On construction of Runge-Kutta type methods for solving ordinary differential equations

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Background

To construct Runge-Kutta type method? This is an old topic since Runge 1895 and Kutta 1901, but

1. The original and seminal idea of Continuous-Stage Runge-Kutta (CSRK) methods was presented by Butcher in 1987;
2. The CSRK method was again mentioned by Hairer in 2010;
3. The CSRK method has been rarely studied until recently:

   - Average vector field (AVF) method (Quispel & McLaren, 2008)
   - Hamiltonian boundary value methods HBVMs(∞, k) (Brugnano et al., 2009)
   - Energy-preserving collocation methods (Hairer 2010)
   - Time finite element methods (TFEM): a unified framework for numerical discretizations of ODEs (Tang & Sun, 2012)
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No RK can preserve the Hamiltonian exactly (Celledoni etc 2009), but CSRK can!
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Questions
Can we construct more CSRK methods? And any other geometric integrators?
Continuous-stage RK methods

Consider the ODEs

\[
\begin{aligned}
\dot{z} &= f(t, z), \quad t \in [t_0, T], \quad z \in \mathbb{R}^d, \\
z(t_0) &= z_0.
\end{aligned}
\]

Definition (CSRK, Hairer 2010)

Let \( A_{\tau, \sigma} \) be a function of two variables \( \tau, \sigma \in [0, 1] \), and \( B_\tau, C_\tau \) be functions of \( \tau \in [0, 1] \) with \( C_\tau = \int_0^1 A_{\tau, \sigma} \, d\sigma \). The one-step method \( \Phi_h : z_0 \mapsto z_1 \) given by

\[
\begin{aligned}
U_\tau &= z_0 + h \int_0^1 A_{\tau, \sigma} f(t_0 + C_\sigma h, U_\sigma) \, d\sigma, \quad \tau \in [0, 1], \\
z_1 &= z_0 + h \int_0^1 B_\tau f(t_0 + C_\tau h, U_\tau) \, d\tau,
\end{aligned}
\]

is called a **continuous-stage Runge-Kutta method**, where \( U_\tau \approx z(t_0 + C_\tau h) \).
Continuous-stage RK methods

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\]

\[
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\]

is called a continuous-stage Runge-Kutta method, where \( U_\tau \approx z(t_0 + C_\tau h) \).

Major premise

We assume \( B_\tau = 1, \ C_\tau = \tau \), because \( \cdots \).
Construction of RK type methods by our approach

The corresponding simplifying assumptions of order conditions are (Hairer 2010)

\[ \bar{B}(\xi) : \int_{0}^{1} B_{\tau} C_{\tau}^{\kappa-1} \, d\tau = \frac{1}{\kappa}, \quad \kappa = 1, \ldots, \xi \]

\[ \bar{C}(\eta) : \int_{0}^{1} A_{\tau, \sigma} C_{\sigma}^{\kappa-1} \, d\sigma = \frac{1}{\kappa} C_{\tau}^{\kappa}, \quad \kappa = 1, \ldots, \eta \]

\[ \bar{D}(\zeta) : \int_{0}^{1} B_{\tau} C_{\tau}^{\kappa-1} A_{\tau, \sigma} \, d\tau = \frac{1}{\kappa} B_{\sigma}(1 - C_{\sigma}^{\kappa}), \quad \kappa = 1, \ldots, \zeta \]

Lemma

If \( \bar{C}(\eta) \) and \( \bar{D}(\zeta) \) are satisfied, then the order of the corresponding CSRK method is \( \min\{2\eta + 2, \eta + \zeta + 1\} \).
Construction of RK type methods by our approach
The corresponding simplifying assumptions of order conditions are (Hairer 2010)

\[ \tilde{B}(\xi) : \int_0^1 B_\tau C_\tau^{\kappa-1} d\tau = \frac{1}{\kappa}, \quad \kappa = 1, \ldots, \xi \]

\[ \tilde{C}(\eta) : \int_0^1 A_{\tau, \sigma} C_\sigma^{\kappa-1} d\sigma = \frac{1}{\kappa} C_\tau^\kappa, \quad \kappa = 1, \ldots, \eta \]

\[ \tilde{D}(\zeta) : \int_0^1 B_\tau C_\tau^{\kappa-1} A_{\tau, \sigma} d\tau = \frac{1}{\kappa} B_\sigma (1 - C_\sigma^\kappa), \quad \kappa = 1, \ldots, \zeta \]

**Lemma**

If \( \tilde{C}(\eta) \) and \( \tilde{D}(\zeta) \) are satisfied, then the order of the corresponding CSRK method is \( \min\{2\eta + 2, \eta + \zeta + 1\} \).

