Title: Symmetric Methods

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Symmetric Methods

Synonym

time reversible

Definition

This entry is concerned with *symmetric methods* for solving ordinary differential equations (ODEs) of the form

$$\dot{y} = f(y) \in \mathbb{R}^n, \quad y(0) = y_0. \tag{1}$$

Throughout this article, we denote by $\varphi_{t,f}(y_0)$ the flow of equation (1) with vector field f, i.e. the exact solution at time t with initial condition $y(0) = y_0$, and we assume that the conditions for its well-definiteness and smoothness for $(y_0, |t|)$ in an appropriate subset Ω of $\mathbb{R}^n \times \mathbb{R}_+$ are satisfied. Numerical methods for (1) implement numerical flows $\Phi_{h,f}$ which, for **small enough** *step sizes* h, approximate $\varphi_{h,f}$. Of central importance in the context of symmetric methods is the concept of *adjoint method*:

Definition 1. *The adjoint method $\Phi^*_{h,f}$ is the inverse of $\Phi_{t,f}$ with reversed time step $-h$:*

$$\Phi^*_{h,f} := \Phi^{-1}_{-h,f} \tag{2}$$

A numerical method Φ_h is then said to be symmetric if $\Phi_{h,f} = \Phi^*_{h,f}$.

Overview

Symmetry is an essential property of numerical methods with regards to *order* of accuracy and *geometric* properties of the solution. We briefly discuss the implications of these two aspects and refer to the corresponding sections for a more involved presentation:

• A method $\Phi_{h,f}$ is said to be of order p if

$$\Phi_{h,f}(y) = \varphi_{h,f}(y) + \mathcal{O}(h^{p+1}),$$

and, if the *local error* has the following first-term expansion

$$\Phi_{h,f}(y) = \varphi_{h,f}(y) + h^{p+1}C(y) + \mathcal{O}(h^{p+2}),$$

then straightforward application of the implicit function theorem leads to

$$\Phi^*_{h,f}(y) = \varphi_{h,f}(y) - (-h)^{p+1}C(y) + \mathcal{O}(h^{p+2}).$$

This implies that **a symmetric method is necessarily of even order** $p = 2q$, since $\Phi_{h,f}(y) = \Phi^*_{h,f}(y)$ means that $(1 + (-1)^{p+1})C(y) = 0$. This property plays a key-role in the construction of *composition* methods by *triple jump techniques* (see section on composition methods) and this is certainly no coincidence that Runge-Kutta methods of *optimal* order (Gauss methods) are symmetric (see section on Runge-Kutta methods). It also explains why symmetric methods are used in conjunction with (Richardson) extrapolation techniques.

• The exact flow $\varphi_{t,f}$ is itself symmetric owing to the *group property* $\varphi_{s+t,f} = \varphi_{s,f} \circ \varphi_{t,f}$. Consider now an isomorphism ρ of the vector space $\mathbb{R}^n$ (the phase space of (1)) and assume that the vector field f satisfies the relation $\rho \circ f = -f \circ \rho$ (see Figure 1). Then, $\Phi_{t,f}$ is said to be ρ-reversible, that it to say the following equality holds:

$$\rho \circ \varphi_{t,f} = \varphi^{-1}_{t,f} \circ \rho. \tag{3}$$

$$\begin{array}{ccc} \mathbb{R}^n & \xrightarrow{f} & \mathbb{R}^n \\ \rho\downarrow & & \downarrow\rho \\ \mathbb{R}^n & \xleftarrow[(-f)]{} & \mathbb{R}^n \end{array} \qquad \begin{array}{ccc} \mathbb{R}^n & \xrightarrow{\varphi_{t,f}} & \mathbb{R}^n \\ \rho\downarrow & & \downarrow\rho \\ \mathbb{R}^n & \xleftarrow[\varphi_{t,f}^{-1}]{} & \mathbb{R}^n \end{array} \qquad \begin{array}{ccc} \mathbb{R}^n & \xrightarrow{\Phi_{h,f}} & \mathbb{R}^n \\ \rho\downarrow & & \downarrow\rho \\ \mathbb{R}^n & \xleftarrow[\Phi_{h,f}^{-1}]{} & \mathbb{R}^n \end{array}$$

Fig. 1. ρ-reversibility of f, $\varphi_{t,f}$ and $\Phi_{h,f}$.

Example 1. Hamiltonian systems

$$\begin{aligned} \dot{y} &= \frac{\partial H}{\partial z}(y,z) \\ \dot{z} &= -\frac{\partial H}{\partial y}(y,z) \end{aligned}$$

with an Hamiltonian function $H(q,p)$ satisfying $H(y,-z) = H(y,z)$ are ρ-reversible for $\rho(y,z) = (y,-z)$.

