapezoidal rule and the fourth-order explicit Runge–Kutta method with uniform random time steps having mean $h_i = 0.125 \cdot 2^{-i}$ with $i = 0, 1, \ldots, 7$. For the explicit trapezoidal rule, we fix $M = 10^3$ and $p = 1$, so that for bigger values of h the first term in the bound presented in Theorem 3 dominates, while in the regime of small h, the higher order of the first term makes the second term larger in mag-

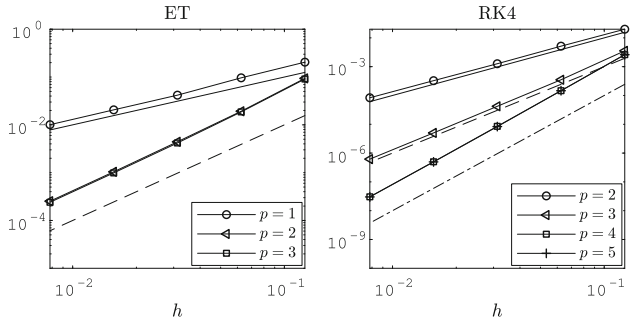

Fig. 5 Mean square order of convergence for the random time-stepping explicit trapezoidal (ET) and fourth-order Runge–Kutta (RK4) as a function of the value of p of Assumption 1. In the left figure, reference slopes 1 and 2 are displayed (solid and dashed lines), while in the right figure reference slopes 2, 3 and 4 are displayed (solid, dashed and dash-dotted lines)

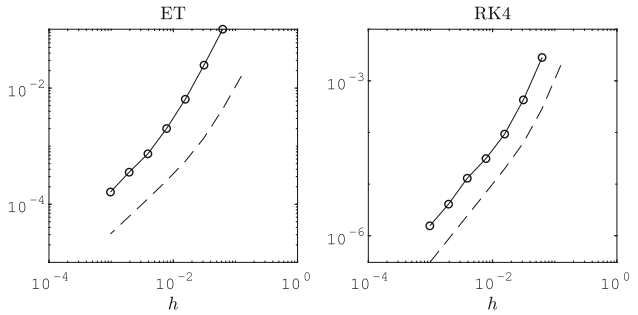

Fig. 6 Convergence of the square root of the MSE of the Monte Carlo estimator for the random time-stepping explicit trapezoidal (ET) (left figure) and fourth-order Runge–Kutta (RK4) (right figure) with respect to the time step h. The dashed line corresponds to the order predicted in Theorem 3 with $M = 10^3$ for ET and $M = 10^4$ for RK4

nitude. This behaviour results in the change of slope in the convergence plot which can be observed in Fig. 6, both in the theoretical estimate and in the numerical results. We perform the same experiment using the fourth-order explicit Runge–Kutta method, fixing $M = 10^4$ and $p = 1.5$, thus obtaining a numerical confirmation of the theoretical result.

As a second experiment, we consider the same setup as above but wish to verify the dependence of the MSE on the number of samples M, which we vary as $M = 2^i$, with $i = 0, 1, \ldots, 9$. For the explicit trapezoidal rule, we consider $p = q = 2$, which is the optimal choice for the intrinsic variability of the RTS-RK method. Moreover, we fix $h = 0.05$. In this case, bound (24) reduces to

$$\mathrm{MSE}(\widehat{Z}_{N,M}) \leq Ch^{2q}\left(1 + \frac{1}{M}\right).$$

In Fig. 7, we show that the convergence of the MSE depends on M as predicted by the theoretical bound. We repeat the same experiment using the fourth-order explicit Runge–Kutta method, for which we take $h = 0.01$ and $p = q = 4$, thus confirming numerically our theoretical result.

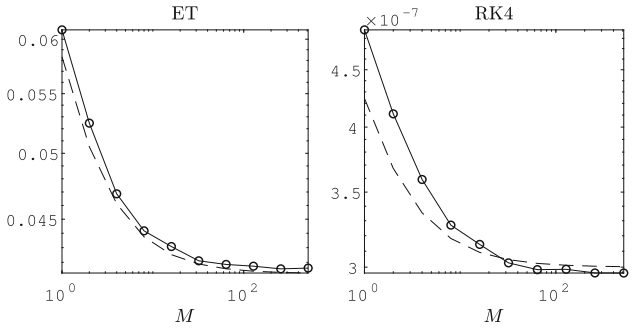

Fig. 7 Convergence of the square root of the MSE of the Monte Carlo estimator for the random time-stepping explicit trapezoidal (ET) (left figure) and fourth-order Runge–Kutta (RK4) (right figure) with respect to the number of trajectories M. The dashed line corresponds to the order predicted in Theorem 3 with $h = 0.05$ for ET and $h = 0.01$ for RK4

9.4 Robustness

In this numerical experiment, we verify the robustness of RTS-RK when applied to chemical reactions. Let us consider the peroxide–oxide chemical reaction, which is macroscopically defined by the following balance equation

$$O_2 + 2\mathrm{NADH} + 2H^+ \rightarrow 2H_2O + 2\mathrm{NAD}^+,$$

where NADH and NAD^+ are the oxidised and reduced form of the nicotinamide adenine dinucleotide (NAD), respectively. This reaction has to be catalysed by an enzyme to take place, which reacts with the reagents to create intermediate products of the reaction. A successful model (Olsen 1983) to describe the time evolution of the chemical system is the following

$$\begin{aligned} &B + X \xrightarrow{k_1} 2X, \quad 2X \xrightarrow{k_2} 2Y, \quad A + B + Y \xrightarrow{k_3} 3X, \\ &X \xrightarrow{k_4} P, \quad Y \xrightarrow{k_5} Q, \quad X_0 \xrightarrow{k_6} X, \\ &A_0 \xleftrightarrow{k_7} A, \quad B_0 \xrightarrow{k_8} B. \end{aligned}$$

Here, A and B are, respectively, $[O_2]$ and [NADH], P, Q are the products, and X, Y are intermediate results of the reaction process. It is therefore possible to model the time evolution of the reaction with the following system of nonlinear ODEs

$$\begin{aligned} A' &= k_7(A_0 - A) - k_3ABY, & A(0) &= 6, \\ B' &= k_8B_0 - k_1BX - k_3ABY, & B(0) &= 58, \\ X' &= k_1BX - 2k_2X^2 + 3k_3ABY - k_4X + k_6X_0, & X(0) &= 0, \\ Y' &= 2k_2X^2 - k_5Y - k_3ABY, & Y(0) &= 0, \end{aligned} \tag{47}$$

where $A_0 = 8$, $B_0 = 1$, $X_0 = 1$ and the real parameters k_i, $i = 1, \ldots, 8$ representing the reaction rates take values

$$k_1 = 0.35, \quad k_2 = 250, \quad k_3 = 0.035, \quad k_4 = 20,$$
$$k_5 = 5.35, \quad k_6 = 10^{-5}, \quad k_7 = 0.1, \quad k_8 = 0.825.$$

It has been shown (Olsen 1983) that for these values of the parameters the system exhibits a chaotic behaviour. In particular, at long time the trajectories lie in a strange attractor, and the system shows a strong sensitivity to perturbations on the initial condition.