**Our approach** is using the orthogonal polynomial expansion technique to deal with \( A_{\tau, \sigma} \). The key tool is the normalized shifted Legendre polynomial defined by

\[ P_\iota(x) = \frac{\sqrt{2\iota + 1}}{\iota!} \frac{d^\iota}{dx^\iota} \left( x^\iota (x - 1)^\iota \right), \quad \iota = 0, 1, 2, \ldots \]

satisfying \( \int_0^1 P_\iota(t) P_\kappa(t) dt = \delta_{\iota\kappa}, \quad \iota, \kappa = 0, 1, 2, \ldots \).
A lemma

Lemma

For the continuous-stage RK method, we have

1. $\bar{C}(\eta)$ (with $\eta \geq 1$) $\iff$ $A_{\tau, \sigma}$ takes the following form

$$A_{\tau, \sigma} = \sum_{i=0}^{\eta-1} \int_{0}^{\tau} P_i(x) \, dx \, P_i(\sigma) + \sum_{i=\eta}^{\infty} \gamma_i(\tau) P_i(\sigma),$$

where $\gamma_i(\tau)$, $i \geq \eta$ are arbitrary;

2. $\bar{D}(\zeta)$ (with $\zeta \geq 1$) $\iff$ $A_{\tau, \sigma}$ takes the following form

$$A_{\tau, \sigma} = \sum_{i=0}^{\zeta-1} \int_{\sigma}^{1} P_i(x) \, dx \, P_i(\tau) + \sum_{i=\zeta}^{\infty} \lambda_i(\sigma) P_i(\tau),$$

where $\lambda_i(\sigma)$, $i \geq \zeta$ are arbitrary.
Construction of CSRK methods

Denote $\xi_\iota := \frac{1}{2\sqrt{4\iota^2-1}}$, $\iota = 1, 2, 3, \cdots$. Note that the set of functions

$$\{ P_i(\tau)P_j(\sigma) : i, j = 0, 1, 2, \cdots \}$$

is linearly independent. By the expansion for $A_{\tau, \sigma}$ we get the following result.

Theorem (Construction of CSRK)

Assume $1 \leq \eta \in \mathbb{Z}$ and $0 \leq \zeta \in \mathbb{Z}$. The following two statements are equivalent:

- both $\bar{C}(\eta)$ and $\bar{D}(\zeta)$ hold;
- $A_{\tau, \sigma}$ takes the following form

$$A_{\tau, \sigma} = \frac{1}{2} + \sum_{\iota=0}^{N_1} \xi_{\iota+1}P_{\iota+1}(\tau)P_{\iota}(\sigma) - \sum_{\iota=0}^{N_2} \xi_{\iota+1}P_{\iota+1}(\sigma)P_{\iota}(\tau) + \sum_{\substack{i \geq \zeta, j \geq \eta}} \omega_{ij}P_i(\tau)P_j(\sigma),$$

here $N_1 = \max \{\eta - 1, \zeta - 2\}$, $N_2 = \max \{\eta - 2, \zeta - 1\}$ and $\omega_{ij}$ are arbitrary real parameters. By convention if $N_2 < 0$ then the second sum vanishes.
Examples (taken from Tang & Sun, 2012)

Four kinds of k-degree time finite element methods (TFEM) can be interpreted as CSRK methods with $B_\tau = 1$, $C_\tau = \tau$ and different $A_{\tau, \sigma}$:

1. For Continuous TFEM, $A_{\tau, \sigma} = \sum_{\ell=0}^{k-1} \int_0^\tau p_\ell(x) \, dx \, p_\ell(\sigma)$;

2. For Left-discontinuous TFEM, $A_{\tau, \sigma} = 1 - \sum_{\ell=0}^{k-1} \int_0^\sigma p_\ell(x) \, dx \left( p_\ell(\tau) - \frac{\sqrt{2\ell+1}}{\sqrt{2k+1}} p_k(\tau) \right)$;

3. For Right-discontinuous TFEM, $A_{\tau, \sigma} = \sum_{\ell=0}^{k-1} \int_0^\tau p_\ell(x) \, dx \left( p_\ell(\sigma) - \frac{\sqrt{2\ell+1}}{\sqrt{2k+1}} p_k(\sigma) \right)$;

4. For Bi-discontinuous TFEM, $A_{\tau, \sigma} = 1 - \sum_{\ell=0}^k p_\ell(\tau) \int_0^\sigma p_\ell(x) \, dx$.

These methods are of superconvergence order $2k$, $2k + 1$, $2k + 1$, $2k + 2$, resp..