Definition 2. *A method Φ_h, applied to a ρ-reversible ordinary differential equation, is said to be ρ-reversible if*

$$\rho \circ \Phi_{h,f} = \Phi_{h,f}^{-1} \circ \rho.$$

Note that if $\Phi_{h,f}$ is symmetric, it is ρ-reversible if and only if the following condition holds:

$$\rho \circ \Phi_{h,f} = \Phi_{-h,f} \circ \rho. \tag{4}$$

Besides, if (4) holds for an invertible ρ, then $\Phi_{h,f}$ is ρ-reversible if and only if it is symmetric.

Example 2. The trapezoidal rule, whose flow is defined by the *implicit* equation

$$\Phi_{h,f}(y) = y + hf\left(\frac{1}{2}y + \frac{1}{2}\Phi_{h,f}(y)\right), \tag{5}$$

is symmetric and is ρ-reversible when applied to ρ-reversible f.

Since most numerical methods satisfy relation (4), symmetry is the required property for numerical methods to share with the exact flow not only time-reversibility but also ρ-reversibility. This illustrates that **a symmetric method mimics geometric properties of**

the exact flow. *Modified differential equations* sustain further this assertion (see next section) and allow for the derivation of deeper results for *integrable reversible* systems such as the **preservation of invariants and the linear growth of errors** by symmetric methods (see Section on reversible KAM theory).

Modified equations for symmetric methods

Constant stepsize backward error analysis. Considering a numerical method Φ_h (not necessarily symmetric) and the sequence of approximations obtained by application of the formula $y_{n+1} = \Phi_{h,f}(y_n), n = 0, 1, 2, ...$, from the initial value y_0, the idea of *backward error analysis* consists in searching for a *modified vector field* f_h^N such that

$$\varphi_{h,f_h^N}(y_0) = \Phi_{h,f}(y_0) + \mathcal{O}(h^{N+2}), \tag{6}$$

where the modified vector field, *uniquely* defined by a Taylor expansion of (6), is of the form

$$f_h^N(y) = f(y) + hf_1(y) + h^2 f_2(y) + \ldots + h^N f_N(y). \tag{7}$$

Theorem 1. *The modified vector field of a symmetric method $\Phi_{h,f}$ has an expansion in even powers of h, i.e. $f_{2j+1} \equiv 0$ for $j = 0, 1, \ldots$ Moreover, if f and $\Phi_{h,f}$ are ρ-reversible, then f_h^N is ρ-reversible as well for any $N \geq 0$.*

Proof. Reversing the time step h in (6) and taking the inverse of both sides, we obtain

$$(\varphi_{-h,f_{-h}^N})^{-1}(y_0) = (\Phi_{-h,f})^{-1}(y_0) + \mathcal{O}(h^{N+2}).$$

Now, the group property of exact flows implies that $(\varphi_{-h,f_{-h}^N})^{-1}(y_0) = \varphi_{h,f_{-h}^N}(y_0)$, so that

$$\varphi_{h,f_{-h}^N}(y_0) = \Phi^*_{h,f}(y_0) + \mathcal{O}(h^{N+2}),$$

and by uniqueness, $(f_h^N)^* = f_{-h}^N$. This proves the first statement. Assume now that f is ρ-reversible, so that (4) holds. It follows from $f_{-h}^N = f_h^N$ that

$$\rho \circ \varphi_{-h,f_h^N} = \rho \circ \varphi_{-h,f_{-h}^N} \overset{\mathcal{O}(h^{N+2})}{=} \rho \circ \Phi_{-h,f} = \Phi_{h,f} \circ \rho \overset{\mathcal{O}(h^{N+2})}{=} \varphi_{h,f_h^N} \circ \rho.$$

where the second and last equalities are valid up to $\mathcal{O}(h^{N+2})$-error terms. Yet the group property then implies that $\rho \circ \varphi_{-nh,f_h^N} = \varphi_{nh,f_h^N} \circ \rho + \mathcal{O}_n(h^{N+2})$ where the constant in the $\mathcal{O}_n$-term depends on n and an interpolation argument shows that for fixed N and small $|t|$

$$\rho \circ \varphi_{-t,f_h^N} = \varphi_{t,f_h^N} \circ \rho + \mathcal{O}(h^{N+1}),$$

where the $\mathcal{O}$-term depends smoothly on t and on N. Finally, differentiating with respect to t, we obtain

$$-\rho \circ f_h^N = \frac{d}{dt}\rho \circ \varphi_{-t,f_h^N}\Big|_{t=0} = \frac{d}{dt}\varphi_{t,f_h^N} \circ \rho\Big|_{t=0} + \mathcal{O}(h^{N+2}) = f_h^N \circ \rho + \mathcal{O}(h^{N+1}),$$

and consequently $-\rho \circ f_h^N = f_h^N \circ \rho$.