Since the components of the solution represent the concentration of chemicals, we require the numerical solution to be positive. Apart from physical considerations, numerically we observe that if one of the components takes negative values, the solution shows strong instabilities. For the RTS-RK method, the distribution of the random time steps can be selected so that the probability of obtaining a negative solution is zero (see e.g. Example 1). In contrast, for the additive noise method we can have disruptive effects even for h small if the solution has a small magnitude, as the probability for negative populations will never be zero. Hence, in this case employing the additive noise method likely produces instabilities regardless of the chosen time step.

Let us apply the additive noise method (3) and the random time-stepping scheme (4) to Eq. (47). We choose $h = 0.05$ as the mean of uniformly distributed time steps for (4) and as the time step for (3), while we employ the Runge–Kutta–Chebyshev method (RKC) (van der Houwen and Sommeijer 1980) as deterministic integrator. Since RKC has order 1, we fix $p = q = 1$. As the problem is stiff, stabilised methods prevent a step size restriction while remaining explicit. We note that the RKC method is a stabilised numerical integrator of first order and that higher-order explicit stabilised methods such as ROCK2 or ROCK4 (Abdulle 2002; Abdulle and Medovikov 2001) could also be used as deterministic solvers for the RTS-RK method. It can be seen in Fig. 8 that the RTS-RK method conserves the positivity of the numerical solution while capturing the chaotic nature of the chemical reaction. In contrast, the additive noise scheme produces negative values, thus showing strong instabilities in the long-time behaviour. In particular, all the numerical trajectories turn negative or diverge before approximately $t = 25$, which is the reason why after this time they are not displayed in Fig. 8.

9.5 Conservation of quadratic first integrals

A simple model for the two-body problem in celestial mechanics is the Kepler system with a perturbation, which reads

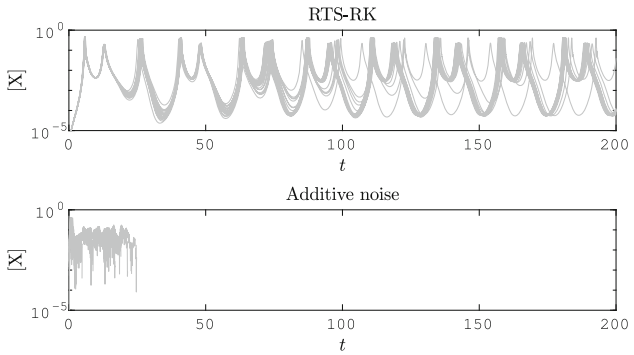

Fig. 8 Fifty trajectories of the numerical value of the concentration of the X species for the random time-stepping and additive noise methods (above and below, respectively)

$$\begin{aligned} w_1' &= v_1, \quad v_1' = -\frac{w_1}{\|q\|^3} - \frac{\delta w_1}{\|q\|^5}, \\ w_2' &= v_2, \quad v_2' = -\frac{w_2}{\|q\|^3} - \frac{\delta w_2}{\|q\|^5}, \end{aligned} \tag{48}$$

where v_1, v_2 are the two components of the velocity and w_1, w_2 are the two components of the position. We set the perturbation parameter δ to be equal to 0.015 and the initial condition to be

$$w_1(0) = 1 - e, \quad w_2(0) = 0, \quad v_1(0) = 0,$$
$$v_2(0) = \sqrt{(1+e)/(1-e)},$$

where $e = 0.6$ is the eccentricity. It is well known that this equation has the Hamiltonian and the angular momentum as quadratic first integrals. In particular, we focus here on the angular momentum, which reads

$$I(v, w) = w_1 v_2 - w_2 v_1. \tag{49}$$

We consider the simplest Gauss collocation method, namely the implicit midpoint rule, as the deterministic Runge–Kutta method. It is known that Gauss collocation methods conserve quadratic first integrals. According to Theorem 4, we expect therefore that the random time-stepping method (4) implemented with Ψ_h given by the implicit midpoint rule also conserves quadratic first integrals. We integrate (48) with uniformly distributed random time steps with mean $h = 0.01$ from time $t = 0$ to time $t = 4000$ which corresponds to approximately 636 revolutions of the system (long-time behaviour). Since the implicit midpoint rule is of order $q = 2$, we choose $p = 2$ for the RTS-RK method. Moreover, we consider the additive noise method (3) with $h = 0.01$, expecting that the first integral will not be conserved. We observe in Fig. 9 that method (4) conserves the angular momentum, while for method (3) the approximate conservation of the quadratic first integral shown in (25) is lost when integrating (48) over long time.

