Title: Splitting methods

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Splitting methods

Synonyms

Operator-splitting methods, fractional step methods

Introduction

Splitting methods constitute a general class of numerical integration schemes for differential equations whose vector field can be decomposed in such a way that each sub-problem is simpler to integrate than the original system. For ordinary differential equations (ODEs) this idea can be formulated as follows. Given the initial value problem

$$x' = f(x), \qquad x_0 = x(0) \in \mathbb{R}^D \tag{1}$$

with $f : \mathbb{R}^D \longrightarrow \mathbb{R}^D$ and solution $\varphi_t(x_0)$, assume that f can be expressed as $f = \sum_{i=1}^{m} f^{[i]}$ for certain functions $f^{[i]}$, such that the equations

$$x' = f^{[i]}(x), \qquad x_0 = x(0) \in \mathbb{R}^D, \qquad i = 1, \ldots, m \tag{2}$$

can be integrated exactly, with solutions $x(h) = \varphi_h^{[i]}(x_0)$ at $t = h$, the time step. The different parts of f may correspond to physically different contributions. Then, by combining these solutions as

$$\chi_h = \varphi_h^{[m]} \circ \cdots \circ \varphi_h^{[2]} \circ \varphi_h^{[1]} \tag{3}$$

and expanding into series in powers of h, one finds that $\chi_h(x_0) = \varphi_h(x_0) + \mathcal{O}(h^2)$, so that χ_h provides a first-order approximation to the exact solution. Higher order approximations can be achieved by introducing more flows with additional coefficients, $\varphi_{a_{ij}h}^{[i]}$, in composition (3).

Splitting methods involve three steps: (i) choosing the set of functions $f^{[i]}$ such that $f = \sum_i f^{[i]}$; (ii) solving either exactly or approximately each equation $x' = f^{[i]}(x)$; and (iii) combining these solutions to construct an approximation for (1) up to the desired order.

The splitting idea can also be applied to partial differential equations (PDEs) involving time and one or more space dimensions. Thus, if the spatial differential operator contains parts of a different character (such as advection and diffusion), then different discretization techniques may be applied to each part, as well as for the time integration.

Splitting methods have a long history and have been applied (sometimes with different names) in many different fields, ranging from parabolic and reaction-diffusion PDEs to quantum statistical mechanics, chemical physics and Hamiltonian dynamical systems [6].

Some of the advantages of splitting methods are the following: they are simple to implement, are explicit if each sub-problem is solved with an explicit method, and often preserve qualitative properties the differential equation might possess.

Splitting methods for ODEs

Increasing the order

Very often in applications the function f in the ODE (1) can be split in just two parts, $f(x) = f^{[a]}(x) + f^{[b]}(x)$. Then both $\chi_h = \varphi_h^{[b]} \circ \varphi_h^{[a]}$ and its adjoint, $\chi_h^* \equiv \chi_{-h}^{-1} = \varphi_h^{[a]} \circ \varphi_h^{[b]}$, are first order integration schemes. These formulae are often called the Lie–Trotter splitting. On the other hand, the symmetric version

$$\mathcal{S}_h^{[2]} \equiv \varphi_{h/2}^{[a]} \circ \varphi_h^{[b]} \circ \varphi_{h/2}^{[a]} \tag{4}$$

provides a second order integrator, known as the Strang–Marchuk splitting, the leapfrog or the Störmer–Verlet method, depending on the context where it is used [2]. Notice that $\mathcal{S}_h^{[2]} = \chi_{h/2}^* \circ \chi_{h/2}$.

More generally, one may consider a composition of the form

$$\psi_h = \varphi_{a_{s+1}h}^{[a]} \circ \varphi_{b_s h}^{[b]} \circ \varphi_{a_s h}^{[a]} \circ \cdots \circ \varphi_{a_2 h}^{[a]} \circ \varphi_{b_1 h}^{[b]} \circ \varphi_{a_1 h}^{[a]}, \tag{5}$$

and try to increase the order of approximation by suitably determining the parameters a_i, b_i. The number s of $\varphi_h^{[b]}$ (or $\varphi_h^{[a]}$) evaluations in (5) is usually referred to as the number of stages of the integrator. This is called time-symmetric if $\psi_h = \psi_h^*$, in which case one has a left-right palindromic composition. Equivalently, in (5) one has

$$a_1 = a_{s+1}, \quad b_1 = b_s, \quad a_2 = a_s, \quad b_2 = b_{s-1}, \ldots \tag{6}$$