Remark 1. The expansion (7) of the modified vector field f_h^N can be computed explicitly at any order N with the *substitution product* of *B-series* [2].

Example 3. Consider the Lotka-Volterra equations in Poisson form

$$\begin{pmatrix} \dot{u} \\ \dot{v} \end{pmatrix} = \begin{pmatrix} 0 & uv \\ -uv & 0 \end{pmatrix} \begin{pmatrix} \nabla_u H(u,v) \\ \nabla_v H(u,v) \end{pmatrix}, \quad H(u,v) = \log(u) + \log(v) - u - v,$$

i.e. $y' = f(y)$ with $f(y) = (u(1-v), v(u-1))^T$. Note that $\rho \circ f = -f \circ \rho$ with $\rho(u,v) = (v,u)$. The modified vector fields $f_{h,\text{iE}}^2$ for the *implicit Euler* method and $f_{h,\text{mr}}^2$ for the implicit midpoint rule read (with $N = 2$)

$$f_{h,\text{iE}}^2 = f + \frac{1}{2}hf'f + \frac{h^2}{12}f''(f,f) + \frac{h^2}{3}f'f'f \text{ and } f_{h,\text{mr}}^2 = f - \frac{h^2}{24}f''(f,f) + \frac{h^2}{12}f'f'f.$$

The exact solutions of the modified ODEs are plotted on Figure 2 together with the corresponding numerical solution. Though the modified vector fields are truncated only at second order, the agreement is excellent. The difference of behaviour of the two solutions is also striking: only the symmetric method captures the periodic nature of the solution[1]. This will be further explored in next section.

[1] The good behaviour of the midpoint rule can not be attributed to its *symplecticity* since the system is a non-canonical Poisson system

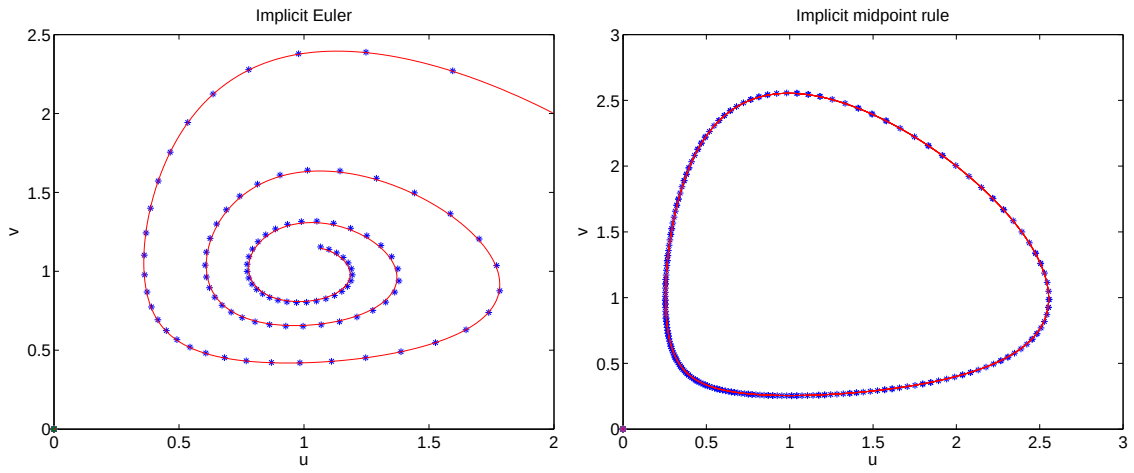


Fig. 2. Exact solutions of modified equations (red lines) versus numerical solutions by Implicit Euler and Midpoint Rule (blue points).

Variable stepsize backward error analysis. In practice, it is often fruitful to resort to variable step-size implementations of the numerical flow $\Phi_{h,f}$. In accordance with [17], we consider step-sizes that are proportional to a function $\epsilon s(y,\epsilon)$ depending only on the current state y and of a parameter ϵ prescribed by the user and aimed at controlling the error. The approximate solution is then given by

$$y_{n+1} = \Phi_{\epsilon s(y_n,\epsilon),f}(y_n), \quad n = 0, \dots,$$

A remarkable feature of this algorithm is that it preserves the symmetry of the exact solution as soon as $\Phi_{h,f}$ is symmetric and s satisfies the relation

$$s(\Phi_{\epsilon s(y,\epsilon),f}(y), -\epsilon) = s(y,\epsilon),$$

and preserves the ρ-reversibility as soon as $\Phi_{h,f}$ is ρ-reversible and satisfies the relation

$$s(\rho^{-1} \circ \Phi_{\epsilon s(y,\epsilon),f}(y), -\epsilon) = s(y,\epsilon).$$

A result similar to Theorem 1 then holds with h replaced by ϵ.