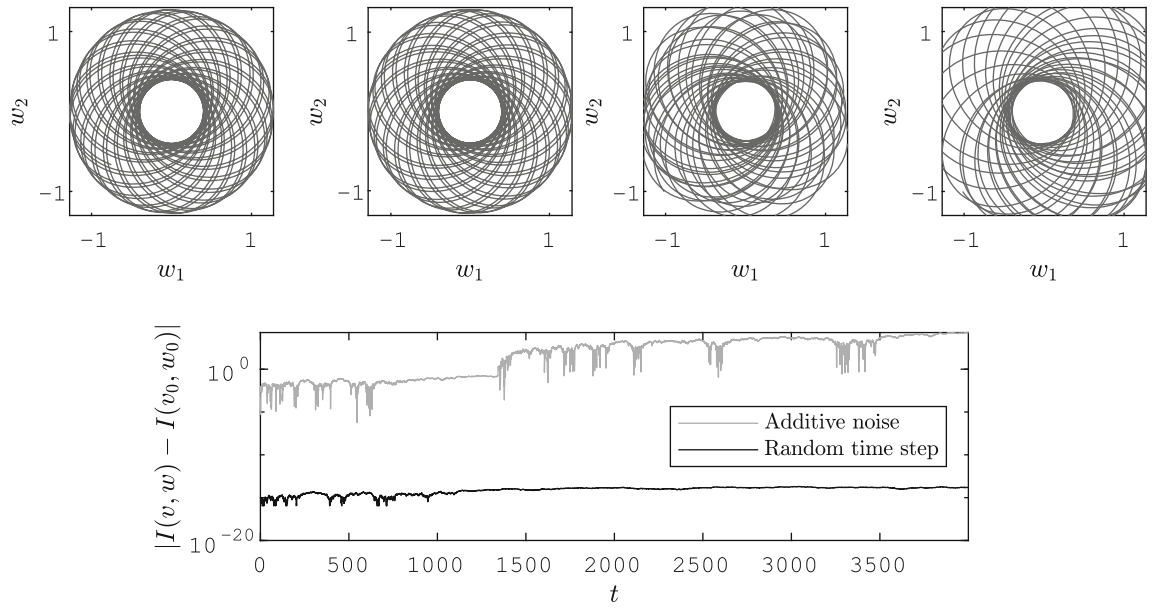

Fig. 9 Trajectories of (48) given by the RTS-RK method (4) for $0 \leq t \leq 200$ and $3800 \leq t \leq 4000$ (first and second figures), and by the additive noise method (3) for $0 \leq t \leq 200$ and $200 \leq t \leq 400$ (third and fourth figures). Error on the angular momentum I defined in (49) for $0 \leq t \leq 4000$ given by the two methods

9.6 Conservation of Hamiltonians

Let us consider the pendulum problem, which is given by the Hamiltonian $Q\colon \mathbb{R}^2 \to \mathbb{R}$ defined by

$$Q(v, w) = \frac{v^2}{2} - \cos w,$$

where $y = (v, w)^\top \in \mathbb{R}^2$. We wish to study the validity of Theorem 6, i.e. showing that the mean error on the Hamiltonian is of order $\mathcal{O}(h^q)$ for time spans of polynomial length, and then it grows proportionally to the square root of time. We consider the initial condition $(v_0, w_0) = (1.5, -\pi)$ and integrate the equation employing RTS-RK based on the implicit midpoint method ($q = 2$) choosing $p = q$, which is the optimal scaling of the noise. We choose uniform time steps, vary their mean $h \in \{0.2, 0.1, 0.05, 0.025\}$, integrate the dynamical system up to the final time $T = 10^6$ and study the time evolution of the mean numerical error on the Hamiltonian Q. Results are shown in Fig. 10, where it is possible to notice that the error is bounded by $\mathcal{O}(h^q)$ (horizontal black lines) for long time spans. After this stationary phase, the error on the Hamiltonian appears to grow as the square root of time. The oscillations of the error which are shown in Fig. 10 are present even when integrating the pendulum system with a deterministic symplectic scheme. Moreover, considering $T = 10^3$, the time step $h \in \{0.2, 0.1\}$ and keeping all other parameters as above, we compute the mean Hamiltonian and represent it in Fig. 10 together with an approximate confidence interval. We arbitrarily compute the confidence interval as $(\mathbb{E}Q(Y_n) - 2\mathrm{Var}\,Q(Y_n)^{1/2}, \mathbb{E}Q(Y_n) + 2\mathrm{Var}\,Q(Y_n)^{1/2})$, and we employ it to show the path-wise variability of the value of the Hamiltonian. As expected, the variability decreases dramatically with respect to the time step h.

9.7 Bayesian inference

For the last numerical experiment we consider the Hénon–Heiles equation, a Hamiltonian system with energy $Q\colon \mathbb{R}^4 \to \mathbb{R}$ defined by

$$Q(v, w) = \frac{1}{2}\|v\|^2 + \frac{1}{2}\|w\|^2 + w_1^2 w_2 - \frac{1}{3}w_2^3, \tag{50}$$

where $v, w \in \mathbb{R}^2$ are the velocity and position, respectively, and where we denote by $y = (v, w)^\top \in \mathbb{R}^4$ the solution. We consider an initial condition such that $Q(y_0) = 0.13$, for which the system exhibits a chaotic behaviour (Hénon and Heiles 1964). In the spirit of Sect. 8, we are interested in recovering the true value of the initial condition y_0 through a single observation y_{obs} of the solution (v, w) at a fixed time $t_{\mathrm{obs}} = 10$. The exact forward operator $\mathcal{G}$ is therefore defined as $\mathcal{G}(y_0) = \varphi_{t_{\mathrm{obs}}}(y_0)$. Noise is then set to be a Gaussian random variable $\varepsilon \sim \mathcal{N}(0, \sigma_\varepsilon^2 I)$, where $\sigma_\varepsilon = 5 \times 10^{-4}$, and we fix a standard Gaussian prior on the initial condition, i.e. $\pi_0 = \mathcal{N}(0, I)$, so that the likelihood is given by

