A TECHNIQUE FOR STUDYING STRONG AND WEAK LOCAL ERRORS OF SPLITTING STOCHASTIC INTEGRATORS*

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Abstract. We present a technique, based on so-called word series, to write down in a systematic way expansions of the strong and weak local errors of splitting algorithms for the integration of Stratonovich stochastic differential equations. Those expansions immediately lead to the corresponding order conditions. Word series are similar to, but simpler than, the B-series used to analyze Runge–Kutta and other one-step integrators. The suggested approach makes it unnecessary to use the Baker–Campbell–Hausdorff formula. As an application, we compare two splitting algorithms recently considered by Leimkuhler and Matthews to integrate the Langevin equations. The word series method clearly bears out reasons for the advantages of one algorithm over the other.

Key words. stochastic differential equations, splitting algorithms, Langevin equations, word series

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1. Introduction. We present a technique, based on so-called *word series*, to write down in a systematic way expansions of the strong and weak local errors of splitting algorithms for the integration of Stratonovich stochastic differential equations (SDEs). Those expansions immediately lead to the corresponding order conditions without any need to use the Baker–Campbell–Haussdorf (BCH) formula. As an application we compare two splitting algorithms recently considered by Leimkuhler and Matthews [21], [22] and Leimkuhler, Matthews, and Stolz [23] to integrate the Langevin equations.

The approach taken in this paper may be seen as patterned after the seminal work of Butcher [7] on the *combinatorics* of the order conditions for Runge–Kutta deterministic integrators. As is well known, in the theory developed by Butcher, the numerical and true solution are expanded with the help of vector-valued mappings called elementary differentials. In the expansions, the elementary differentials are weighted by so-called elementary weights. These are real numbers that change with the integrator but are independent of the system being integrated. There are an elementary differential and an elementary weight for each rooted tree, and both are easily written down because their structure is a transcription of that of the rooted tree. The elementary differentials change with the differential system being integrated but are common for all Runge–Kutta integrators and also for the true solution; this has important implications because when designing new integrators or comparing different integrators one may focus on the elementary weights. B-series [19], series of elementary differential with arbitrary coefficients, are a way of systematizing Butcher's

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approach and extending it to more general integrators. A key result in [19] is the rule for composing B-series. B-series have found many applications in numerical analysis, in particular in relation with modified equations [8] and geometric integration [9], [33], [18]. For applications of B-series outside numerical mathematics, see [10], [11]. Burrage and Burrage [6] have analyzed à la Butcher weak and strong errors of Runge–Kutta integrators for SDEs. The paper [34] surveys the history of these developments.

The importance of splitting algorithms [4] has been increasing in recent years, essentially as a consequence of their capability of exploiting the structure of the problem being integrated. In the deterministic case, there are several ways of investigating the consistency properties of a splitting integrator:

- The best known technique, described in, e.g., [32], applies the BCH formula. This method has several shortcomings, including the *huge combinatorial complexity* of the BCH formula itself (see [3], [26] for a discussion).
- An approach that parallels Butcher's treatment of Runge–Kutta formulas has been introduced in [26] (a summary is available in [18, section III.3]). As in Butcher's work, the approach is based on the use of rooted trees. The *B-series* expansions found in this way are also made of elementary differentials and scalar coefficients.
- More recently, *word series* expansions [25], [12], [13], [27], [28], [29] have been suggested as an alternative to B-series. The scope of applicability of word series is narrower than that of B-series: splitting methods may be treated with word series, but Runge–Kutta formulas may not. When applicable, word series are more convenient than B-series. They are more compact than B-series and have a composition rule (see Theorem 3) much simpler than the recipe used to compose B-series.

In the present work we extend the third technique above to cater for splitting integrators for Stratonovich SDEs, thus avoiding the complicated combinatorics involved in the BCH formula. In section 2 we present the tools required in the rest of the paper. In section 3 we show how to expand a composition of exact solutions by using the formula for composing word series. For clarity, the idea is presented in the deterministic case where several complications of the Stratonovich scenario are absent. In section 4 we provide formulas for the expansion of both strong and weak local errors and write down the associated order conditions. In section 5 the material is applied to the case of Langevin dynamics. Leimkuhler and Matthews [21], [22] have considered two closely related splitting algorithms and found, numerically and theoretically, that one is clearly superior to the other. We show that a word series analysis identifies *additional* reasons for that superiority. Section 6 describes additional possible uses of word series in the analysis of SDE integrators.

It is well known that error expansions like those considered in section 4 in general do not converge. This does not diminish their usefulness: by truncating the series one obtains the Taylor polynomials that are needed to write down the order conditions. Of course when *bounds* of the weak or strong local error are required it is necessary to estimate the remainder term in the error expansion. Although the emphasis of this paper is in the combinatorics of the expansion rather than on error estimates, we have included an appendix that illustrates how to derive error bounds for word series expansions (cf. [12], [13], [27]).

For simplicity, except in the appendix, all mappings are assumed to be indefinitely differentiable. Of course, when that is not the case, the formulas presented below only make sense up to the order where the derivatives that appear exist.

2. Preliminaries. In this section we describe word series. The presentation is very concise. References are grouped in section 2.5.

2.1. Words. Let $\mathcal{A}$ be a finite set, which we shall call the *alphabet*. The elements $a \in \mathcal{A}$ are called *letters*. A *word* w is an arbitrary finite sequence of letters $a_1 a_2 \ldots a_n$, $a_i \in \mathcal{A}$. We denote by $\mathcal{W}$ the set of all words, including the empty word $\emptyset$, i.e., the word with zero letters. No distinction is made between the letter a and the word having a as its only letter, so that $\mathcal{A}$ is seen as a subset of $\mathcal{W}$.

We work with mappings $\delta : \mathcal{W} \to \mathbb{R}$ and use the notation δ_w to refer to the real value that δ takes at $w \in \mathcal{W}$. The set $\mathbb{R}^{\mathcal{W}}$ consists of all such mappings. Given $\delta, \delta' \in \mathbb{R}^{\mathcal{W}}$, we associate with them their *convolution product* $\delta \star \delta' \in \mathbb{R}^{\mathcal{W}}$, defined by $(\delta \star \delta')_\emptyset = \delta_\emptyset \delta'_\emptyset$ and, for nonempty words,

$$(\delta \star \delta')_{a_1 a_2 \ldots a_n} = \delta_\emptyset \delta'_{a_1 a_2 \ldots a_n} + \sum_{j=1}^{n-1} \delta_{a_1 a_2 \ldots a_j} \delta'_{a_{j+1} \ldots a_n} + \delta_{a_1 a_2 \ldots a_n} \delta'_\emptyset.$$

Note that in the right-hand side there is a term for each of the ways in which $a_1 a_2 \ldots a_n$ may be split into two subwords (in more technical language *deconcatenated* into two subwords). The operation $\star$ is not commutative, but it is associative; to find the value of $\delta \star \delta' \star \delta'' = (\delta \star \delta') \star \delta'' = \delta \star (\delta' \star \delta'')$ at a word w we sum all the values $\delta_v \delta'_{v'} \delta''_{v''}$ corresponding to triples v, v', v'' that concatenated yield w. The element $\mathbb{1} \in \mathbb{R}^{\mathcal{W}}$ specified by $\mathbb{1}_\emptyset = 1$ and $\mathbb{1}_w = 0$ for each nonempty word w is the unit of the operation $\star$.