Remark 2. A recipe to construct such a function s, suggested by Stoffer in [17], consists in requiring that the local error estimate is kept constantly equal to a tolerance parameter. For the details of the implementation, we refer to the original paper or to Chap. VIII.3 of [10].

Reversible Kolmogorov-Arnold-Moser theory

The theory of *integrable Hamiltonian* systems has its counterpart for *reversible integrable* ones. A reversible system

$$\dot{y} = f(y,z),\ \dot{z} = g(y,z) \text{ where } \rho \circ (f,g) = -(f,g) \circ \rho \text{ with } \rho(y,z) = (y,-z), \quad (8)$$

is reversible integrable if it can be brought, through a reversible transformation $(a,\theta) = (I(y,z),\Theta(y,z))$, to the *canonical* equations

$$\dot{a} = 0, \quad \dot{\theta} = \omega(a).$$

An interesting instance is the case of *completely integrable Hamiltonian* systems

$$\dot{y} = \frac{\partial H}{\partial z}(y,z), \quad \dot{z} = -\frac{\partial H}{\partial y}(y,z),$$

with first integrals I_j's in involution[2] such that $I_j \circ \rho = I_j$. In the conditions where Arnold-Liouville Theorem (see Chapter X.1.3. of [10]) can be applied, then, under the additional assumption that

$$\exists (y^*,0) \in \{(y,z), \forall j, I_j(y,z) = I_j(y_0,z_0)\}, \quad (9)$$

such a system is reversible integrable. In this situation, ρ-reversible methods constitute a very interesting way around symplectic method, as the following result shows:

Theorem 2. *Let $\Phi_{h,(f,g)}$ be a reversible numerical method of order p applied to an integrable reversible system (8) with real-analytic f and g. Consider $a^\bullet = (I_1(y^\bullet,z^\bullet),\ldots,I_d(y^\bullet,z^\bullet))$: If the condition*

$$\forall k \in \mathbb{Z}^d/\{0\},\ |k \cdot \omega(a^\bullet)| \geq \gamma \left(\sum_{i=1}^{d} |k_i| \right)^{-\nu}$$

is satisfied for some positive constants γ and ν, then there exist positive C, c and h_0 such that the following assertion holds:

[2] That is to say such that $(\nabla_y I_i) \cdot (\nabla_z I_j) = (\nabla_z I_i) \cdot (\nabla_y I_j)$ for all i,j.

$$\forall h \le h_0, \forall (x_0, y_0) \textit{ such that } \max_{j=1,\dots,d} |I_j(y_0, z_0) - a^\bullet| \le c|\log h|^{-\nu-1}, \tag{10}$$

$$\forall t = nh \le h^{-p}, \begin{cases} \|\Phi^n_{h,(f,g)}(x_0, y_0) - (y(t), z(t))\| \le Cth^p \\ |I_j(\Phi^n_{h,(f,g)}(y_0, z_0)) - I_j(y_0, z_0)| \le Ch^p \textit{ for all } j \end{cases}$$

Analogously to symplectic methods, ρ-reversible methods thus preserve invariant tori $I_j = cst$ over long intervals of times and the error growth is linear in t. Remarkably and in contrast with symplectic methods, this result remains valid for reversible variable stepsize implementations (see Chapter X.I.3 of [10]). However, it is important to note that for an Hamiltonian reversible system, the Hamiltonian ceases to be preserved when condition (9) is not fullfilled. This situation is illustrated on Figure 3 for the Hamiltonian system with $H(q,p) = \frac{1}{2}p^2 + \cos(q) + \frac{1}{5}\sin(2q)$, an example borrowed from [4].

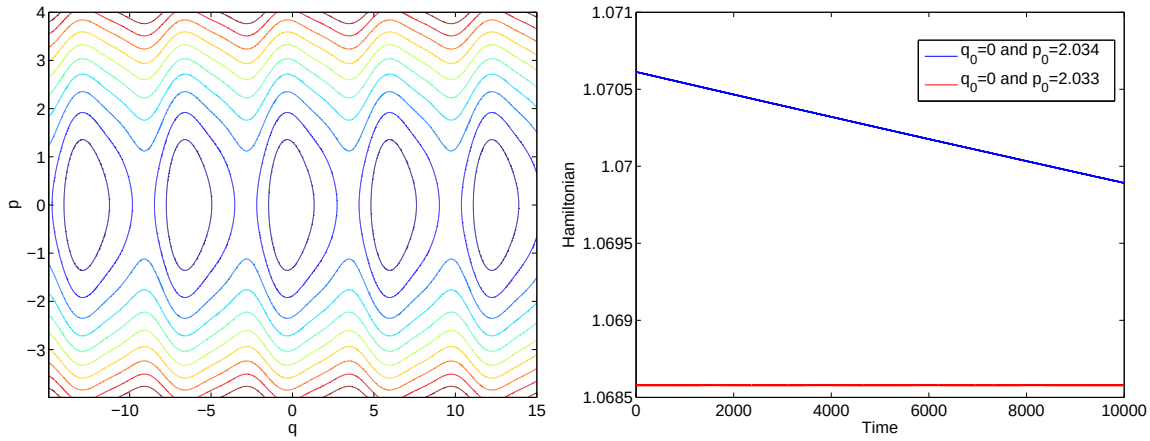


Fig. 3. Level sets of H (left) and evolution of H w.r.t. time for two different initial values