The order conditions the parameters a_i, b_i have to satisfy can be obtained by relating the previous integrator ψ_h with a formal series Ψ_h of differential operators [1]: it is

known that, the h-flow φ_h of the original system $x' = f^{[a]}(x) + f^{[b]}(x)$ satisfies, for each $g \in C^\infty(\mathbb{R}^D, \mathbb{R})$, the identity $g(\varphi_h(x)) = \mathrm{e}^{h(F^{[a]}+F^{[b]})}[g](x)$, where $F^{[a]}$ and $F^{[b]}$ are the Lie derivatives corresponding to $f^{[a]}$ and $f^{[b]}$ respectively, acting as

$$F^{[a]}[g](x) = \sum_{j=1}^{D} f_j^{[a]}(x) \frac{\partial g}{\partial x_j}(x), \qquad F^{[b]}[g](x) = \sum_{j=1}^{D} f_j^{[b]}(x) \frac{\partial g}{\partial x_j}(x). \tag{7}$$

Similarly, the approximation $\psi_h(x) \approx \varphi_h(x)$ given by the splitting method (5) satisfies the identity $g(\psi_h(x)) = \Psi(h)[g](x)$, where

$$\Psi(h) = \mathrm{e}^{a_1 h F^{[a]}} \, \mathrm{e}^{b_1 h F^{[b]}} \cdots \mathrm{e}^{a_s h F^{[a]}} \, \mathrm{e}^{b_s h F^{[b]}} \, \mathrm{e}^{a_{s+1} h F^{[a]}}. \tag{8}$$

Hence, the coefficients a_i, b_i must be chosen in such a way that the operator $\Psi(h)$ is a good approximation of $\mathrm{e}^{h(F^{[a]}+F^{[b]})}$, or equivalently, $h^{-1}\log(\Psi) \approx F^{[a]} + F^{[b]}$.

Applying repeatedly the Baker–Campbell–Hausdorff (BCH) formula [2] one arrives at

$$\begin{aligned} \frac{1}{h}\log(\Psi(h)) = {} & (v_a F^{[a]} + v_b F^{[b]}) + h v_{ab} F^{[ab]} + h^2 (v_{abb} F^{[abb]} + v_{aba} F^{[aba]}) \\ & + h^3 (v_{abbb} F^{[abbb]} + v_{abba} F^{[abba]} + v_{abaa} F^{[abaa]}) + \mathcal{O}(h^4), \end{aligned} \tag{9}$$

where

$$\begin{aligned} F^{[ab]} &= [F^{[a]}, F^{[b]}], \quad F^{[abb]} = [F^{[ab]}, F^{[b]}], \quad F^{[aba]} = [F^{[ab]}, F^{[a]}], \\ F^{[abbb]} &= [F^{[abb]}, F^{[b]}], \quad F^{[abba]} = [F^{[abb]}, F^{[a]}], \quad F^{[abaa]} = [F^{[aba]}, F^{[a]}], \end{aligned}$$

the symbol $[\cdot, \cdot]$ stands for the Lie bracket, and $v_a, v_b, v_{ab}, v_{abb}, v_{aba}, v_{abbb}, \ldots$ are polynomials in the parameters a_i, b_i of the splitting scheme (5). In particular, one gets $v_a = \sum_{i=1}^{s+1} a_i$, $v_b = \sum_{i=1}^{s} b_i$, $v_{ab} = \frac{1}{2} - \sum_{i=1}^{s} b_i \sum_{j=1}^{i} a_j$. The order conditions then read $v_a = v_b = 1$ and $v_{ab} = v_{abb} = v_{aba} = \cdots = 0$ up to the order considered. To achieve order $r = 1, 2, 3, \ldots, 10$ the number of conditions to be fulfilled is $\sum_{j=1}^{r} n_j$, where $n_j = 2, 1, 2, 3, 6, 9, 18, 30, 56, 99$. This number is smaller for $r > 3$ when dealing with second order ODEs of the form $y'' = g(y)$ when they are rewritten as (1) [1].

For time-symmetric methods, the order conditions at even orders are automatically satisfied, which leads to $n_1 + n_3 + \cdots + n_{2k-1}$ order conditions to achieve order $r = 2k$. For instance, $n_1 + n_3 = 4$ conditions need to be fulfilled for a symmetric method (5)-(6) to be of order four.