- The same ideas of TFEMs extended to PDEs such as Reed & Hill 1973 (DG), Cockburn & Shu 1989-1998 (Local DG for conservation laws), ···
Construction of classical RK methods

CSRK can be reduced to classical RK methods by using a quadrature formula \((b_i, c_i)_{i=1}^s\) and the Butcher tableau is

\[
\begin{array}{c|cc}
  c & (b_j A_{c_i, c_j})_{s \times s} \\
  & \quad b^T \\
\end{array}
\]

Note that \(A_{\tau, \sigma}\) is a bivariate polynomial when truncating the Legendre expansion.

**Theorem (Construction of classical RK methods)**

Suppose that the quadrature formula \((b_i, c_i)_{i=1}^s\) is of order \(p\) (i.e., it is exact for polynomials of degree \(p - 1\)) and \(A_{\tau, \sigma}\) is a bivariate polynomial with degree \(r\) in \(\tau\) and with degree \(v\) in \(\sigma\), satisfying \(\bar{C}(\eta)\) and \(\bar{D}(\zeta)\), then the \(s\)-stage RK method generated by \((b_j A_{c_i, c_j}, b_i, c_i)\) is of order \(\min(p, 2\alpha + 2, \alpha + \beta + 1)\), where \(\alpha = \min(\eta, p - v)\) and \(\beta = \min(\zeta, p - r)\).
Comparison to W-transformation

Definition (W-transformation, Hairer & Wanner 1981,1991)

Let $\eta, \zeta$ be given integers between 0 and $s - 1$. We say that an $s \times s$ matrix $W$ satisfies $T(\eta, \zeta)$ for the quadrature formula $(b_i, c_i)_{i=1}^{s}$ if

(a) $W$ is nonsingular,

(b) $w_{ij} = P_{j-1}(c_i)$, $i = 1, \ldots, s$, $j = 1, \ldots, \max(\eta, \zeta) + 1$,

(c) $W^T B W = \begin{pmatrix} I & 0 \\ 0 & R \end{pmatrix}$, where $B := \text{diag}(b_1, \cdots, b_s)$, $I$ is the $(\zeta + 1) \times (\zeta + 1)$ identity matrix and $R$ is an arbitrary $(s - \zeta - 1) \times (s - \zeta - 1)$ matrix.

Remark

- Generally, the RK methods constructed by classical W-transformation can also be retrieved by our approach;
- The RK coefficient matrix can be explicitly expressed and conveniently calculated. Remarkably, we have avoided computing the inverse of $W$ or $R$;
- The matrix $W$ by our approach is free of the constrains $T(\eta, \zeta)$. 
Construction of geometric integrators

Consider a Hamiltonian differential equation

\[ \dot{z} = J^{-1} \nabla H(z), \quad z(t_0) = z_0 \in \mathbb{R}^{2d}, \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}, \quad z = (p, q)^T. \]

Some important properties:

1. the Hamiltonian $H$ (or energy) is constant;
2. the exact flow $\varphi_t$ is symplectic transformation;
3. if $H(-p, q) = H(p, q)$, then the system is $\rho$-reversible ($\rho(p, q) = (-p, q)$).

Negative results

1. No numerical integrator can preserve the energy and symplecticity at the same time for general Hamiltonian systems (Ge & Marsden 1988);
2. No (classical) RK method can preserve the energy for general Hamiltonian systems (Celledoni et al., 2009).

Numerical discretization preserving these properties:

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Numerical discretization preserving these properties:

Energy-preserving integrators

Theorem (Energy conservation)

Suppose that $g_\iota(x) = \sum_{j=0}^{\infty} a_{\iota j} P_j(x)$, $a_{\iota j} \in \mathbb{R}$ and

$$A_{\tau, \sigma} = \sum_{\iota=0}^{\infty} \omega_{\iota} \left( \int_0^{\tau} g_\iota(x) \, dx \, g_\iota(\sigma) \right), \quad \omega_{\iota} \in \mathbb{R}.$$

1. \(\bar{C}(\eta) \) (with \(1 \leq \eta \in \mathbb{Z}\)) is satisfied iff \(\omega_{\iota}\) and \(a_{\iota \kappa}\) \((\iota, \kappa = 0, 1, 2, \cdots)\) satisfy

$$\sum_{\iota=0}^{\infty} \omega_{\iota} a_{\iota i} a_{\iota j} = \begin{cases} \delta_{ij}, & 0 \leq i, j \leq \eta - 1, \\ 0, & 0 \leq i \leq \eta - 1, j \geq \eta; \end{cases}$$