Given two words w and w' with m and n letters, respectively, their *shuffle product* $w \sqcup\!\!\sqcup w'$ is the formal sum of the $(m+n)!/(m!n!)$ words with $m+n$ letters that may be obtained by interleaving the letters of w and w' while preserving the order in which the letters appear in w and w'. For instance, $a \sqcup\!\!\sqcup b = ab + ba$, $a \sqcup\!\!\sqcup a = aa + aa = 2aa$, $ab \sqcup\!\!\sqcup c = abc + acb + cab$, $ab \sqcup\!\!\sqcup cd = abcd + acbd + cabd + acdb + cadb + cdab$.

We shall denote by $\mathcal{G}_{sh}$ (*sh* for shuffle) the subset of $\mathbb{R}^{\mathcal{W}}$ that comprises all the elements $\gamma \in \mathbb{R}^{\mathcal{W}}$ satisfying the so-called *shuffle relations:* $\gamma_\emptyset = 1$ and, for each pair of words w, w', if

$$(1) \qquad w \sqcup\!\!\sqcup w' = \sum_j w_j,$$

then

$$(2) \qquad \gamma_w \gamma_{w'} = \sum_j \gamma_{w_j}.$$

For instance, $\gamma_a \gamma_b = \gamma_{ab} + \gamma_{ba}$, $\gamma_a^2 = 2\gamma_{aa}$, $\gamma_{ab}\gamma_c = \gamma_{cab} + \gamma_{acb} + \gamma_{abc}$, etc. For the convolution product, $\mathcal{G}_{sh}$ is a *noncommutative group* with unit $\mathbb{1}$.

2.2. Word series. Assume now that for each letter $a \in \mathcal{A}$, $f_a : \mathbb{R}^d \to \mathbb{R}^d$ is a map. With every word $w \in \mathcal{W}$ we associate a *word basis function* $f_w : \mathbb{R}^d \to \mathbb{R}^d$. If $w = a_1 a_2 \ldots a_n$, $n > 1$, then f_w is defined recursively by

$$(3) \qquad f_{a_1 a_2 \ldots a_n}(x) = \big(\partial_x f_{a_2 \ldots a_n}(x)\big) f_{a_1}(x),$$

where $\partial_x f_{a_2 \ldots a_n}(x)$ denotes the value at the point x of the Jacobian matrix of $f_{a_2 \ldots a_n}$. For the empty word, $f_\emptyset$ is simply the identity map $x \mapsto x$. With every $\delta \in \mathbb{R}^{\mathcal{W}}$ we associate a *word series*. This is the formal series

$$W_\delta(x) = \sum_{w \in \mathcal{W}} \delta_w f_w(x).$$

The δ_w are the *coefficients* of the series. The notation $W_\delta(x)$ does not incorporate the dependence on the f_a, which are given once and for all.

As a very important example, consider the d-dimensional initial value problem

$$(4) \qquad \frac{d}{dt}x = \sum_{a \in \mathcal{A}} \lambda_a(t) f_a(x), \qquad x(t_0) = x_0,$$

where, for each $a \in \mathcal{A}$, λ_a is a real-valued function of t. For each t, the solution value $x(t) \in \mathbb{R}^d$ has a word series expansion

$$(5) \qquad x(t) = W_{\alpha(t;t_0)}(x_0) = \sum_{w \in \mathcal{W}} \alpha_w(t;t_0) f_w(x_0),$$

with coefficients given by

$$(6) \qquad \alpha_\emptyset(t;t_0) = 1, \qquad \alpha_a(t;t_0) = \int_{t_0}^t \lambda_a(s)\,ds, \quad a \in \mathcal{A},$$

and, for words with $n > 1$ letters, recursively,

$$(7) \qquad \alpha_{a_1 a_2 \cdots a_n}(t;t_0) = \int_{t_0}^t \alpha_{a_1 a_2 \cdots a_{n-1}}(s;t_0) \lambda_{a_n}(s)\,ds.$$

Thus, for a word with $n > 0$ letters, $\alpha_w(t;t_0)$ is an n-fold iterated integral or, equivalently, an integral over a simplex in $\mathbb{R}^n$.

As we shall see later, for splitting numerical integrators, the numerical solution after a single step also possesses a word series expansion.

For future reference we point out that, as $t \to t_0$, for each word of n letters,

$$(8) \qquad \alpha_{a_1 a_2 \ldots a_n}(t;t_0) = \mathcal{O}\big((t-t_0)^n\big).$$

In the simplest case where the alphabet consists of a single letter $\mathcal{A} = \{a\}$ and $\lambda_a(t) = 1$ for each t, there is one word $a^n = a \ldots a$ with n letters, $n = 0, 1, \ldots$, and the corresponding coefficient is

$$(9) \qquad \alpha_{a^n} = \frac{(t-t_0)^n}{n!};$$

the word series representation (5) just coincides with the standard Taylor expansion of $x(t)$ around t_0 with the derivatives of x expressed by means of the mapping f_a, e.g.,

$$\frac{d}{dt}x = f_a(x),$$
$$\frac{d^2}{dt^2}x = \big(\partial_x f_a(x)\big)\frac{d}{dt}x = \big(\partial_x f_a(x)\big)f_a(x) = f_{aa}(x),$$
$$\frac{d^3}{dt^3}x = \big(\partial_x f_{aa}(x)\big)\frac{d}{dt}x = \big(\partial_x f_{aa}(x)\big)f_a(x) = f_{aaa}(x),$$
$$\cdots = \cdots$$

For an alphabet with N letters, if $\lambda_a(t) = 1$ for each letter and each t, then $\alpha_w = (t-t_0)^n/n!$ for any of the N^n words w with n letters. In this case, (5) is the Taylor series for $x(t)$ with the derivatives of $x(t)$ written in terms of the f_a, $a \in \mathcal{A}$.

It is also important to note that, in (5), the coefficients α_w depend on the functions λ_a, $a \in \mathcal{A}$, and are independent of the f_a in (4); on the contrary, the word basis functions f_w are independent of the λ_a and change with f_a. This will make it possible to compare later different splitting integrators by expressing them in terms of one common set of word basis functions.

The following two results will be required in the next section.

PROPOSITION 1. *For any choice of the functions λ_a, $a \in \mathcal{A}$, and any t, t_0, the coefficients $\alpha_w(t; t_0)$ computed in (6)–(7) satisfy the shuffle relations; i.e., the element $\alpha(t; t_0) \in \mathbb{R}^{\mathcal{W}}$ lies in the group $\mathcal{G}_{sh} \subset \mathbb{R}^{\mathcal{W}}$.*

PROPOSITION 2. *Assume that $t_0 < t_1 < t_2$; then, for any choice of the functions λ_a, $a \in \mathcal{A}$, with the notation as above,*

$$\alpha(t_2; t_0) = \alpha(t_1; t_0) \star \alpha(t_2; t_1).$$

As an example, for the two-letter word ab, the proposition yields, since $\alpha_\emptyset(t_1; t_0) = \alpha_\emptyset(t_2; t_1) = 1$,

$$\alpha_{ab}(t_2; t_0) = \alpha_{ab}(t_2; t_1) + \alpha_a(t_1; t_0)\alpha_b(t_2; t_1) + \alpha_{ab}(t_1; t_0),$$

an equality that may be obtained elementarily by writing the left-hand side as a double integral over a triangle and then decomposing the triangle into two smaller triangles and a rectangle.