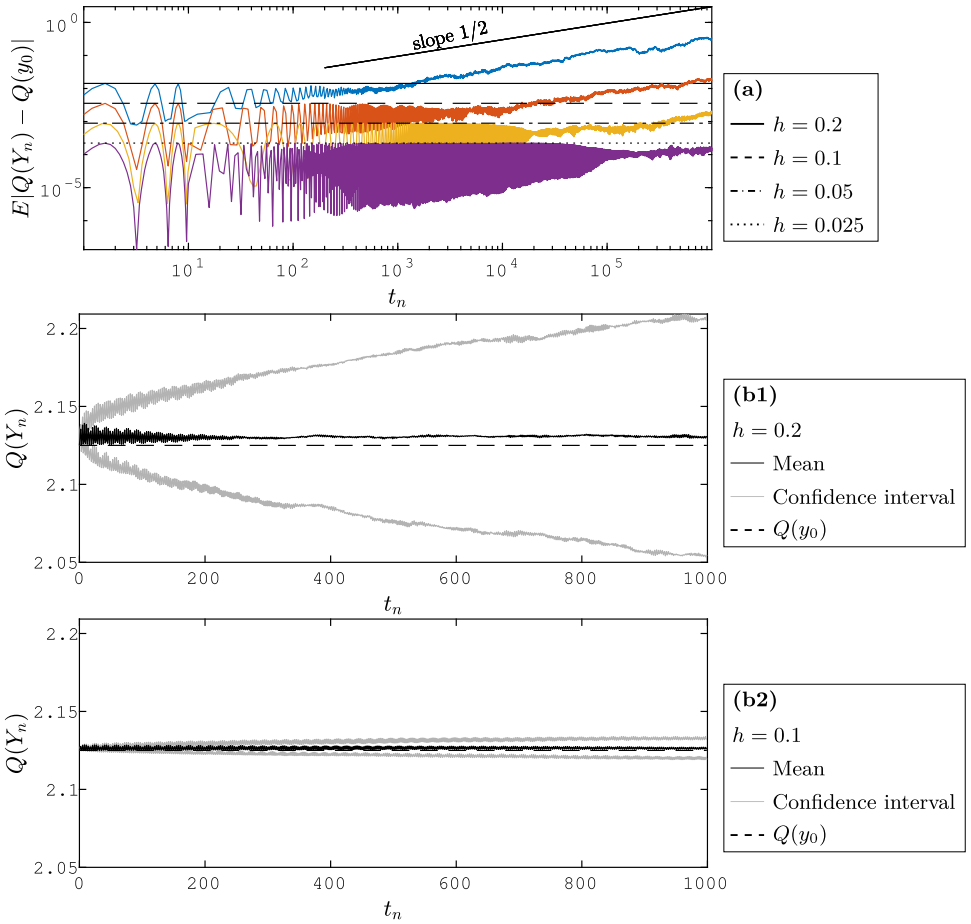

Fig. 10 **a** Time evolution of the mean error for the pendulum problem and different values of the time step h. The black lines represent the theoretical estimate given by Theorem 6, while the coloured lines represent the experimental results. The mean was computed by averaging 20 realisations of the numerical solution. **b1**, **b2**:Time evolution of the mean Hamiltonian for two different values of the time step. The mean Hamiltonian is depicted together with an approximate confidence interval, whose width is proportional to the standard deviation of the Hamiltonian over 200 trajectories. (Color figure online)

(39). We choose the observational noise to have a small variance [i.e. of order $\mathcal{O}(10^{-8})$] as in this case classical solvers present the misleading overconfident behaviour explained in Sect. 8.

Since the equation is Hamiltonian, we choose to employ a classical second-order ($q = 2$) symplectic method, the Störmer–Verlet scheme (Hairer et al. 2006; Störmer 1907; Verlet 1967), for which one step is defined in the general case as

$$\begin{aligned} v_{n+1/2} &= v_n - \frac{h}{2}\nabla_w Q(v_n, w_n), \\ w_{n+1} &= w_n + \frac{h}{2}\big(\nabla_v Q(v_{n+1/2}, w_n) \\ &\quad + \nabla_v Q(v_{n+1/2}, w_{n+1})\big), \\ v_{n+1} &= v_{n+1/2} - \frac{h}{2}\nabla_w Q(v_{n+1/2}, w_{n+1}). \end{aligned}$$

As the Hamiltonian Q given by (50) is separable, i.e. $Q(v, w) = Q_1(v) + Q_2(w)$, where $Q_1, Q_2 \colon \mathbb{R}^2 \to \mathbb{R}$, the Stömer–Verlet scheme simplifies to

$$\begin{aligned} v_{n+1/2} &= v_n - \frac{h}{2}\nabla_w Q_2(w_n), \\ w_{n+1} &= w_n + h\nabla_v Q_1(v_{n+1/2}), \\ v_{n+1} &= v_{n+1/2} - \frac{h}{2}\nabla_w Q_2(w_{n+1}). \end{aligned}$$

Hence, in the separable case the Störmer–Verlet scheme is explicit and the evaluation of the flow consists only of three evaluations of the derivatives of Q. We then employ this method both with a fixed time step h and as a basic integrator for the RTS-RK method (with uniformly distributed time steps and $p = 2$), thus computing the posterior distributions $\pi^h(y_0 \mid y_{\text{obs}})$ and $\pi^h_{\text{prob}}(y_0 \mid y_{\text{obs}})$ defined in Sect. 8, respectively. Moreover, we compute the posterior distribution given by a non-symplectic method, the Heun's scheme, which is a classical second-order method. The time step h is varied for the three methods above in order to study whether the approximate posterior concentrates towards the true posterior distribution $\pi(y_0 \mid y_{\text{obs}})$.

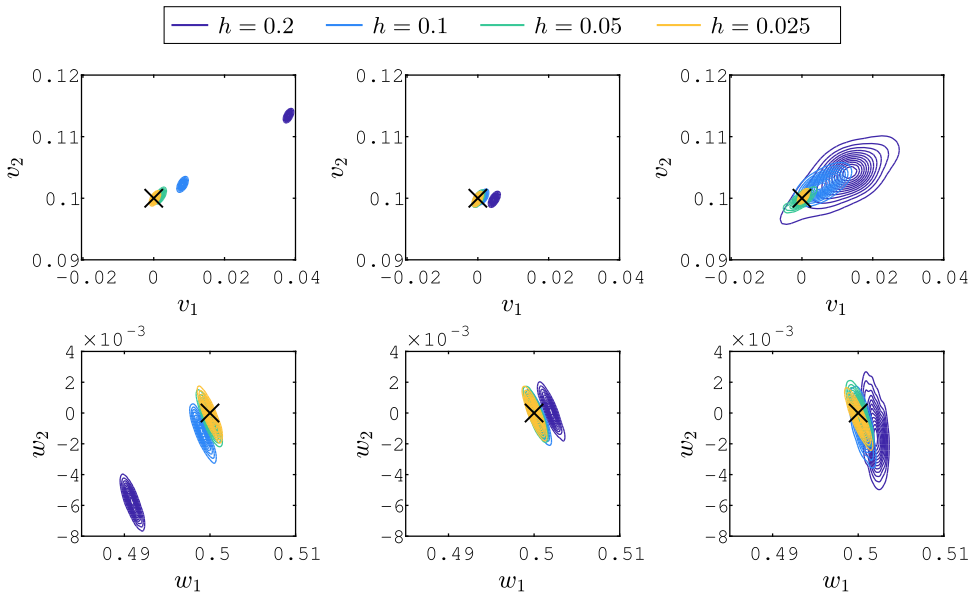

Fig. 11 Posterior distributions for the initial position and velocity of the Hénon–Heiles system with different values of $h = \{0.2, 0.1, 0.05, 0.025\}$. First row: initial velocity v_0. Second row: initial position w_0. First column: deterministic Heun's method. Second column: deterministic Störmer–Verlet scheme. Third column: RTS-RK Störmer–Verlet ($p = 2$)