Symmetric methods of Runge-Kutta type

Runge-Kutta methods form a popular class of numerical integrators for (1). Owing to their importance in applications, we consider general systems (1) and subsequently partitioned systems.

Methods for general systems. We start with the following

Definition 3. *Consider a matrix $A = (a_{i,j}) \in \mathbb{R}^s \times \mathbb{R}^s$ and a vector $b = (b_j) \in \mathbb{R}^s$. The Runge-Kutta method denoted (A, b) is defined by*

$$Y_i = y + h \sum_{j=1}^{s} a_{i,j} f(Y_j), \quad i = 1, \ldots, s \tag{11}$$

$$\tilde{y} = y + h \sum_{j=1}^{s} b_j f(Y_j). \tag{12}$$

Note that strictly speaking, the method is properly defined only for small $|h|$. In this case, the corresponding numerical flow $\Phi_{h,f}$ maps y to $\tilde{y}$. Vector Y_i approximates the solution at intermediate point $t_0 + c_i h$, where $c_i = \sum_j a_{i,j}$ and it is customary since [1] to represent a method by its *tableau*:

$$\begin{array}{c|ccc} c_1 & a_{1,1} & \ldots & a_{1,s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s,1} & \ldots & a_{s,s} \\ \hline & b_1 & \ldots & b_s \end{array} \tag{13}$$

Runge-Kutta methods automatically satisfy the ρ-compatibility condition (4): changing h into $-h$ in (11, 12), we have indeed by linearity of ρ and by using $\rho \circ f = -f \circ \rho$

$$\rho(Y_i) = \rho(y) - h \sum_{j=1}^{s} a_{i,j} f\Big(\rho(Y_j)\Big), \quad i = 1, \ldots, s$$

$$\rho(\tilde{y}) = \rho(y) - h \sum_{j=1}^{s} b_j f\Big(\rho(Y_j)\Big).$$

By construction, this is $\rho(\Phi_{-h,f}(y))$ and by previous definition $\Phi_{h,f}(\rho(y))$. As a consequence, ρ-reversible Runge-Kutta methods coincide with symmetric methods. Nevertheless, symmetry requires an additional algebraic condition stated in next theorem:

Theorem 3. *A Runge-Kutta method (A, b) is symmetric if*

$$PA + AP = eb^T \text{ and } b = Pb, \tag{14}$$

where $e = (1, \ldots, 1)^T \in \mathbb{R}^s$ and P is the permutation matrix defined by $p_{i,j} = \delta_{i,s+1-j}$.

Proof. Denoting $Y = \Big(Y_1^T, \ldots, Y_s^T\Big)^T$ and $F(Y) = \Big(f(Y_1)^T, \ldots, f(Y_s)^T\Big)^T$, a more compact form for (11, 12) is

$$Y = e \otimes y + h(A \otimes I)F(Y), \tag{15}$$

$$\tilde{y} = y + h(b^T \otimes I)F(Y). \tag{16}$$

On the one hand, premultiplying (15) by $P \otimes I$ and noticing that

$$(P \otimes I)F(Y) = F\Big((P \otimes I)Y\Big),$$

it is straightforward to see that $\Phi_{h,f}$ can also be defined by coefficients PAP^T and Pb. On the other hand, exchanging h and $-h$, y and $\tilde{y}$, it appears that $\Phi^*_{h,f}$ is defined by coefficients $A^* = eb^T - A$ and $b^* = b$. The flow $\Phi_{h,f}$ is thus symmetric as soon as $eb^T - A = PAP$ and $b = Pb$, which is nothing but condition (14).

Remark 3. For methods without redundant stages, condition (14) is also necessary.