2.3. Word series operators. Real-valued functions χ defined in $\mathbb{R}^d$ shall be called *observables*. For every letter a, D_a is the linear differential operator that maps the observable χ into the new observable $D_a\chi$ defined by

$$D_a\chi(x) = \sum_{i=1}^{d} f_a^i(x)\frac{\partial}{\partial x_i}\chi(x), \qquad x \in \mathbb{R}^d.$$

For each word $w = a_1 a_2 \ldots a_n$ with more than one letter, we define the operator D_w by composing the operators associated with the letters of w:

$$D_{a_1 a_2 \ldots a_n} = D_{a_1} \circ D_{a_2} \circ \cdots \circ D_{a_n}.$$

For the empty word, the corresponding operator is the identity: $D_\emptyset\chi(x) = \chi(x)$. Note that the dependence of the D_w on the functions f_a is not incorporated into the notation. Given $\delta \in \mathbb{R}^{\mathcal{W}}$, we define its *word series operator* as the formal linear differential operator:

$$D_\delta = \sum_{w \in \mathcal{W}} \delta_w D_w.$$

It is trivial to check that convolution product $\star$ is defined in such a way that it corresponds to the composition of the associated word series operators:

$$D_\delta \circ D_{\delta'} = D_{\delta \star \delta'}, \qquad \delta, \delta' \in \mathbb{R}^{\mathcal{W}}.$$

The differential operators D_w, $w \in \mathcal{W}$, may also be applied in a componentwise way to vector-valued observables defined in $\mathbb{R}^d$. By considering the application of D_w to the identity map id : $x \mapsto x$, $x \in \mathbb{R}^d$, we find that the word basis function f_w and the operator D_w are related through the formula $f_w = D_w$id. By implication, $W_\delta(x) = D_\delta$id(x) for $\delta \in \mathbb{R}^{\mathcal{W}}$ and $x \in \mathbb{R}^d$.

2.4. Handling word series and word series operators. The following theorem provides rules for handling word series and word series operators. Note the order in which γ and δ appear in (11).

THEOREM 3. *Let γ be an element of the group $\mathcal{G}_{sh}$. Then the following hold:*
- *(Composition of a word series and an observable.) For any (real- or vector-valued) observable χ,*

$$\chi\big(W_\gamma(x)\big) = D_\gamma \chi(x). \tag{10}$$

- *(Composition of word series.) For every $\delta \in \mathbb{R}^\mathcal{W}$, we have*

$$W_\delta\big(W_\gamma(x)\big) = W_{\gamma \star \delta}(x). \tag{11}$$

It is important to emphasize that the hypothesis $\gamma \in \mathcal{G}_{sh}$ is essential for the result to hold; the conclusions are not true if $\gamma \in \mathbb{R}^\mathcal{W}$ does not belong to the group. According to Proposition 1, the coefficients $\alpha_w(t; t_0)$ may play the role of γ in the theorem. This is the key to the analysis of splitting integrators, as we show in section 3.

2.5. References and discussion. The material in section 2.2 is connected to several algebraic theories, even though, for the benefit of more applied readers, those connections have been downplayed in our exposition. The vector space $\mathbb{R}^\mathcal{W}$ is the dual of the shuffle Hopf algebra, and the group $\mathcal{G}_{sh}$ is the group of characters of such algebra; see [27] and its references. The monograph [31] contains many relevant results on the combinatorics of words.

Series indexed by the words of an alphabet were introduced and studied extensively by Chen; see, e.g., [14]. Sometimes the series are presented as combining words themselves; i.e., they are of the form $\sum_w \delta_w w$ with $\delta \in \mathbb{R}^\mathcal{W}$ (Chen series). In other applications, notably in control theory [16], the series combine differential operators as in our $D_\delta = \sum_w \delta_w D_w$ above. Word series [25], [11], [13], [27] while essentially equivalent to Chen series are series of mappings, and therefore, in numerical analysis, they may be used in the same way as B-series. Word series may also be used to study analytically dynamical systems: [27], [28], [29]. Chen series also play an important role in Lyons rough path theory; see, e.g., [2].

Each series basis function f_w may be decomposed as a sum of elementary differentials [27]. After such a decomposition each word series becomes a B-series; the B-series has a term for each colored rooted tree. Since there are far more colored rooted trees with n vertices than words with n letters, the B-series format is less compact. An additional advantage of word series over B-series is the simplicity of the operation $\star$; the rule for composing B-series is substantially more complicated. On the other hand, word series have a more limited scope than B-series: not all B-series may be rewritten as word series. Splitting integrators may be described by word series, but that is not the case for Runge–Kutta algorithms or additive Runge–Kutta algorithms [1].

A proof of Theorem 3 may be seen in [27]. The fact that iterated integrals satisfy the shuffle relations (Proposition 1) was first noted by Ree [30]. Proposition 2 is due to Chen [14]; in view of (5) and (11), the result expresses in terms of words the composition rule for solution operators $\phi_{t_2;t_0} = \phi_{t_2;t_1} \circ \phi_{t_1;t_0}$.

3. Composing exact solutions with the help of word series. Theorem 3 leads to a technique to represent the local error of splitting integrators both for deterministic and Stratonovich equations. Even though the idea is completely general, for notational convenience we shall present it by means of a very simple (deterministic)

example. Consider the particular case where in the system (4) the alphabet consists of three letters $\mathcal{A} = \{a, b, c\}$, i.e.,

$$\frac{d}{dt} x = \lambda_a(t) f_a(x) + \lambda_b(t) f_b(x) + \lambda_c(t) f_c(x),$$

and denote by $\phi_{t,t_0} : \mathbb{R}^d \to \mathbb{R}^d$ the solution mapping, i.e., the mapping such that, for each x_0, $\phi_{t,t_0}(x_0)$ is the value at t of the solution with initial condition $x(t_0) = x_0$. Assume that the split systems

$$\frac{d}{dt} x = \lambda_a(t) f_a(x) + \lambda_b(t) f_b(x), \quad \frac{d}{dt} x = \lambda_c(t) f_c(x)$$

may be integrated analytically, and denote by $\phi_{t,t_0}^{(1)} : \mathbb{R}^d \to \mathbb{R}^d$ and $\phi_{t,t_0}^{(2)} : \mathbb{R}^d \to \mathbb{R}^d$ their solution mappings. The simplest splitting integrator advances the numerical solution from t_0 to $t_0 + h$, $h > 0$, by means of the mapping

$$\widetilde{\phi}_{t_0+h,t_0} = \phi_{t_0+h,t_0}^{(2)} \circ \phi_{t_0+h,t_0}^{(1)}.$$

From (5) we have the word series representation (we write α_w instead of $\alpha_w(t_0 + h; t_0)$)

$$\begin{aligned}
\phi_{t_0+h,t_0}(x_0) &= W_{\alpha(t_0+h;t_0)}(x_0) \\
&= x_0 + \alpha_a f_a(x_0) + \alpha_b f_b(x_0) + \alpha_c f_c(x_0) \\
&\quad + \alpha_{aa} f_{aa}(x_0) + \alpha_{ab} f_{ab}(x_0) + \alpha_{ac} f_{ac}(x_0) + \cdots
\end{aligned}$$