Splitting and composition methods

When the original system (1) is split in $m > 2$ parts, higher order schemes can be obtained by considering a composition of the basic first order splitting method (3) and its adjoint $\chi_h^* = \varphi_h^{[1]} \circ \cdots \circ \varphi_h^{[m-1]} \circ \varphi_h^{[m]}$. More specifically, compositions of the general form

$$\psi_h = \chi^*_{\alpha_{2s}h} \circ \chi_{\alpha_{2s-1}h} \circ \cdots \circ \chi^*_{\alpha_2 h} \circ \chi_{\alpha_1 h}, \tag{10}$$

can be considered with appropriately chosen coefficients $(\alpha_1, \ldots, \alpha_{2s}) \in \mathbb{R}^{2s}$ so as to achieve a prescribed order of approximation.

In the particular case when system (1) is split in $m = 2$ parts, so that $\chi_h = \varphi_h^{[b]} \circ \varphi_h^{[a]}$, method (10) reduces to (5) with $a_1 = \alpha_1$ and

$$b_j = \alpha_{2j-1} + \alpha_{2j}, \qquad a_{j+1} = \alpha_{2j} + \alpha_{2j+1}, \qquad \text{for} \quad j = 1, \ldots, s, \tag{11}$$

where $\alpha_{2s+1} = 0$. In that case, the coefficients a_i and b_i are such that

$$\sum_{i=1}^{s+1} a_i = \sum_{i=1}^{s} b_i. \tag{12}$$

Conversely, any splitting method (5) satisfying (12) can be written in the form (10) with $\chi_h = \varphi_h^{[b]} \circ \varphi_h^{[a]}$.

Moreover, compositions of the form (10) make sense for an arbitrary basic first order integrator χ_h (and its adjoint χ_h^*) of the original system (1). Obviously, if the coefficients α_j of a composition method (10) are such that ψ_h is of order r for arbitrary basic integrators χ_h of (1), then the splitting method (5) with (11) is also of order r. Actually, as shown in [7], the integrator (5) is of order r for ODEs of the form (1) with

$f = f^{[a]} + f^{[b]}$ if and only if the integrator (10) (with coefficients α_j obtained from (11)) is of order r for arbitrary first order integrators χ_h.

This close relationship allows one to establish in an elementary way a defining feature of splitting methods (5) of order $r \geq 3$: at least one a_i and one b_i are necessarily negative [1]. In other words, splitting schemes of order $r \geq 3$ always involve backward fractional time steps.

Preserving properties

Assume that the individual flows $\varphi_h^{[i]}$ share with the exact flow φ_h some defining property which is preserved by composition. Then it is clear that any composition of the form (5) and (10) with χ_h given by (3) also possesses this property. Examples of such features are symplecticity, unitarity, volume preservation, conservation of first integrals, etc. [6]. In this sense, splitting methods form an important class of geometric numerical integrators [2]. Repeated application of the BCH formula can be used (see (9)) to show that there exists a modified (formal) differential equation

$$\tilde{x}' = f_h(\tilde{x}) \equiv f(\tilde{x}) + h f_2(\tilde{x}) + h^2 f_3(\tilde{x}) + \cdots, \quad \tilde{x}(0) = x_0, \tag{13}$$

associated to any splitting method ψ_h such that the numerical solution $x_n = \psi_h(x_{n-1})$ $(n = 1, 2, \ldots)$ satisfies $x_n = \tilde{x}(nh)$ for the exact solution $\tilde{x}(t)$ of (13). An important observation is that the vector fields f_k in (13) belong to the Lie algebra generated by $f^{[1]}, \ldots, f^{[m]}$. In the particular case of autonomous Hamiltonian systems, if $f^{[i]}$ are Hamiltonian, then each f_k is also Hamiltonian. Then one may study the long-time behavior of the numerical integrator by analyzing the solutions of (13) viewed as a small perturbation of the original system (1) and obtain rigorous statements with techniques of backward error analysis [2].