We can observe in Fig. 11 that the posterior distributions given by Heun's method are concentrated away from the true value of the initial condition for the larger values of the time step. In fact, Heun's method is not symplectic, and a deviation on the energy Q is produced when integrating the dynamical system forward in time. Hence, initial conditions with a different energy level with respect to the observation are mapped by the approximate forward model to points which are close to the observations, and as a result the posterior distribution is concentrated far from the true value. This behaviour is corrected using the Störmer–Verlet method due to its symplecticity. However, we remark that the posterior distribution for $h = 0.2$ is still concentrated on a biased value of the initial condition, without any indication of this bias given by the posterior's variance. Applying the RTS-RK method together with PMMH instead gives nested posterior distributions whose variance quantifies the uncertainty of the numerical solver. This favourable behaviour is possible due to the numerical error quantification of probabilistic methods, which has been already shown in Cockayne et al. (2017) and Conrad et al. (2017), together with the good energy conservation properties of the RTS-RK method when a symplectic integrator is used as its deterministic component as proved in Theorem 6.

10 Conclusion

In this work, we introduced the RTS-RK method, a novel probabilistic integrators for ODEs built on Runge–Kutta numerical integrators with random time steps. In particular, we analysed its weak and mean square convergence properties, as well as the quality of Monte Carlo estimators drawn from the probabilistic solution. Geometric properties such as the conservation of first integrals and the approximation of Hamiltonians over long time intervals have been extensively treated theoretically. Finally, we showed heuristically the advantageous properties of the probabilistic approach in Bayesian inference problems with respect to the classic deterministic approach when the discretisation is not in the asymptotic regime $h \to 0$. The validity of our theoretical contributions is strengthened by an extensive series of numerical examples.

The RTS-RK method is partially inspired by the probabilistic method based on additive noise perturbations presented in Conrad et al. (2017) and further analysed in Lie et al. (2019), with which it shares convergence properties and the advantageous behaviour in inverse problems. Nonetheless, our method fills the void of geometry-aware probabilistic integrators for ODEs, and thus it represents a step forward in the field of probabilistic numerics for differential equations.

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Appendix

A modified stochastic differential equation

In Remark 5, we claim the existence of a modified stochastic differential equation (SDE) whose solution is well approximated by the RTS-RK method. Let us denote by $\widetilde{f}$ the function defining the modified equation corresponding to the numerical flow Ψ_h truncated after l terms, i.e.

$$\widetilde{f}(y) = f(y) + h^q f_{q+1}(y) + h^{q+1} f_{q+2}(y) + \cdots + h^l f_{l+1}(y).$$

Details about the construction of such a function can be found in Sect. 7.2. In particular, analyticity of the function f is needed for a rigorous backward error analysis to hold. Therefore, we will refer in this section to Assumption 5 (see Sect. 7.2). For the additive noise method presented in Conrad et al. (2017), the authors consider the SDE

$$\mathrm{d}Y = \widetilde{f}(Y)\,\mathrm{d}t + \sqrt{Qh^{2p}}\,\mathrm{d}W, \tag{51}$$

where W is a d-dimensional standard Brownian motion. It is possible to show (Conrad et al. 2017, Theorem 2.4) that the solution of (51) satisfies

$$|\mathbb{E}\big(\Phi(Y_N) - \Phi(Y(T)) \mid Y_0 = y\big)| \leq Ch^{2p},$$

where $T = Nh$ and Y_N is the numerical solution given by the additive noise method after N steps. Here, we present a similar construction for the RTS-RK method. In particular, let us consider the modified SDE

$$\begin{aligned}\mathrm{d}\widetilde{Y} = &\Big(\widetilde{f}(\widetilde{Y}) + \frac{1}{2}Ch^{2p}\partial_{tt}\Psi_h(\widetilde{Y})\Big)\,\mathrm{d}t \\ &+ \sqrt{Ch^{2p}\partial_t\Psi_h(\widetilde{Y})\partial_t\Psi_h(\widetilde{Y})^\top}\,\mathrm{d}W,\end{aligned} \tag{52}$$

where C is given in Assumption 1(iii). Let us denote by $\widetilde{\mathcal{L}}$ the generator of (52), which can be written explicitly as

$$\widetilde{\mathcal{L}} = \Big(\widetilde{f} + \frac{1}{2}Ch^{2p}\partial_{tt}\Psi_h\Big)\cdot\nabla + \frac{1}{2}Ch^{2p}\partial_t\Psi_h\partial_t\Psi_h^\top : \nabla^2,$$

and, adopting the semi-group notation, it satisfies

$$\mathbb{E}\big(\Phi(\widetilde{Y}(h)) \mid \widetilde{Y}(0) = y\big) = \mathrm{e}^{h\widetilde{\mathcal{L}}}\Phi(y).$$

In the following lemma, we consider the error over one step between the numerical solution given by the RTS-RK method and the solution of (52) in the weak sense. The proof is inspired by the calculations presented in Conrad et al. (2017, Section 2.4).

Lemma 9 *Under the assumptions of Lemma 1 and if Assumption 5 holds, then*

$$|\mathbb{E}\big(\Phi(Y_1) - \Phi(\widetilde{Y}(h)) \mid Y_0 = y\big)| \leq Ch^{2p+1},$$

where C is a positive constant independent of h and of y, $\widetilde{Y}$ is the solution of (52) and Y_1 is the numerical solution given by the RTS-RK method after one step.

Proof Let us consider the modified ODE

$$\widehat{y}'(t) = \widetilde{f}(\widehat{y}), \tag{53}$$

and denote its flow as $\widehat{\varphi}_t$. The generator $\widehat{\mathcal{L}} = \widetilde{f}\cdot\nabla$ satisfies, adopting the semi-group notation,

$$\Phi(\widehat{\varphi}_h(y)) = \mathrm{e}^{h\widehat{\mathcal{L}}}\Phi(y).$$

We can now compute the distance between the solution to (52) and (53) as

$$\begin{aligned}&\mathrm{e}^{h\widetilde{\mathcal{L}}}\Phi(y) - \mathrm{e}^{h\widehat{\mathcal{L}}}\Phi(y) = \mathrm{e}^{h\widetilde{f}\cdot\nabla} \\ &\Big(\mathrm{e}^{\frac{1}{2}Ch^{2p+1}\partial_{tt}\Psi_h\cdot\nabla + \frac{1}{2}Ch^{2p+1}\partial_t\Psi_h\partial_t\Psi_h^\top:\nabla^2} - I\Big)\Phi(y) \\ &= \big(1+\mathcal{O}(h)\big)\Big(\frac{1}{2}Ch^{2p+1}\partial_{tt}\Psi_h\cdot\nabla + \frac{1}{2}Ch^{2p+1}\partial_t\Psi_h\partial_t\Psi_h^\top : \nabla^2 \\ &\quad + \mathcal{O}\big(h^{4p+1}\big)\Big)\Phi(y) \\ &= \frac{1}{2}Ch^{2p+1}\partial_{tt}\Psi_h\cdot\nabla\Phi(y) + \frac{1}{2}Ch^{2p+1}\partial_t\Psi_h\partial_t\Psi_h^\top : \nabla^2\Phi(y) \\ &\quad + \mathcal{O}\big(h^{4p+1}\big).\end{aligned}$$