Example 4. The *implicit midpoint rule*, defined by $A = \frac{1}{2}$ and $b = 1$ is a symmetric method of order 2. More generally, the s-stage Gauss collocation method based on the roots of the s^{th} shifted Legendre polynomial, is a symmetric method of order $2s$. For instance, the 2-stage and 3-stage Gauss methods of orders 4 and 6 have the following coefficients:

$$\begin{array}{c|cc} \frac{1}{2}-\frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4}-\frac{\sqrt{3}}{6} \\ \frac{1}{2}+\frac{\sqrt{3}}{6} & \frac{1}{4}+\frac{\sqrt{3}}{6} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \qquad \begin{array}{c|ccc} \frac{1}{2}-\frac{\sqrt{15}}{10} & \frac{5}{36} & \frac{2}{9}-\frac{\sqrt{15}}{15} & \frac{5}{36}-\frac{\sqrt{15}}{30} \\ \frac{1}{2} & \frac{5}{36}+\frac{\sqrt{15}}{24} & \frac{2}{9} & \frac{5}{36}-\frac{\sqrt{15}}{24} \\ \frac{1}{2}+\frac{\sqrt{15}}{10} & \frac{5}{36}+\frac{\sqrt{15}}{30} & \frac{2}{9}+\frac{\sqrt{15}}{15} & \frac{5}{36} \\ \hline & \frac{5}{18} & \frac{4}{9} & \frac{5}{18} \end{array} \tag{17}$$

Methods for partitioned systems. For systems of the form

$$\dot{y} = f(z), \quad \dot{z} = g(y), \tag{18}$$

it is natural to apply two different Runge-Kutta methods to variables y and z: Written in compact form, a partitioned Runge-Kutta method reads:

$$Y = e \otimes y + h(A \otimes I)F(Z), \quad Z = e \otimes y + h(\hat{A} \otimes I)G(Y),$$

$$\tilde{y} = \quad y + h(b^T \otimes I)F(Z), \qquad \tilde{z} = \quad y + h(\hat{b}^T \otimes I)G(Y),$$

and the method is symmetric if both (A, b) and $(\hat{A}, \hat{b})$ are. An important feature of partitioned Runge-Kutta method is that they can be symmetric and *explicit* for systems of the form (18).

Example 5. The Verlet method is defined by the following two Runge-Kutta tableaux:

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & \frac{1}{2} & \frac{1}{2} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \quad \text{and} \quad \begin{array}{c|cc} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \tag{19}$$

The method becomes explicit owing to the special structure of the partitioned system:

$$\begin{aligned} &Y_1 = y_0, && Z_1 = z_0 + \tfrac{h}{2} f(Y_1), \\ &Y_2 = y_0 + h g(Z_1), && Z_2 = Z_1, \\ &y_1 = Y_2, && z_1 = z_0 + \tfrac{h}{2}\Big(f(Y_1) + f(Y_2)\Big) \end{aligned}$$

The Verlet method is the most elementary method of the class of partitioned Runge-Kutta methods known as Lobatto IIIA-IIIB. Unfortunately, methods of higher orders within this class are no longer explicit in general, even for the equations of the form (18). It is nevertheless possible to construct symmetric explicit Runge-Kutta methods, which turn out to be equivalent to compositions of Verlet's method, and whose introduction is for this reason postponed to next section.

Note that a particular instance of partitioned systems are second-order differential equations of the form

$$\dot{y} = z, \quad \dot{z} = g(y), \tag{20}$$

which covers many situations of practical interest (for instance mechanical systems governed by Newton's law in absence of friction).

Symmetric methods obtained by composition

Another class of symmetric methods is constituted of symmetric *compositions* of low-order methods. The idea consists in applying a basic method $\Phi_{h,f}$ with a sequence of prescribed step-sizes: Given s real numbers $\gamma_1, \ldots, \gamma_s$, its composition with step sizes $\gamma_1 h, \ldots, \gamma_s h$ gives rise to a new method

$$\Psi_{h,f} = \Phi_{\gamma_s h,f} \circ \ldots \circ \Phi_{\gamma_1 h,f}. \tag{21}$$

Noticing that the local error of $\Psi_{h,f}$, defined by $\Psi_{h,f}(y) - \varphi_{h,f}(y)$, is of the form

$$(\gamma_1^{p+1} + \ldots + \gamma_s^{p+1}) h^{p+1} C(y) + \mathcal{O}(h^{p+2}),$$

as soon as $\gamma_1 + \ldots + \gamma_s = 1$, $\Psi_{h,f}$ is of order at least $p+1$ if

$$\gamma_1^{p+1} + \ldots + \gamma_s^{p+1} = 0.$$

This observation is the key to *triple jump* compositions, as proposed by a series of authors [3; 5; 18; 21]: Starting from a symmetric method $\Phi_{h,f}$ of (even) order $2q$, the new method obtained for

$$\gamma_1 = \gamma_3 = \frac{1}{2 - 2^{1/(2q+1)}} \text{ and } \gamma_2 = \frac{2^{1/(2q+1)}}{2 - 2^{1/(2q+1)}}$$

is symmetric

$$\Psi^*_{h,f} = \Phi^*_{\gamma_1 h,f} \circ \Phi^*_{\gamma_2 h,f} \circ \Phi^*_{\gamma_3 h,f} = \Phi_{\gamma_3 h,f} \circ \Phi_{\gamma_2 h,f} \circ \Phi_{\gamma_1 h,f} = \Psi_{h,f}$$