(note that for simplicity only three of the nine terms with two letters have been displayed). For the first split system, still using the alphabet $\{a, b, c\}$ and including all words with two letters,

$$\begin{aligned}
\phi_{t_0+h,t_0}^{(1)}(x_0) &= W_{\alpha^{(1)}(t_0+h;t_0)}(x_0) \\
&= x_0 + \alpha_a f_a(x_0) + \alpha_b f_b(x_0) \\
&\quad + \alpha_{aa} f_{aa}(x_0) + \alpha_{ab} f_{ab}(x_0) \\
&\quad + \alpha_{ba} f_{ba}(x_0) + \alpha_{bb} f_{bb}(x_0) + \cdots,
\end{aligned}$$

when computing the coefficients $\alpha_w^{(1)}$ by means of (6)–(7) we have to take $\lambda_c(t) = 0$, so that $\alpha_w^{(1)} = \alpha_w$ if w does not contain the letter c and $\alpha_w^{(1)} = 0$ otherwise. Similarly,

$$\begin{aligned}
\phi_{t_0+h,t_0}^{(2)}(x_0) &= W_{\alpha^{(2)}(t_0+h;t_0)}(x_0) \\
&= x_0 + \alpha_c f_c(x_0) + \alpha_{cc} f_{cc}(x_0) + \cdots,
\end{aligned}$$

where the dots stand for words with three or more letters. Now, after invoking Proposition 1 and (11), we find that

$$(12) \qquad\qquad \widetilde{\phi}_{t_0+h,t_0}(x_0) = W_{\widetilde{\alpha}(t_0+h;t_0)}(x_0),$$

with

$$\widetilde{\alpha}(t_0 + h; t_0) = \alpha^{(1)}(t_0 + h; t_0) \star \alpha^{(2)}(t_0 + h; t_0) \in \mathcal{G}_{sh}.$$

By using the definition of the convolution product $\star$, we compute

$$\begin{aligned}
\widetilde{\phi}_{t_0+h,t_0}(x_0) &= x_0 + \alpha_a f_a(x_0) + \alpha_b f_b(x_0) + \alpha_c f_c(x_0) \\
&\quad + \alpha_{aa} f_{aa}(x_0) + \alpha_{ab} f_{ab}(x_0) + \alpha_a \alpha_c f_{ac}(x_0) \\
&\quad + \alpha_{ba} f_{ba}(x_0) + \alpha_{bb} f_{bb}(x_0) + \alpha_b \alpha_c f_{bc}(x_0) + \alpha_{cc} f_{cc}(x_0) + \cdots.
\end{aligned}$$

It is extremely easy to find the coefficients in the last expansion. If w is a concatenation $w'w''$, where the (possibly empty) word w' does not include the letter c and the (possibly empty) word w'' does not include the letters a or b, then $\widetilde{\alpha}_w = \alpha_{w'}\alpha_{w''}$; if w is not a concatenation of that form, then the coefficient is 0.

The fact that the expansion of the integrator mapping $\widetilde{\phi}$ and the solution mapping ϕ agree for words with < 2 letters implies, via (8), that both differ by $\mathcal{O}(h^2)$, i.e., that the integrator is consistent. The local error may be expanded as a word series

$$\widetilde{\phi}_{t_0+h,t_0}(x_0) - \phi_{t_0+h,t_0}(x_0) = W_{\delta(t_0,h)}(x_0)$$

with

$$\delta(t_0,h) = \alpha^{(1)}(t_0+h;t_0) \star \alpha^{(2)}(t_0+h;t_0) - \alpha(t_0+h,t_0).$$

In particular, the leading $\mathcal{O}(h^2)$ term, corresponding to two-letter words, is given by

$$(\alpha_a\alpha_c - \alpha_{ac})f_{ac}(x_0) + (\alpha_b\alpha_c - \alpha_{bc})f_{bc}(x_0) - \alpha_{ca}f_{ca}(x_0) - \alpha_{cb}f_{cb}(x_0).$$

In some circumstances (for instance, when studying conservation of energy or other invariants of motion) it is of interest to look at the error in an observable χ after a single step:

$$\chi\left(\widetilde{\phi}_{t_0+h,t_0}(x_0)\right) - \chi\left(\phi_{t_0+h,t_0}(x_0)\right).$$

Expansions of errors of this kind are easily derived with the help of (10). In our example, we may write, *without any additional computation*,

$$\chi\left(\widetilde{\phi}_{t_0+h,t_0}(x_0)\right) - \chi\left(\phi_{t_0+h,t_0}(x_0)\right) = (\alpha_a\alpha_c - \alpha_{ac})D_{ac}\chi(x_0)$$
$$+ (\alpha_b\alpha_c - \alpha_{bc})D_{bc}\chi(x_0)$$
$$- \alpha_{ca}D_{ca}\chi(x_0) - \alpha_{cb}D_{cb}\chi(x_0) + \cdots.$$

For this simple example the results presented here could have been found easily by elementary means. However, as pointed out above, the word series technique works for arbitrary splitting coefficients leading to high-order algorithms and arbitrary ways of splitting the right-hand side of (4) into two or more parts.

4. Splitting methods for stochastic differential equations. In this section we show how word series may be used to analyze local errors of splitting integrators for SDEs.

4.1. Expanding the true solution. Consider the d-dimensional Stratonovich SDE,

$$(13) \qquad dx = \sum_{a \in \mathcal{A}_{det}} f_a(x)\,dt + \sum_{A \in \mathcal{A}_{stoch}} f_A(x) \circ dB_A(t),$$

where $\mathcal{A}_{det}$ and $\mathcal{A}_{stoch}$ are finite sets without common elements and the $B_A(t)$, $A \in \mathcal{A}_{stoch}$, are independent scalar Wiener processes defined on the same filtered probability space. We shall use the material above with the alphabet $\mathcal{A} = \mathcal{A}_{det} \cup \mathcal{A}_{stoch}$. The letters in $\mathcal{A}_{det}$ (respectively, in $\mathcal{A}_{stoch}$) are called *deterministic* (respectively, *stochastic*). The *weight* $\|w\|$ of the letter w is defined as the number of deterministic letters of w plus half the number of stochastic letters. The weight thus takes values in the set $(1/2)\mathbb{N} = \{0, 1/2, 1, 3/2, \ldots\}$. Note that if the w_j are the words resulting from shuffling w and w' as in (1), then, for each j, $\|w_j\| = \|w\| + \|w'\|$. Also, when

two words are concatenated, the weight of the result is the sum of the weights of the factors.

Since Stratonovich integrals follow the rules of ordinary calculus, from (5) we conclude that the solution of (13) with initial condition $x(t_0) = x_0$ has the expansion $t > t_0 \geq 0$,

$$(14) \qquad\qquad x(t) = W_{J(t;t_0)}(x_0),$$

where the $J_w(t; t_0)$ are the well-known Stratonovich iterated integrals (wa and wA are the words obtained by appending the letter a or A at the end of w):

$$J_\emptyset(t; t_0) = 1,$$

$$J_a(t; t_0) = \int_{t_0}^t ds = t - t_0, \qquad a \in \mathcal{A}_{det},$$

$$J_A(t; t_0) = \int_{t_0}^t \circ dB_A(s) = B_A(t_1) - B_A(t_0), \qquad A \in \mathcal{A}_{stoch},$$

$$J_{wa}(t, t_0) = \int_{t_0}^t J_w(s; t_0)\, ds, \qquad a \in \mathcal{A}_{det},$$

$$J_{wA}(t; t_0) = \int_{t_0}^t J_w(s; t_0) \circ dB_A(s), \qquad A \in \mathcal{A}_{stoch}.$$

The expansion (14) of course coincides with the familiar Stratonovich–Taylor expansion (see, e.g., [20, Chapter 5]).