Further extensions

Several extensions can be considered to reduce the number of stages necessary to achieve a given order and get more efficient methods. One of them is the use of a processor or corrector. The idea consists in enhancing an integrator ψ_h (the kernel) with a map π_h (the processor) as $\hat{\psi}_h = \pi_h \circ \psi_h \circ \pi_h^{-1}$. Then, after n steps one has $\hat{\psi}_h^n = \pi_h \circ \psi_h^n \circ \pi_h^{-1}$, and so only the cost of ψ_h is relevant. The simplest example of a processed integrator is provided by the Störmer–Verlet method (4). In that case $\psi_h = \chi_h = \varphi_h^{[b]} \circ \varphi_h^{[a]}$ and $\pi_h = \varphi_{h/2}^{[a]}$. The use of processing allows one to get methods with fewer stages in the kernel and smaller error terms than standard compositions [1].

The second extension uses the flows corresponding to other vector fields in addition to $F^{[a]}$ and $F^{[b]}$. For instance, one could consider methods (5) such that, in addition to $\varphi_h^{[a]}$ and $\varphi_h^{[b]}$, use the h-flow $\varphi_h^{[abb]}$ of the vector field $F^{[abb]}$ when its computation is straightforward. This happens, for instance, for second-order ODEs $y'' = g(y)$ [1; 6].

Splitting is particularly appropriate when $\|f^{[a]}\| \ll \|f^{[b]}\|$ in (1). Introducing a small parameter ε, we can write $x' = \varepsilon f^{[a]}(x) + f^{[b]}(x)$, so that the error of scheme (5) is $\mathcal{O}(\varepsilon)$. Moreover, since in many practical applications $\varepsilon < h$, one is mainly interested in eliminating error terms with small powers of ε instead of satisfying all the order conditions. In this way it is possible to get more efficient schemes. In addition, the use of a processor allows one to eliminate the errors of order εh^k for all $1 < k < n$ and all n [6].

Although only autonomous differential equations have been considered here, several strategies exist for adapting splitting methods also to non-autonomous systems without deteriorating their overall efficiency [1].

Some good 4th-order splitting methods

In the next table we collect the coefficients of a few selected fourth-order symmetric methods of the form (5)-(6). Higher order and more elaborated schemes can be found in [1; 2; 6] and references therein. They are denoted as X_s4, where s indicates the number of stages. $\mathrm{S}_6 4$ is a general splitting method, whereas $\mathrm{SN}_6 4$ refers to a method tailored for second-order ODEs of the form $y'' = g(y)$ when they are rewritten as a first order system (1) and the coefficients a_i are associated to $g(y)$. Finally, $\mathrm{SNI}_5 4$ is a method especially designed for problems of the form $x' = \varepsilon f^{[a]}(x) + f^{[b]}(x)$. With $s = 3$ stages, there is only one solution, $\mathrm{S}_3 4$, given by $a_1 = b_1/2,\ b_1 = 2/(2 - 2^{1/3})$. In all cases, the remaining coefficients are fixed by symmetry and consistency ($\sum_i a_i = \sum_i b_i = 1$).

$\mathrm{S}_6 4$	a_1=0.07920369643119565	$b_1 = 0.209515106613362$
	$a_2 = 0.353172906049774$	$b_2 = -0.143851773179818$
	$a_3 = -0.04206508035771952$	
$\mathrm{SN}_6 4$	a_1=0.08298440641740515	$b_1 = 0.245298957184271$
	$a_2 = 0.396309801498368$	$b_2 = 0.604872665711080$
	$a_3 = -0.3905630492234859$	
$\mathrm{SNI}_5 4$	a_1=0.81186273854451628884	$b_1 = -0.0075869131187744738$
	$a_2 = -0.67748039953216912289$	$b_2 = 0.31721827797316981388$

Numerical example: a perturbed Kepler problem

To illustrate the performance of the previous splitting methods, we apply them to the time integration of the perturbed Kepler problem described by the Hamiltonian

$$H = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{r} - \frac{\varepsilon}{2r^5}\left(q_2^2 - 2q_1^2\right), \tag{14}$$

where $r = \sqrt{q_1^2 + q_2^2}$. We take $\varepsilon = 0.001$ and integrate the equations of motion $q_i' = p_i,\ p_i' = -\partial H/\partial q_i,\ i = 1, 2$, with initial conditions $q_1 = 4/5,\ q_2 = p_1 = 0,$