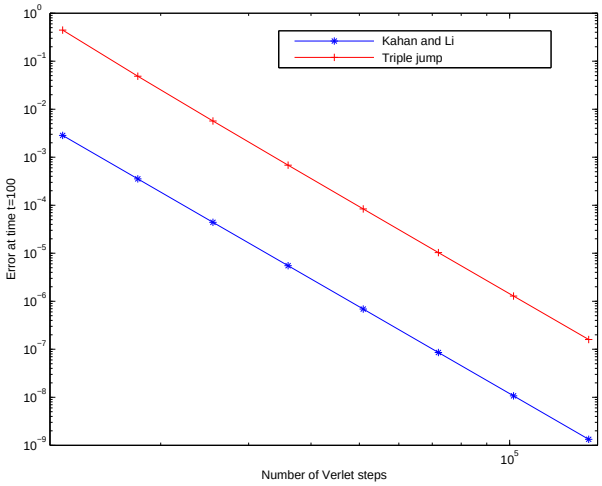
and of order at least $2q+1$. Since the order of a symmetric method is even, $\Psi_{h,f}$ is in fact of order $2q+2$. The procedure can then be repeated recursively to construct arbitrarily high-order symmetric methods of orders $2q+2$, $2q+4$, $2q+6$, ..., with respectively 3, 9, 27, ..., compositions of the original basic method $\Phi_{h,f}$. However, the construction is far from being the most efficient, for the combined coefficients become large, some of which being negatives. A partial remedy is to envisage compositions with $s = 5$. We hereby give the coefficients obtained by Suzuki [18]:

$$\gamma_1 = \gamma_2 = \gamma_4 = \gamma_5 = \frac{1}{4 - 4^{1/(2q+1)}} \text{ and } \gamma_3 = -\frac{4^{1/(2q+1)}}{4 - 4^{1/(2q+1)}}$$

which give rise to very efficient methods for $q = 1$ and $q = 2$. The most efficient high-order composition methods are nevertheless obtained by solving the full system of order conditions, i.e. by raising the order directly from 2 to 8 for instance, without going through the intermediate steps described above. This requires much more effort though, first to derive

the order conditions, and then to solve the resulting polynomial system. It is out of the scope of this article to describe the two steps involved and we rather refer to the paper [15] on the use of ∞B-series for order conditions and to Chapter V.3.2. of [10] for various examples and numerical comparisons. An excellent method of order 6 with 9 stages has been obtained by Kahan and Li [12] and we reproduce here its coefficients:

$$\gamma_1 = \gamma_9 = 0.3921614440073141,$$
$$\gamma_2 = \gamma_8 = 0.3325991367893594,$$
$$\gamma_3 = \gamma_7 = -0.7062461725576393,$$
$$\gamma_4 = \gamma_6 = 0.0822135962935508,$$
$$\gamma_5 = 0.7985439909348299.$$



For the sake of illustration, we have computed the solution of Kepler's equations with this method and the method of order six obtained by the triple jump technique. In both cases, the basic method is Verlet's scheme. The gain offered by the method of Kahan and Li is impressive (it amounts to two digits of accuracy on this example). Other methods can be found for instance in [10; 14].

Remark 4. It is also possible to consider symmetric compositions of non-symmetric methods. In this situation, raising the order necessitates to compose the basic method and its adjoint.

Symmetric methods for highly-oscillatory problems

In this Section, we present methods aimed at solving problems of the form

$$\ddot{q} = -\nabla V_{fast}(q) - \nabla V_{slow}(q) \tag{22}$$

where V_{fast} and V_{slow} are two potentials acting on different time scales, typically such that $\nabla^2 V_{fast}$ is positive semi-definite and $\|\nabla^2 V_{fast}\| >> \|\nabla^2 V_{slow}\|$. Explicit standard methods

suffer from severe stability restrictions due to the presence of high-oscillations at the slow time scale and necessitate small steps and many evaluations of the forces. Since slow forces $-\nabla V_{slow}$ are in many applications much more expensive to evaluate than fast ones, efficient methods in this context are thus devised to require significantly fewer evaluations per step of the slow force.

Example 6. In applications to molecular dynamics for instance, fast forces deriving from V_{fast} (short-range interactions) are much cheaper to evaluate than slow forces deriving from V_{slow} (long-range interactions). Other examples of applications are presented in [11].