The following result summarizes some properties of the $J_w(t; t_0)$ which will be required later. The first item expresses the shuffle relations of iterated integrals; see also Proposition 1. The second, third, and fifth items are well known. The fourth is a trivial consequence of the second and third.

PROPOSITION 4. *The iterated stochastic Stratonovich integrals $J_w(t; t_0)$ possess the following properties;*
- *$J(t; t_0) \in \mathcal{G}_{sh}$.*
- *The joint distribution of any finite subfamily of the family of random variables $\{h^{-\|w\|}J_w(t_0 + h; t_0)\}_{w \in \mathcal{W}}$ is independent of $t_0 \geq 0$ and $h > 0$.*
- *$\mathbb{E}\, |\, J_w(t_0 + h; t_0)\, |^p < \infty$ for each $w \in \mathcal{W}$, $t_0 \geq 0$, $h > 0$, and $p \in [0, \infty)$.*
- *For each $w \in \mathcal{W}$ and any finite $p \geq 1$, the (t_0-independent) L^p norm of the random variable $J_w(t_0 + h; t_0)$ is $\mathcal{O}(h^{\|w\|})$ as $h \downarrow 0$.*
- *$\mathbb{E}\, J_w(t_0 + h; t_0) = 0$ whenever $\|w\|$ is not an integer.*

In view of the proposition, when the word series in (14) is rewritten as

$$x(t) = \sum_{n \in (1/2)\mathbb{N}} \sum_{\|w\|=n} J_w(t; t_0) f_w(x_0),$$

for each $n \in (1/2)\mathbb{N}$, the term in the inner sum is $\mathcal{O}((t - t_0)^n)$ in any L^p norm, $p < \infty$. This should be compared with the deterministic case, where, as we saw above, the bound (8) leads to grading the expansion (5) by the number of letters of the words.

We shall need below the following auxiliary result (Π of course denotes a product).

LEMMA 5. *Assume that $w_1, \ldots, w_\ell$ are words with $\sum_j \|w_j\| \notin \mathbb{N}$. Then, for each $t_0 \geq 0$ and $h > 0$,*

$$\mathbb{E}\big(\Pi_j J_{w_j}(t_0 + h; t_0)\big) = 0.$$

Proof. By using repeatedly the shuffle relations (1)–(2), the product of iterated integrals may be rewritten as a sum of iterated integrals corresponding to the words w_i' resulting from shuffling the w_j, $j = 1, \ldots, \ell$. As noted above, each w_i' has the noninteger weight $\sum_j \|w_j\|$ and we may use the last item of Proposition 4. $\square$

The idea of the proof (i.e., the use of the shuffle relations to rewrite products of iterated integrals as sums) has been used in [17] as a means to evaluate the moments of iterated stochastic integrals. An instance of the shuffle relations for iterated stochastic integrals is presented in Proposition 5.2.10 of [20]; this well-known monograph does not relate the formula presented there to the algebra of word shuffles. A number of recent papers have also exploited the connection between the Stratonovich calculus and the shuffle Hopf algebra; see, e.g., [15] and its references.

4.2. Expanding the numerical solution. In a splitting integrator, a time step $t_0 \to t_0 + h$, $h > 0$, is performed by applying a mapping ϕ_{t_0+h,t_0} defined as a composition of several solution mappings

$$\phi^{(i)}_{t_0+c_i h, t_0+d_i h}, \qquad i = 1, \ldots, I,$$

corresponding to SDEs resulting from splitting the right-hand side of (13). The c_i and d_i are real constants associated with the particular integrator. By proceeding as in the deterministic case, the use of the operation $\star$ leads to a word-series representation (cf. (12)),

$$\widetilde{\phi}_{t_0+h,t_0}(x_0) = W_{\widetilde{J}(t_0+h;t_0)}(x_0), \qquad i = 1, \ldots, I,$$

where, for each nonempty $w \in \mathcal{W}$, $\widetilde{J}_w(t_0 + h; t_0)$ is either zero or a sum of products of iterated Stratonovich integrals corresponding to words whose concatenation is w. Therefore, in each product, the iterated integrals being multiplied correspond to words whose weights add up to $\|w\|$.

PROPOSITION 6. *The coefficients $\widetilde{J}_w(t_0+h; t_0)$, $w \in \mathcal{W}$, associated with a splitting integrator possess the properties of the exact values $\widetilde{J}_w(t_0 + h; t_0)$ listed in Proposition 4.*

Proof. The first four items of this proposition are consequences of Proposition 4 and the representation of each $\widetilde{J}_w(t_0 + h; t_0)$, $w \neq \emptyset$, as a sum of products of iterated integrals. For the last item, in view of the linearity of the expectation, it is enough to prove that, for any $t_j < t_j^*$,

$$\sum_j \|w_j\| \notin \mathbb{N} \quad \Rightarrow \quad \mathbb{E}\left(\prod_j J_{w_j}(t_j^*; t_j) \right) = 0.$$

Furthermore, we may assume that we are in the particular case where any two intervals $(t_j, t_j^*) \subset \mathbb{R}$ are either disjoint or equal to each other; the general situation may be reduced to the particular case by decomposing with the help of Proposition 2. Under this assumption, let us group together the iterated integrals sharing the same (t_j, t_j^*) and write

$$\prod_j J_{w_j}(t_j^*; t_j) = \prod_k \prod_{j \in I_k} J_{w_j}(t_k^*; t_k);$$

here, as k varies, any two intervals $(t_k, t_k^*) \subset \mathbb{R}$ are disjoint, and, for each value of k, the set I_k comprises the indices j for which $(t_j^*; t_j)$ coincides with $(t_k^*; t_k)$. Now, by

independence,

$$\mathbb{E}\left(\prod_j J_{w_j}(t_j^*; t_j)\right) = \prod_k \mathbb{E}\left(\prod_{j \in I_k} J_{w_j}(t_k^*; t_k)\right),$$

and the proof will be completed if we show that there is at least a value of k for which

$$\mathbb{E}\left(\prod_{j \in I_k} J_{w_j}(t_k^*; t_k)\right) = 0.$$

Since

$$\sum_k \sum_{j \in I_k} \|w_j\| = \sum_j \|w_j\| \notin \mathbb{N},$$

at least one of the inner sums is not an integer and we may apply Lemma 5.   □

4.3. The local error. The preparations above have proved the main result of this paper.

THEOREM 7. *For a splitting integrator as above, the local error possesses a word series expansion*

$$(15) \quad \widetilde{\phi}_{t_0+h,t_0}(x_0) - \phi_{t_0+h,t_0}(x_0) = W_{\delta(t_0,h)}(x_0) = \sum_{n \in (1/2)\mathbb{N}} \sum_{\|w\|=n} \delta_w(t_0,h) f_w(x_0),$$

with coefficients

$$\delta_w(t_0,h) = \widetilde{J}_w(t_0 + h; t_0) - J_w(t_0 + h; t_0), \qquad w \in \mathcal{W},$$

that, in any L^p norm, $1 \le p < \infty$, satisfy, uniformly in $t_0 \ge 0$,

$$\|\delta_w(t_0,h)\|_p = \mathcal{O}(h^{\|w\|}), \qquad h \downarrow 0.$$

In addition, for each observable χ, conditional on x_0,

$$(16) \qquad \mathbb{E}\chi\big(\widetilde{\phi}_{t_0+h,t_0}(x_0)\big) - \mathbb{E}\chi\big(\phi_{t_0+h,t_0}(x_0)\big) = \sum_{n \in \mathbb{N}} \sum_{\|w\|=n} \big(\mathbb{E}\delta_w(t_0,h)\big) D_w \chi(x_0).$$

The theorem implies that the *strong order conditions*

$$(17) \qquad \widetilde{J}_w(t_0 + h; t_0) = J_w(t_0 + h; t_0), \qquad \|w\| = 0, 1/2, 1, \ldots, \mu, \quad \mu \in (1/2)\mathbb{N},$$

ensure that the series in (15) only comprises terms of size $\mathcal{O}(h^{\mu+1/2})$. In fact, under suitable assumptions on (13), the fulfillment of the order conditions ensures that the local error possesses an $\mathcal{O}(h^{\mu+1/2})$ bound (see the appendix).