Let us recall that equation (10) gives

$$\begin{aligned}\mathrm{e}^{h\mathcal{L}_h}\Phi(y) - \Phi(\Psi_h(y)) = &\frac{1}{2}Ch^{2p+1}\partial_{tt}\Psi_h(y)\cdot\nabla\Phi(y) \\ &+ \frac{1}{2}Ch^{2p+1}\partial_t\Psi_h(y)\partial_t\Psi_h(y)^\top : \nabla^2\Phi(y) + \mathcal{O}(h^{2p+1}),\end{aligned}$$

which implies that

$$\mathrm{e}^{h\widetilde{\mathcal{L}}}\Phi(y) - \mathrm{e}^{h\mathcal{L}_h}\Phi(y) = \mathrm{e}^{h\widehat{\mathcal{L}}}\Phi(y) - \Phi(\Psi_h(y)) + \mathcal{O}(h^{2p+1}).$$

Now, the theory of backward error analysis (see Sect. 7.2 or e.g. Hairer et al. 2006, Chapter IX) guarantees that

$$\mathrm{e}^{h\widehat{\mathcal{L}}}\Phi(y) - \Phi(\Psi_h(y)) = \mathcal{O}(h^{q+l+2}).$$

Choosing $l = 2p - q - 1$, we have therefore

$$\mathrm{e}^{h\widetilde{\mathcal{L}}}\Phi(y) - \mathrm{e}^{h\mathcal{L}_h}\Phi(y) = \mathcal{O}(h^{2p+1}),$$

which is the desired result. □

The error can be then propagated to final time as in Theorem 1, as presented in the following theorem.

Theorem 7 *Under the assumptions of Lemma 9 and Theorem 1, and if there exists a constant $L > 0$ independent of h such that for all $\Phi \in \mathcal{C}_b^\infty(\mathbb{R}^d, \mathbb{R})$*

$$\sup_{u\in\mathbb{R}^d} |e^{h\widetilde{\mathcal{L}}}\Phi(u)| \leq (1 + Lh) \sup_{u\in\mathbb{R}^d} |\Phi(u)|,$$

then it holds

$$|\mathbb{E}\big(\Phi(Y_N) - \Phi(\widetilde{Y}(T)) \mid Y_0 = y\big)| \leq Ch^{2p},$$

where $T = Nh$ and C is a positive constant independent of h and of y, $\widetilde{Y}$ is the solution of (52) and Y_N is the numerical solution given by the RTS-RK method after N steps.

Proof The proof follows by replacing $\mathcal{L}$ with $\widetilde{\mathcal{L}}$ and Lemma 1 with Lemma 9 in the proof of Theorem 1. □

Proof of Lemma 6

In the following, we denote by $[\![a, b]\!]$ the interval $[\![a, b]\!] = [a, b]$ if $a < b$ and $[\![a, b]\!] = [b, a]$ if $a \geq b$. Let us first consider $r \geq 2$ and the function $\gamma_r(x) = x^r \mathrm{e}^{-r\kappa/x}$, whose first derivative is given by

$$\gamma_r'(x) = rx^{r-2}(x+\kappa)\mathrm{e}^{-r\kappa/x}.$$

Under Assumption 6, we have that $H_j \leq Mh$ almost surely, and hence for any $t \in [\![h, H_j]\!]$

$$|\gamma_r'(t)| \leq r(Mh)^{r-2}(Mh+\kappa)\mathrm{e}^{-r\kappa/(Mh)},$$

where we exploited that $\mathrm{e}^{-r\kappa/x}$ is a growing function of x. The fundamental theorem of calculus gives

$$\begin{aligned}|\gamma_r(H_j)| &= \left|\gamma_r(h) + \int_h^{H_j} \gamma_r'(t)\,\mathrm{d}t\right| \\ &\leq \gamma_r(h) + r(Mh)^{r-2}(Mh+\kappa)\mathrm{e}^{-r\kappa/(Mh)}|H_j - h|,\end{aligned}$$

Taking expectation on both sides and since by (33) it holds $|\eta_j|^r \leq C\gamma_r(H_j)$, we obtain

$$\mathbb{E}|\eta_j|^r \leq C\left(\gamma_r(h) + rM^{r-2}h^{p+r-3/2}(Mh+\kappa)\mathrm{e}^{-r\kappa/(Mh)}\right),$$

which proves the desired inequality. This is because Assumption 6 and Assumption 1(ii) imply that $M \geq 1$, and because Mh can be bounded by M. Let us now consider $r = 1$. In this case, we have for $t \in [\![h, H_j]\!]$

$$|\gamma_1'(t)| \leq (mh)^{-1}(Mh+\kappa)\mathrm{e}^{-\kappa/(Mh)}, \quad \text{almost surely.}$$

Hence, we apply the same reasoning as above and obtain almost surely

$$|\gamma_1(H_j)| \leq \gamma_1(h) + (mh)^{-1}(Mh+\kappa)\mathrm{e}^{-\kappa/(Mh)}|H_j - h|,$$

which implies the desired result by proceeding as above. □

Proof of Lemma 7

We first expand the square as

$$\begin{aligned}\left(\sum_{j=0}^{n-1}\left(\sum_{k=q}^{N-1} a_{jk} + b_j\right)\right)^2 &= \sum_{j=0}^{n-1}\left(\sum_{k=q}^{N-1} a_{jk} + b_j\right)^2 \\ &+ 2\sum_{j=1}^{n-1}\sum_{i=0}^{j-1}\left(\sum_{k=q}^{N-1} a_{jk} + b_j\right)\left(\sum_{k=q}^{N-1} a_{ik} + b_i\right).\end{aligned} \tag{54}$$