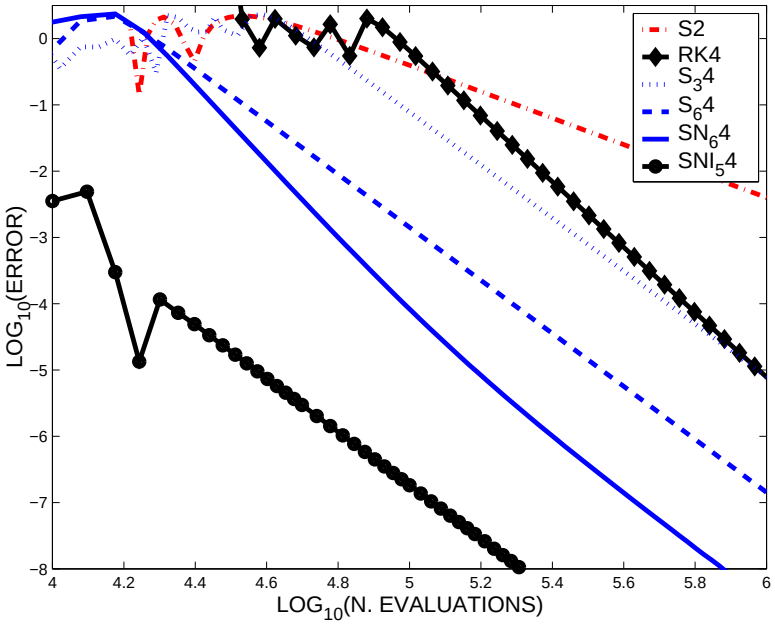

Fig. 1. Error in the solution $(q_1(t_f), q_2(t_f))$ vs. the number of evaluations for different 4th-order splitting methods (the extra cost in the method $\mathrm{SNI}_5 4$, designed for perturbed problems, is not taken into account).

$p_1 = \sqrt{3/2}$. Splitting methods are used with the partition into kinetic and potential energy. We measure the 2-norm error in the position at $t_f = 2000$, $(q_1, q_2) = (0.318965403761932, 1.15731646810481)$, for different time steps and plot the corresponding error as a function of the number of evaluations for each method in Figure 1. Notice that although the generic method $\mathrm{S}_6 4$ has three more stages than the minimum given by $\mathrm{S}_3 4$, this extra cost is greatly compensated by a higher accuracy. On the other hand, since this system corresponds to the second order ODE $q'' = g(q)$, method $\mathrm{SN}_6 4$ leads to a higher accuracy with the same computational cost. Finally, $\mathrm{SNI}_5 4$ takes profit of the near-integrable character of the Hamiltonian (14) and the two extra stages to achieve an even higher efficiency. It requires solving the Kepler problem separately from the perturbation. This requires a more elaborated algorithm with a slightly increase in the computational cost (not reflected in the figure). Results provided by the leap-frog method S2 and the standard fourth-order Runge-Kutta integrfator RK4 are also included for reference.

Splitting methods for PDEs

In the numerical treatment of evolutionary PDEs of parabolic or mixed hyperbolic-parabolic type, splitting time-integration methods are also widely used. In this setting the overall evolution operator is formally written as a sum of evolution operators, typically representing different aspects of a given model. Consider an evolutionary PDE formulated as an abstract Cauchy problem in a certain function space $\mathcal{U} \subset \{u : \mathbb{R}^D \times \mathbb{R} \to \mathbb{R}\}$,

$$u_t = L(u), \qquad u(t_0) = u_0, \tag{15}$$

where L is a spatial partial differential operator. For instance,

$$\frac{\partial}{\partial t}u(x,t) = \sum_{j=1}^{d} \frac{\partial}{\partial x_j}\left(\sum_{i=1}^{d} c_i(x)\frac{\partial}{\partial x_i}u(x,t)\right) + f(x,u(x,t)), \qquad u(x,t_0) = u_0(x)$$

or in short, $L(x,u) = \nabla \cdot (c\nabla u) + f(u)$, corresponds to a diffusion-reaction problem. In that case it makes sense to split the problem into two sub-equations, corresponding to the different physical contributions,

$$u_t = L_a(u) \equiv \nabla \cdot (c\nabla u), \qquad u_t = L_b(u) \equiv f(u), \tag{16}$$

solve numerically each equation in (16), thus giving $u^{[a]}(h) = \varphi_h^{[a]}(u_0)$, $u^{[b]}(h) = \varphi_h^{[b]}(u_0)$, respectively for a time step h, and then compose the operators $\varphi_h^{[a]}$, $\varphi_h^{[b]}$ to construct an approximation to the solution of (15). Thus, $u(h) \approx \varphi_h^{[b]}(\varphi_h^{[a]}(u_0))$ provides a first-order approximation, whereas the Strang splitting $u(h) \approx \varphi_{h/2}^{[a]}(\varphi_h^{[b]}(\varphi_{h/2}^{[a]}(u_0)))$ is formally second-order accurate for sufficiently smooth solutions. In this way, especially adapted numerical methods can be used to integrate each sub-problem, even in parallel [3; 4].