It should be pointed out that, since both $J(t_0 + h; t_0)$ and $\widetilde{J}(t_0 + h; t_0)$ satisfy the shuffle relations, the conditions in (17) corresponding to different words are not independent from one another. For instance, from the shuffle $a \sqcup a = 2aa$, $a \in \mathcal{A}$, we may write

$$\big(J_a(t_0 + h; t_0)\big)^2 = 2J_{aa}(t_0 + h; t_0), \quad \big(\widetilde{J}_a(t_0 + h; t_0)\big)^2 = 2\widetilde{J}_{aa}(t_0 + h; t_0),$$

and therefore the order condition for the word aa is fulfilled if and only if the same happens for a. Lyndon words [31] may be used to identify subsets of independent order conditions (cf. [26]), but we shall not concern ourselves with such an investigation.

If, for a given alphabet $\mathcal{A}$ and given coefficients $\widetilde{J}_w(t_0 + h; t_0)$, one demands that the series in (15) only comprise terms of size $\mathcal{O}(h^{\mu+1/2})$ for *all possible choices* of the vector fields f_a, f_A, then the conditions (17) are not only sufficient but also *necessary*. This happens because, as it is easy to show, in such a scenario, the word basis functions are mutually independent. However, this consideration is not of much practical value; splitting integrators are useful because they are adapted to the specific structure of the problem being solved, and therefore one is interested in the behavior for individual problems, not in catering for all possible choices of f_a, f_A. The best way to deal with specific problems is to write down, up to the desired order, the word series expansions of the true and numerical solutions and compare them after taking into account the shuffle relations and the specific expressions of the word basis functions; this will be illustrated in the next section. For instance, if, for the problem at hand, a word basis function f_w vanishes identically, then it is clearly not necessary to impose the associated order condition in (17).

Similar considerations apply to the *weak order conditions*

$$(18) \qquad \mathbb{E}\widetilde{J}_w(t_0 + h; t_0) = \mathbb{E}J_w(t_0 + h; t_0), \qquad \|w\| = 0, 1, 2, \ldots, \nu, \quad \nu \in \mathbb{N},$$

which ensure that the series in (16) only comprises terms of size $\mathcal{O}(h^{\nu+1})$.

The conditions (17)–(18) are similar to those found in [6] for stochastic Runge–Kutta integrators (however, [6] only shows that a condition corresponding to (18) implies that the expectation of the local error is $\mathcal{O}(h^{\nu+1})$; arbitrary observables χ are not considered there).

5. Application to Langevin dynamics. We shall illustrate the application of the foregoing material by considering the Langevin equations

$$dq = M^{-1}p \, dt,$$
$$dp = F(q) \, dt - \gamma p \, dt + \sigma M^{1/2} dB(t),$$

where M is the $d \times d$ diagonal mass matrix with diagonal entries $m_i > 0$, $\gamma > 0$ is the friction coefficient, σ governs the fluctuation due to noise, B is a d-dimensional Wiener process, and the force F originates from a potential; i.e., $F = -\nabla V$ for a suitable scalar-valued function V. Since the noise is additive, there is no distinction between the Stratonovich and Ito interpretations.

5.1. Splitting the Langevin dynamics. After setting $x = (q, p) \in \mathbb{R}^d \times \mathbb{R}^d$, the equations are the particular instance of (13) given by

$$(19) \qquad dx(t) = f_a(x)dt + f_b(x)dt + f_c(x)dt + \sum_{i=1}^{d} f_{A_i}(x) \circ dB_i(t)$$

with

$$f_a(q, p) = (M^{-1}p, 0), \quad f_b(q, p) = (0, F(q)), \quad f_c(q, p) = (0, -\gamma p),$$

and, for $i = 1, \ldots, d$,

$$f_{A_i}(q, p) = (0, \sigma\sqrt{m_i}e_i),$$

where e_i is the ith unit vector in $\mathbb{R}^d$. The deterministic letters a, b, and c are, respectively, associated with inertia, potential forces, and friction; as will become apparent below, the word basis functions f_w, $w \in \mathcal{W}$, also have clear physical meaning.

The system (19) is split into three parts corresponding to $\{f_a\}$, $\{f_b\}$, and $\{f_c, f_{A_1}, \ldots, f_{A_d}\}$.[1] Each of the three split systems may be integrated explicitly. With a terminology common in molecular dynamics, the solution of the first is a "drift" in position, $q \mapsto q + (t - t_0)M^{-1}p$ (p remains constant). The solution of the second is a "kick" in momentum $p \mapsto p + (t - t_0)F(q)$ (q remains constant). The third split system defines an Ornstein–Uhlenbeck process in p. Leimkuhler and Matthews [21], [22] use the letters A, B, and O to refer to these split systems and the acronym ABOBA for the Strang-like algorithm

$$\widetilde{\phi}^{ABOBA} = \phi^A_{t_0+h;t_0+h/2} \circ \phi^B_{t_0+h;t_0+h/2} \circ \phi^O_{t_0+h;t_0} \circ \phi^B_{t_0+h/2;t_0} \circ \phi^A_{t_0+h/2;t_0}.$$

With the help of an analysis of the large friction limit and numerical experiments, these authors find that the very similar BAOAB algorithm

$$\widetilde{\phi}^{BAOAB} = \phi^B_{t_0+h;t_0+h/2} \circ \phi^A_{t_0+h;t_0+h/2} \circ \phi^O_{t_0+h;t_0} \circ \phi^A_{t_0+h/2;t_0} \circ \phi^B_{t_0+h/2;t_0}$$

substantially improves on ABOBA. In this section we analyze by means of word series the local error of both algorithms. Our findings complement (rather than duplicate) those in [21], [22], [23].

5.2. The word basis functions. The structure of the Langevin equations implies that many word basis functions are identically zero. The vector fields f_a, f_b, f_c, and f_{A_i} have many null components, and additional simplifications are due to f_{A_i} being constant, f_a and f_c being linear in p and independent of q, and f_b being independent of p. In particular, the relation $f_{ba}(q, p) = (M^{-1}F(q), 0)$ shows that f_{ba} is a function of q alone and, since the q components of f_c and f_{A_i} vanish, we have, in view of (3),

(20) $$f_{cba}(q,p) = 0, \qquad f_{A_iba}(q,p) = 0, \quad i = 1, \ldots, d,$$

for each q and p. Physically, (20) means that the value $M^{-1}F(q)$ of the acceleration created by the potential forces would not be affected if noise or friction changed instantaneously the momentum of the system. On the other hand, in general,

(21) $$f_{cab}(q,p) \neq 0, \qquad f_{A_iab}(q,p) \neq 0, \quad i = 1, \ldots, d.$$

The second block of $f_{ab}(q,p) = (0, \partial_q F(q)M^{-1}p) = (0, (d/dt)F(q))$ is the contribution to $(d^2/dt^2)p$ that arises from the potential forces. This contribution is a function of q *and* p, and its value would be affected if friction or noise changed instantaneously the momentum. It is also useful to note at this point that, according to (3), if f_w vanishes identically, then the same is true for all words of the form $w'w$, i.e., for all words that have w as a suffix. Table 1 lists the words w with weight < 3 and nonvanishing basis function.