Methods for general problems with nonlinear fast potentials. Introducing the variable $p = \dot{q}$ in (22), the equation reads

$$\underbrace{\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix}}_{\dot{y}} = \underbrace{\begin{pmatrix} p \\ 0 \end{pmatrix}}_{f_K(y)} + \underbrace{\begin{pmatrix} 0 \\ -\nabla_q V_{fast}(q) \end{pmatrix}}_{f_F(y)} + \underbrace{\begin{pmatrix} 0 \\ -\nabla_q V_{slow}(q) \end{pmatrix}}_{f_S(y)}$$

The usual Verlet method [20] would consist in composing the flows $\varphi_{h,(f_F+f_S)}$ and φ_{h,f_K} as follows

$$\varphi_{\frac{h}{2},(f_F+f_S)} \circ \varphi_{h,f_K} \circ \varphi_{\frac{h}{2},(f_F+f_S)}$$

or, if necessary, numerical approximations thereof, and would typically be restricted to very small step-sizes. The Impulse Method [8; 19; 6] combines the three pieces of the vector field differently

$$\varphi_{\frac{h}{2},f_S} \circ \varphi_{h,(f_K+f_F)} \circ \varphi_{\frac{h}{2},f_S}.$$

Note that φ_{h,f_S} is explicit

$$\varphi_{h,f_S} \begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} q \\ p - h\nabla_q V_{slow}(q) \end{pmatrix}$$

while $\varphi_{h,(f_K+f_F)}$ may require to be approximated by a numerical method $\Phi_{h,(f_K+f_F)}$ which uses step-sizes that are fractions of h. If $\Phi_{h,(f_K+f_F)}$ is symmetric (and/or symplectic), the overall method is symmetric as well (and/or symplectic) and allows for larger step-sizes.

However, it still suffers from resonances and a better option is given by the mollified Impulse methods, which considers a the mollified potential $\bar{V}_{slow}(q) = V_{slow}(a(q))$ in loco of $V_{slow}(q)$, where $a(q)$ and $a'(q)$ are *averaged* values given by

$$a(q) = \frac{1}{h}\int_0^h x(s)ds, \quad a'(q) = \frac{1}{h}\int_0^h X(s)ds$$

where

$$\ddot{x} = -\nabla V_{fast}(x), x(0) = q, \dot{x}(0) = p, \quad \ddot{X} = -\nabla^2 V_{fast}(x)X, X(0) = I, \dot{X}(0) = 0 \tag{23}$$

The resulting method uses the mollified force $-a'(q)^T(\nabla_q V_{slow})(a(q))$ and is still symmetric (and/or symplectic) provided (23) is solved with a symmetric (and/or symplectic) method.

Methods for problems with quadratic fast potentials In many applications of practical importance, the potential V_{fast} is quadratic of the form $V_{fast}(q) = \frac{1}{2}q^T\Omega^2 q$. In this case, the mollified impulse method falls into the class of trigonometric symmetric methods of the form

$$\Phi_h \begin{pmatrix} p \\ q \end{pmatrix} = R(h\Omega)\begin{pmatrix} p \\ q \end{pmatrix} - \frac{1}{2}h\begin{pmatrix} \psi_0(h\Omega)\nabla V_{slow}\Big(\phi(h\Omega)q_0\Big) + \psi_1(h\Omega)\nabla V_{slow}\Big(\phi(h\Omega)q_1\Big) \\ h\psi(h\Omega)\nabla V_{slow}\Big(\phi(h\Omega)q_0\Big) \end{pmatrix}$$

where $R(h\Omega)$ is the block-matrix given by

$$R(h\Omega) = \begin{pmatrix} \cos(h\Omega) & -\Omega\sin(h\Omega) \\ \Omega^{-1}\sin(h\Omega) & \cos(h\Omega) \end{pmatrix}$$

and the functions ϕ, ψ, ψ_0 and ψ_1 are even functions such that

$$\psi(z) = \frac{\sin(z)}{z}\psi_1(z), \quad \psi_0(z) = \cos(z)\psi_1(z), \quad \text{and } \psi(0) = \phi(0) = 1.$$

Various choices of functions ψ and ϕ are possible and documented in the litterature. Two particularly interesting ones are $\psi(z) = \frac{\sin^2(z)}{z^2}$, $\phi(z) = 1$ (see [9]) or $\psi(z) = \frac{\sin^3(z)}{z^3}$, $\phi(z) = \frac{\sin(z)}{z}$ (see [7]).

Conclusion

This entry should be regarded as an introduction to the subject of symmetric methods. Several topics have not been exposed here, such as symmetric projection for ODEs on manifolds, DAEs of index 1 or 2, symmetric multistep methods, symmetric splitting methods, symmetric Lie-group methods, ... and we refer the interested reader to [10; 16; 13] for a comprehensive presentation of these topics.

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