Then, we expand the square in the first sum and obtain

$$\begin{aligned}\left(\sum_{k=q}^{N-1} a_{jk} + b_j\right)^2 &= \left(\sum_{k=q}^{N-1} a_{jk}\right)^2 + b_j^2 + 2b_j\sum_{k=q}^{N-1} a_{jk} \\ &= \sum_{k=q}^{N-1} a_{jk}^2 + 2\sum_{k=q+1}^{N-1}\sum_{l=q}^{k-1} a_{jk}a_{jl} + b_j^2 + 2b_j\sum_{k=q}^{N-1} a_{jk} \\ &= a_{jq}^2 + \sum_{k=q+1}^{N-1} a_{jk}^2 + 2\sum_{k=q+1}^{N-1}\sum_{l=q}^{k-1} a_{jk}a_{jl} + b_j^2 + 2b_j\sum_{k=q}^{N-1} a_{jk}.\end{aligned} \tag{55}$$

We then rewrite the term appearing in the double sum in (54) as

$$\begin{aligned}\left(\sum_{k=q}^{N-1} a_{jk} + b_j\right)\left(\sum_{k=q}^{N-1} a_{ik} + b_i\right) &= a_{jq}a_{iq} + \sum_{k=q}^{N-1}\sum_{\substack{l=q \\ l+k>2q}}^{N-1} a_{jk}a_{il} \\ &+ b_j\sum_{k=q}^{N-1} a_{ik} + b_i\sum_{k=q}^{N-1} a_{jk} + b_ib_j.\end{aligned} \tag{56}$$

Substituting expressions (55) and (56) in (54), we finally get almost surely.

$$\begin{aligned}\left(\sum_{j=0}^{n-1}\left(\sum_{k=q}^{N-1} a_{jk} + b_j\right)\right)^2 &= \sum_{j=0}^{n-1} a_{jq}^2 \\ &+ 2\sum_{j=1}^{n-1}\sum_{i=0}^{j-1} a_{jq}a_{iq} + R(a) + S(a,b),\end{aligned}$$

where the remainder $R(a)$ can be written as $R = R_1 + R_2 + R_3$ where

$$\begin{aligned}R_1(a) &= \sum_{j=0}^{n-1}\sum_{k=q+1}^{N-1} a_{jk}^2, \\ R_2(a) &= 2\sum_{j=0}^{n-1}\sum_{k=q+1}^{N-1}\sum_{l=q}^{k-1} a_{jk}a_{jl}, \\ R_3(a) &= 2\sum_{j=1}^{n-1}\sum_{i=0}^{j-1}\sum_{k=q}^{N-1}\sum_{\substack{l=q \\ l+k>2q}}^{N-1} a_{jk}a_{il},\end{aligned}$$

and the remainder $S(a, b)$ can be written as $S = S_1 + S_2 + S_3 + S_4$ where

$$\begin{aligned}S_1(a,b) &= \sum_{j=0}^{n-1} b_j^2, \\ S_2(a,b) &= 2\sum_{j=1}^{n-1}\sum_{i=0}^{j-1} b_ib_j,\end{aligned}$$

$$S_3(a,b) = 2\sum_{j=1}^{n-1}\sum_{k=q}^{N-1} b_j a_{jk},$$

$$S_4(a,b) = 2\sum_{j=1}^{n-1}\sum_{i=0}^{n-1}\left(b_j\sum_{k=q}^{N-1} a_{ik} + b_i\sum_{k=q}^{N-1} a_{jk}\right).$$

which proves the desired result. □

Proof of Lemma 8

In the following, all the constants are independent of h and n, but can depend on N and q. Moreover, since $h < 1$, we often apply $h^r \le h^s$ for $r \ge s$. We first notice that, under Assumption 2 and Assumption 5, we get for all $j = 0,\dots,n-1$ and $k = q,\dots,N-1$

$$\begin{aligned}|\Delta_{j,k}| &= |Q_{k+1}(Y_j) - Q_{k+1}(Y_{j+1})| \\ &\le C\|\Psi_0(Y_j) - \Psi_{H_j}(Y_j)\| \\ &\le C_\Delta |H_j|,\end{aligned} \tag{57}$$

almost surely and where C_Δ is independent of h. Above, we exploited that Q_{k+1} is Lipschitz continuous for all $k = q,\dots,N+1$ due to Assumption 5. Let us now consider $R(\Delta)$. Due to (57) and to Assumption 6, we have

$$\begin{aligned}\mathbb{E}(H_j^k - h^k)^2\Delta_{j,k}^2 &\le C_\Delta^2\mathbb{E}(H_j^{k+1} - H_j h^k)^2 \\ &= C_\Delta^2\big(h^{2(k+1)} + C_{2(k+1)}h^{2p+2(k+1)-1} \\ &\quad + h^{2(k+1)} + C_2 h^{2p+2k+1} \\ &\quad - 2h^{2k+2} - 2C_{k+2}h^{2p+2k+1}\big) \\ &= C_\Delta^2\big((C_{2(k+1)} + C_2 - 2C_{k+2})h^{2p+2k+1}\big) \\ &\le Ch^{2p+2k+1},\end{aligned} \tag{58}$$

where $C > 0$ is a positive constant. Now, since $k \ge q+1$, we get

$$\mathbb{E}(H_j^k - h^k)^2\Delta_{j,k}^2 \le Ch^{2(p+q+1)}.$$

Hence, for $R_1(\Delta)$ there exists a constant $\widetilde{C}_1$ such that

$$\mathbb{E}R_1(\Delta) \le \widetilde{C}_1 nh^{2(p+q+1)}.$$

We now proceed to the second remainder $R_2(\Delta)$. Applying the Cauchy–Schwarz inequality and (58), we get

$$\begin{aligned}\mathbb{E}\left((H_j^k - h^k)\Delta_{j,k}(H_j^l - h^l)\Delta_{j,l}\right) &\le \left(\mathbb{E}\big((H_j^k - h^k)^2\Delta_{j,k}^2\big)\right)^{1/2} \\ &\quad \left(\mathbb{E}\big((H_j^l - h^l)^2\Delta_{j,l}^2\big)\right)^{1/2} \\ &\le Ch^{2p+k+l+1},\end{aligned}$$

where $C > 0$ is a positive constant. Now, since in the definition of $R_2(a)$ in (57) we have $k \ge q+1$ and $l \ge q$, we have here $k + l \ge 2q+1$. Therefore, there exists a constant $\widetilde{C}_2$ such that

$$\mathbb{E}R_2(\Delta) \le \widetilde{C}_2 nh^{2(p+q+1)}.$$

We now consider the term $R_3(\Delta)$. Since H_i and H_j are independent for $i \ne j$, we have

$$\begin{aligned}&\mathbb{E}\big((H_j^k - h^k)\Delta_{j,k}(H_i^l - h^l)\Delta_{i,l}\big) \\ &\quad = \mathbb{E}(H_j^k - h^k)\Delta_{j,k}\mathbb{E}(H_i^l - h^l)\Delta_{i,l}.\end{aligned}$$