5.3. Coefficients. Once the relevant word basis functions have been identified, we proceed to find the coefficients. Let us begin with ABOBA. From the definition of the operation $\star$, it is clear that if w is not of the form $a^k b^\ell w' b^m a^n$, with k, ℓ, m, n nonnegative integers and w' a word not including the letters a or b, then $\widetilde{J}^{ABOBA}_w = 0$. For a word that may be written in that form in a unique way (e.g., $abccba$), the value

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[1] The splitting considered here is not the only meaningful way to split the Langevin equations; a Hamiltonian/Ornstein–Uhlenbeck splitting is considered in, e.g., [5]. See also [23].

Coefficients of the splitting methods ABOBA and BAOBA for words w with weight $\|w\| < 3$ and nonvanishing basis function f_w. A check mark signals agreement with the exact J_w. All iterated stochastic integrals have domain $(t_0 + h; t_0)$.

$\|w\|$	w	$\widetilde{J}_w^{ABOBA}$	$\widetilde{J}_w^{BAOAB}$	Exact?
0	$\emptyset$	1	1	✓
1/2	A_j	J_{A_j}	J_{A_j}	✓
1	a, b, c	h	h	✓
3/2	$A_i a$	$h J_{A_i}/2$	$h J_{A_i}/2$	
	$A_i c$	$J_{A_i c}$	$J_{A_i c}$	✓
2	ab, ba, bc, ca, cc	$h^2/2$	$h^2/2$	✓
5/2	$A_i ab$	0	$h^2 J_{A_i}/4$	
	$A_i ca$	$h J_{A_i c}/2$	$h J_{A_i c}/2$	
	$A_i cc$	$J_{A_i cc}$	$J_{A_i cc}$	✓

of $\widetilde{J}_w^{ABOBA}$ is

$$J_{a^k}(t_0 + h/2; t_0) J_{b^\ell}(t_0 + h/2; t_0) J_{w'}(t_0 + h; t_0)$$
$$\times J_{b^m}(t_0 + h; t_0 + h/2) J_{a^n}(t_0 + h; t_0 + h/2)$$

or, from (9),

$$= \frac{1}{k!\ell!m!n!} \left(\frac{h}{2}\right)^{k+\ell+m+n} J_{w'}.$$

For a word that may be written in the form $a^k b^\ell w' b^m a^n$ in several ways, we sum over all possible ways (e.g., for aa, we have $\ell = m = 0$, $w' = \emptyset$, and three possibilities $(k, n) = (2, 0)$, $(k, n) = (1, 1)$, $(k, n) = (0, 2)$ leading to a coefficient $(1/2)(h/2)^2 + (h/2)^2 + (1/2)(h/2)^2 = h^2/2$). Similar considerations, with the roles of a and b interchanged, apply to the alternative BAOAB method. It now takes next to no time to find the coefficients in the third and fourth columns of the table.

5.4. Comparing the algorithms. At this point, we are in a position to compare the algorithms. Since at the words $A_i a$, $i = 1, \ldots, d$, both methods are in error, for both of them, the local error expansion in (15) begins with $\mathcal{O}(h^{3/2})$ terms. Furthermore, ABOBA and BAOAB share the same coefficient values $\widetilde{J}_w$ at the leading (i.e., $\mathcal{O}(h^{3/2})$) order and also at the next order (corresponding to words of weight 2). In fact, for the words that are featured in the table, the only difference between both integrators corresponds to the words $A_i ab$, $i = 1, \ldots, d$. For these, the exact solution has coefficient

$$J_{A_i ab} \sim \mathcal{N}\left(0, \frac{h^5}{20}\right),$$

BAOAB has

$$\widetilde{J}_{A_i ab}^{BAOAB} = \frac{h^2}{4} J_{A_i} \sim \mathcal{N}\left(0, \frac{h^5}{16}\right),$$

while, as noted above,

$$\widetilde{J}_{A_i ab}^{ABOBA} = 0,$$

due to the pattern ab after the stochastic letter. The joint distribution of $J_{A_i ab}$ and $\widetilde{J}_{A_i ab}^{BAOAB}$ is Gaussian with covariance $h^5/24$, and therefore the correlation between both variables is

$$\frac{h^5/24}{\sqrt{h^5/20}\sqrt{h^5/16}} = \frac{\sqrt{5}}{3} \approx 0.74,$$

while $J_{A_i ab}$ and $\widetilde{J}_{A_i ab}^{ABOBA}$ are obviously uncorrelated. Thus, for this word, ABOBA provides a very poor approximation to the exact coefficient. Due to the symmetric role played by the letters a and b in the algebra of words, for $A_i ba$, it is BAOAB that has an identically zero coefficient. However, this is irrelevant for the present discussion because, for that word, the basis function vanishes, as noted in (20).

Cases where $f_w \neq 0$, $\widetilde{J}_w^{ABOBA} = 0$, but $\widetilde{J}_w^{BAOAB}$ provides a nontrivial approximation to J_w, occur for higher values of the weight. For the deterministic word cba, $\widetilde{J}_{cab}^{BAOAB} = h^3/4$ and $\widetilde{J}_{A_i cab}^{ABOBA} = 0$ (the correct value is $h^3/6$). For $A_i cab$ with weight $7/2$, the exact solution has

$$J_{A_i cab} \sim \mathcal{N}\left(0, \frac{h^7}{252}\right),$$

while

$$\widetilde{J}_{A_i cab}^{BAOAB} \sim \mathcal{N}\left(0, \frac{h^7}{148}\right),$$

and, again due to the ab pattern,

$$\widetilde{J}_{A_i cab}^{ABOBA} = 0.$$

Now the correlation between the BAOAB coefficient and the true value is $\sqrt{21}/5 \approx 0.91$.

Why does ABOBA provide poor approximations for words like $A_i ba$, cba, $A_i cba$? By looking at the physical meaning of the corresponding word basis functions (see, e.g., the discussion of (21) presented above), we see that the *above shortcomings of ABOBA stem from the following algorithmic source.* In any given time step, ABOBA uses the *same* value of F in both kicks (q is not updated between those kicks) and, furthermore, that common value of F only depends on the values of q and p at the beginning of the step. Thus, over the whole step, the momentum increment hF due to the potential forces does not "see" the presence of friction or noise in the current step. On the contrary, in BAOAB the change in p at substep O (friction and noise) causes the kicking force to vary from the first kick to the second.[2]

6. Further developments. We have presented a systematic method, based on word series, for writing down expansions of strong and weak local errors of splitting integrators for Stratonovich SDEs. The method has been illustrated with a comparison between two related algorithms for the Langevin equations. The material may be adapted to study Ito equations, where the quasi-shuffle algebra replaces the shuffle algebra used here.

In the deterministic case, word series may also be applied to the computation of modified equations of integrators, as in [27]. Similarly, the word series approach may also be extended to investigate modified equations for Ito or Stratonovich SDEs. In addition, word series may be helpful in finding invariant densities of numerical algorithms. These developments will be dealt with in future work.