Systems of hyperbolic conservation laws, such as

$$u_t + f(u)_x + g(u)_x = 0, \qquad u(x,t_0) = u_0(x)$$

can also be treated with splitting methods, in this case by fixing a step size h and applying a especially tailored numerical scheme to each scalar conservation law $u_t + f(u)_x = 0$

and $u_t + g(u)_x = 0$. This is a particular example of dimensional splitting where the original problem is approximated by solving one space direction at a time. Early examples of dimensional splitting are the so-called locally one-dimensional (LOD) methods (such as LOD-backward Euler and LOD Crank–Nicolson schemes) and alternating direction implicit (ADI) methods (e.g., the Peaceman–Rachford algorithm) [4].

Although the formal analysis of splitting methods in this setting can also be carried out by power series expansions, several fundamental difficulties arise, however. First, nonlinear PDEs in general possess solutions that exhibit complex behavior in small regions of space and time, such as sharp transitions and discontinuities. Second, even if the exact solution of the original problem is smooth, it might happen that the composition defining the splitting method provides non-smooth approximations. Therefore, it is necessary to develop sophisticated tools to analyze whether the numerical solution constructed with a splitting method leads to the correct solution of the original problem or not [3].

On the other hand, even if the solution is sufficiently smooth, applying splitting methods of order higher than two is not possible for certain problems. This happens, in particular, when there is a diffusion term in the equation, since then the presence of negative coefficients in the method leads to an ill-posed problem. When $c = 1$ in (16), this order-barrier has been circumvented, however, with the use of complex-valued coefficients with positive real parts: the operator $\varphi_{zh}^{[a]}$ corresponding to the Laplacian L_a is still well defined in a reasonable distribution set for $z \in \mathbb{C}$, provided that $\Re(z) \geq 0$.

There exist also relevant problems where high order splitting methods can be safely used as is in the integration of the time dependent Schrödinger equation $iu_t = -\frac{1}{2m}\Delta u + V(x)u$ split into kinetic $T = -(2m)^{-1}\Delta$ and potential V energy operators and with periodic boundary conditions. In this case, the combination of the Strang splitting in time and the Fourier collocation in space is quite popular in chemical

physics (with the name of split-step Fourier method). These schemes have appealing structure-preserving properties, such as unitarity, symplecticity and time-symmetry [5]. Moreover, it has been shown that for a method (5) of order r with the splitting into kinetic and potential energy and under relatively mild assumptions on T and V, one has a rth-order error bound $\|\psi_h^n u_0 - u(nh)\| \leq Cnh^{r+1} \max_{0\leq s\leq nh} \|u(s)\|_r$ in terms of the rth-order Sobolev norm [5].

Cross-references

Composition methods; Symplectic methods; One-step methods, order, convergence; Stoermer-Verlet; Symmetric methods;

References

1. Blanes S, Casas F, and Murua A (2008) Splitting and composition methods in the numerical integration of differential equations. *Bol. Soc. Esp. Mat. Apl.* **45**: 89-145
2. Hairer E, Lubich C, and Wanner G (2006) *Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations*, 2nd Ed, Springer (Berlin)
3. Holden H, Karlsen K H, Lie K A, and Risebro N H (2010) *Splitting Methods for Partial Differential Equations with Rough Solutions*, European Mathematical Society (Zürich)
4. Hundsdorfer W, Verwer J G (2003) *Numerical Solution of Time-Dependent Advection-Diffusion-Reaction Equations*, Springer (Berlin)
5. Lubich C (2008) *From Quantum to Classical Molecular Dynamics: Reduced Models and Numerical Analysis*, European Mathematical Society (Zürich)
6. McLachlan R I, Quispel R (2002) Splitting methods, *Acta Numer.* **11**: 341–434
7. McLachlan R I (1995), On the numerical integration of ordinary differential equations by symmetric composition methods, *SIAM J. Numer. Anal.*, **16**: 151–168