Computing the two factors singularly, we have due to (57) and to Assumption 6

$$\begin{aligned}\mathbb{E}(H_j^k - h^k)\Delta_{j,k} &\le C_\Delta\mathbb{E}(H_j^{k+1} - H_j h^k) \\ &= C_\Delta C_{k+1}h^{2p+k},\end{aligned} \tag{59}$$

and analogously for $\mathbb{E}(H_i^l - h^l)\Delta_{i,l}$. Then, since $k + l \ge 2q+1$

$$\begin{aligned}&\mathbb{E}\big((H_j^k - h^k)\Delta_{j,k}(H_i^l - h^l)\Delta_{i,l}\big) \\ &\quad \le C_\Delta^2 C_{k+1}C_{l+1}h^{2(2p+q+1/2)}.\end{aligned} \tag{60}$$

Hence, we have for a constant $\widetilde{C}_3 > 0$

$$\mathbb{E}R_3(\Delta) \le \widetilde{C}_3 n^2 h^{2(2p+q+1/2)}.$$

Finally, replacing $t_n = nh$, we can write for a constant $C > 0$

$$\begin{aligned}\mathbb{E}R(\Delta) &\le (\widetilde{C}_1 + \widetilde{C}_2)nh^{2(p+q+1)} + \widetilde{C}_3 n^2 h^{2(2p+q+1/2)} \\ &= (\widetilde{C}_1 + \widetilde{C}_2)t_n h^{2(p+q+1/2)} + \widetilde{C}_3 t_n^2 h^{2(2p+q-1/2)}.\end{aligned}$$

Let us now consider $S(\Delta,\eta)$. First, we notice that under the assumption $p \ge 3/2$ we have for any $r \ge 1$, $\min\{r, p+r-3/2\} = r$, and therefore Lemma 6 simplifies to

$$\mathbb{E}|\eta_j|^r \le Ch^r \mathrm{e}^{-r\kappa/(Mh)}.$$

We first consider $S_1(\Delta,\eta)$. Applying Lemma 6 with $r = 2$, we obtain for a constant $\widehat{C}_1 > 0$

$$\mathbb{E}S_1(\Delta,\eta) \le \widehat{C}_1 nh^2 \mathrm{e}^{-2\kappa/(Mh)}.$$

For the second term $S_2(\Delta,\eta)$, we have by (33) that $|\eta_i| \le CH^i\mathrm{e}^{-\kappa/H_i}$ and $\eta_j \le CH^j\mathrm{e}^{-\kappa/H_j}$ almost surely. These two bounds are independent for $i \ne j$, and therefore, applying Lemma 6 with $r = 1$, we have for a constant $\widehat{C}_2 > 0$

$$\mathbb{E}S_2(\Delta,\eta) \le \widehat{C}_2 n^2 h^2 \mathrm{e}^{-2\kappa/(Mh)}.$$

We now consider the third remainder $S_3(\Delta,\eta)$. Applying the Cauchy–Schwarz inequality, we obtain

$$\mathbb{E}\eta_j(H_j^k - h^k)\Delta_{j,k} \le (\mathbb{E}\eta_j^2)^{1/2}(\mathbb{E}(H_j^k - h^k)^2\Delta_{j,k}^2)^{1/2}.$$

Applying Lemma 6 with $r = 2$ to the first factor and (58) to the second, we get

$$\begin{aligned}\mathbb{E}\eta_j(H_j^k - h^k)\Delta_{j,k} &\leq Ch\mathrm{e}^{-\kappa/(Mh)}h^{p+k+1/2}\\ &= Ch^{p+k+3/2}\mathrm{e}^{-\kappa/(Mh)}\end{aligned}$$

Now, since $k \geq q$, we have for a constant $\widehat{C}_3 > 0$

$$\mathbb{E}S_3(\Delta, \eta) \leq \widehat{C}_3 nh^{p+q+3/2}\mathrm{e}^{-\kappa/(Mh)}.$$

Finally, we consider the last term $S_4(\Delta, \eta)$. Since by (33) it holds $|\eta_j| \leq CH_j\mathrm{e}^{-\kappa/H_j}$ almost surely, and this bound is independent of H_i for $i \neq j$, applying (59) and Lemma 6 we have

$$\begin{aligned}\mathbb{E}\eta_j(H_i^k - h^k)\Delta_{i,k} &= \mathbb{E}\eta_j\mathbb{E}(H_i^k - h^k)\Delta_{i,k}\\ &\leq Ch\mathrm{e}^{-\kappa/(Mh)}h^{2p+k},\end{aligned}$$

which, since $k \geq q$, implies that there exists a constant $\widehat{C}_4 > 0$ such that

$$\mathbb{E}S_4(\Delta, \eta) \leq \widehat{C}_4 n^2 h^{2p+q+1}\mathrm{e}^{-\kappa/(Mh)}.$$

Finally, replacing $t_n = nh$, we can write

$$\begin{aligned}\mathbb{E}S(\Delta, \eta) &\leq (\widehat{C}_1 nh^2 + \widehat{C}_2 n^2 h^2)\mathrm{e}^{-2\kappa/(Mh)}\\ &\quad + (\widehat{C}_3 nh^{p+q+3/2} + \widehat{C}_4 n^2 h^{2p+q+1})\mathrm{e}^{-\kappa/(Mh)}\\ &= (\widehat{C}_1 t_n h + \widehat{C}_2 t_n^2)\mathrm{e}^{-2\kappa/(Mh)}\\ &\quad + (\widehat{C}_3 t_n h^{p+q+1/2} + \widehat{C}_4 t_n^2 h^{2p+q-1})\mathrm{e}^{-\kappa/(Mh)},\end{aligned}$$

which completes the proof. □

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