Appendix: Error bounds. In what follows, the deterministic vector fields f_a, $a \in \mathcal{A}_{det}$, and the stochastic vector fields f_A, $A \in \mathcal{A}_{stoch}$, in (13) are assumed to be globally Lipschitz, thus guaranteeing existence and uniqueness of the initial value

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[2]Note that BAOBA in the first kick of the next step reuses the value of $F(q)$ employed in the second kick of the present step, so that both ABOBA and BAOAB use each evaluation of the potential force twice.

problem for (13) itself and for the split systems. The theorems below provide bounds
for the weak local error and the mean square local error.

We begin with weak approximations. The third hypothesis used below is the same
as inequality (2.17) in [24], which is key in establishing Theorem 2.5 in that reference.
The first and second hypotheses just make explicit the differentiability requirements
on f_a, f_A, and χ that have to be imposed to guarantee that $D_w\chi$ makes sense when
w has weight $\nu + 1$.

THEOREM 8. *Let ν be a positive integer. Assume the following:*
- *The deterministic vector fields f_a, $a \in \mathcal{A}_{det}$, are of class $C^{2\nu}$, while the stochastic vector fields f_A, $A \in \mathcal{A}_{stoch}$, are of class $C^{2\nu+1}$.*
- *The observable χ is of class $C^{2\nu+2}$ in $\mathbb{R}^d$.*
- *There is a constant $C > 0$ such that for each $x \in \mathbb{R}^d$ and each word w of weight $\nu + 1$,*
$$|D_w\chi(x)| \leq C(1 + |x|^2)^{1/2}.$$

- *The weak error conditions* (18) *hold.*

Then there exists a constant $K > 0$ such that for each x_0, each $t_0 \geq 0$, and each $h > 0$,
$$|\mathbb{E}\chi\big(\widetilde{\phi}_{t_0+h,t_0}(x_0)\big) - \mathbb{E}\chi\big(\phi_{t_0+h,t_0}(x_0)\big)| \leq K(1 + |x_0|^2)^{1/2}h^{\nu+1}$$

(the expectation is conditional on x_0).

Proof. Define the residuals
$$R_{t_0,h}(x_0) = \chi\big(\phi_{t_0+h,t_0}(x_0)\big) - \sum_{\substack{n\in\mathbb{N}/2, \\ n\leq\nu}} \sum_{\|w\|=n} J_w(t_0,h)D_w\chi(x_0)$$

and
$$\widetilde{R}_{t_0,h}(x_0) = \chi\big(\widetilde{\phi}_{t_0+h,t_0}(x_0)\big) - \sum_{\substack{n\in\mathbb{N}/2, \\ n\leq\nu}} \sum_{\|w\|=n} \widetilde{J}_w(t_0,h)D_w\chi(x_0)$$

associated with the true and numerical solutions, respectively. If the weak order
conditions hold, we have, after using the fifth item in Proposition 4 and its counterpart
in Proposition 6,
$$\mathbb{E}\chi\big(\widetilde{\phi}_{t_0+h,t_0}(x_0)\big) - \mathbb{E}\chi\big(\phi_{t_0+h,t_0}(x_0)\big) = \mathbb{E}\widetilde{R}_{t_0,h}(x_0) - \mathbb{E}R_{t_0,h}(x_0),$$

and our task is to successively bound the two terms on the right-hand side.

For the theoretical solution, the standard stochastic Taylor expansion (see, e.g.,
[20, section 5.6] or [24, section 1.2]) provides the following representation as an iterated
Stratonovich integral:
$$R_{t_0,h}(x_0) = \sum_w \int_{t_0}^{t_0+h} \circ dB_{\ell_r}(s_r) \int_{t_0}^{s_r} \circ dB_{\ell_{r-1}}(s_{r-1}) \cdots$$
$$\int_{t_0}^{s_2} \circ dB_{\ell_1}(s_1)D_w\chi\big(\phi_{s_1,t_0}(x_0)\big);$$

here the ℓ_i are deterministic or stochastic letters, and the sum is extended to all
words of the form $w = \ell_1 \ldots \ell_r$, where $\|\ell_2 \ldots \ell_r\| = \nu$ and it is understood that, for a
deterministic letter ℓ_i, $dB_\ell(s_i)$ means ds. We next rewrite the iterated Stratonovich
integrals as combinations of iterated Ito integrals, as in [20, Remark 5.2.8]; in each
resulting iterated integral the sum of the weights of the letters of the Brownian motions

that appear is $\nu + 1$. An application of [24, Lemma 2.2] then shows that, for a suitable constant L, $\mathbb{E}|R_{t_0,h}(x_0)|^2 \leq L^2(1 + |x_0|^2)h^{2\nu+2}$, which implies $\mathbb{E}|R_{t_0,h}(x_0)| \leq L(1 + |x_0|^2)^{1/2}h^{\nu+1}$.

We now turn to the residual in the numerical solution. As in the proof of Theorem 4 in [27], we observe that, given an initial condition $x_0 = x(t_0)$ and any splitting algorithm, the numerical solution after one step $t_0 \to t_0 + h$ is the same as the value of the true solution at $t_0 + h$ of a time-dependent SDE in which the originally given vector fields are switched on and off as time evolves. For instance, in the simplest case where the SDE is $dx = f_a(x)dt + f_A(x) \circ dB_A(t)$ and the (Lie–Trotter) numerical scheme consists of advancing with $dx = f_A(x) \circ dB_A(x)$ and then with $dx = f_a(x)dt$, the time-dependent SDE is

$$dx = 1_{\{t_0+h/2 < t \leq t_0+h\}} f_a(x)2dt + 1_{\{t_0 \leq t \leq t_0+h/2\}} f_A(x) \circ dB_A(t_0 + 2(t - t_0)),$$

where $t_0 \leq t \leq t_0 + h$ and $1_{\{\cdot\}}$ denotes an indicator function. Using this observation the numerical residual may be bounded by reproducing the steps taken above to bound the residual of the true solution. $\qquad\square$

The last result refers to the mean square error. The proof is parallel to that we have just presented and will be omitted.

THEOREM 9. *Let μ be a positive integer multiple of $1/2$. Assume the following:*
- *The deterministic vector fields f_a, $a \in \mathcal{A}_{det}$, are of class $C^{2\mu}$, while the stochastic vector fields f_A, $A \in \mathcal{A}_{stoch}$, are of class $C^{2\mu+1}$.*
- *There is a constant $C > 0$ such that for each $x \in \mathbb{R}^d$ and each word w of weight $\mu + 1$,*
$$|f_w(x)| \leq C(1 + |x|^2)^{1/2}.$$

- *The strong error conditions* (17) *hold.*

Then there exists a constant $K > 0$ such that for each x_0, each $t_0 \geq 0$, and each $h > 0$,
$$\left(\mathbb{E}|\widetilde{\phi}_{t_0+h,t_0}(x_0) - \phi_{t_0+h,t_0}(x_0)|^2\right)^{1/2} \leq K(1 + |x_0|^2)^{1/2} h^{\mu+1/2}$$

(the expectation is conditional on x_0).

These local error bounds, in tandem with standard results (see, e.g., [24]), lead to bounds for the *global error*. For instance, for the Langevin equations considered in section 5, the order conditions are fulfilled with $\mu = 1$ and $\nu = 2$. It then follows that both integrators are convergent with mean square global errors $\mathcal{O}(h)$ and weak global errors $\mathcal{O}(h^2)$ if the force $F(q)$ satisfies the corresponding smoothness and growth hypotheses.

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