2. The CSRK method $\Phi_h$ can preserve the Hamiltonian exactly and the order is $2\eta_M$, where $\eta_M = \max\{\eta \in \mathbb{Z} : \bar{C}(\eta) \text{ is satisfied for } \Phi_h\}$, provided that $\eta_M$ is subject to $1 \leq \eta_M < \infty$. And $\zeta_M = \max\{\zeta \in \mathbb{Z} : \bar{D}(\zeta) \text{ is satisfied for } \Phi_h\} = \eta_M - 1$. 
Connection to EP collocation method (EPCM)

Based on the quadrature formula \((b_i, c_i)_{i=1}^s\), the EPCM (Hairer, 2010) is

\[
\begin{aligned}
    \mathbf{u}(t_0) &= \mathbf{z}_0, \\
    \dot{\mathbf{u}}(t_0 + c_i h) &= \frac{1}{b_i} \int_0^1 l_i(\tau) \mathbf{f}(\mathbf{u}(t_0 + \tau h)) \, d\tau, \quad i = 1, \ldots, s, \\
    \mathbf{z}_1 &= \mathbf{u}(t_0 + h).
\end{aligned}
\]

which is equivalent to the CSRK method with

\[
A_{\tau, \sigma} = \sum_{i=1}^s \frac{1}{b_i} \int_0^\tau l_i(x) \, dx \, l_i(\sigma), \quad B_\tau = 1, \quad C_\tau = \tau.
\]

Here \(l_i(x)\) can be expanded as a linear combination of \(\{P_\ell(x)\}_{\ell=0}^{s-1}\).

The order \(p\) of EPCM is even, i.e., \(p = 2\eta = 2 \min(s, p - s + 1)\).
Example (A one-parameter family of EP integrators of order $2k$)

$$A_{\tau, \sigma} = \sum_{\iota=0}^{k-1} \int_0^\tau P_\iota(x) \, dx \, P_\iota(\sigma) + \theta \left( \int_0^\tau P_{k+1}(x) \, dx \, P_k(\sigma) + \int_0^\tau P_k(x) \, dx \, P_{k+1}(\sigma) \right),$$

here $\theta$ is an real parameter.
Example for new EP integrators

**Example** (A one-parameter family of EP integrators of order $2k$)

$$A_{\tau, \sigma} = \sum_{l=0}^{k-1} \int_0^\tau P_l(x) \, dx \, P_l(\sigma) + \theta \left( \int_0^\tau P_{k+1}(x) \, dx \, P_k(\sigma) + \int_0^\tau P_k(x) \, dx \, P_{k+1}(\sigma) \right),$$

here $\theta$ is an real parameter.

When $\theta = 0$, the corresponding method is equivalent to

- $k$-degree continuous time finite element method (Hulme 1972, Betsch & Steinmann 2000, Tang & Chen & Liu 2006, Tang & Sun 2012);
- AVF method when $k = 1$ (Quispel & McLaren 2008);
- HBVMs$(\infty, k)$ (Brugnano et al. 2010);
- EP collocation methods of maximal order $2k$ (Hairer 2010).
Symplectic and symmetric integrators

Theorem (Characterizations for symplecticity)

A CSRK method is symplectic if $A_{\tau, \sigma}$ takes the following form

$$A_{\tau, \sigma} = \frac{1}{2} + \sum_{0 \leq i < j \in \mathbb{Z}} \omega_{ij} (P_i(\sigma)P_j(\tau) - P_i(\tau)P_j(\sigma)), \quad \omega_{ij} \in \mathbb{R}.$$ 

Applying the quadrature formula $(b_i, c_i)_{i=1}^s$ to the CSRK with the coefficient above truncated up to a certain term gives an $s$-stage symplectic RK method.

Theorem (Characterizations for symmetry)

A CSRK method is symmetric if $A_{\tau, \sigma}$ takes the following form

$$A_{\tau, \sigma} = \frac{1}{2} + \sum_{0 \leq i, j \in \mathbb{Z}} \omega_{ij} P_i(\tau)P_j(\sigma), \quad \omega_{ij} \in \mathbb{R}.$$ 

Applying the quadrature formula $(b_i, c_i)_{i=1}^s$ with $b_{s+1-i} = b_i$ and $c_{s+1-i} = 1 - c_i$ to the CSRK with the coefficient above truncated up to a certain term gives an $s$-stage symmetric RK method.
A corollary

Corollary (Characterizations for symplecticity and symmetry)

Based on the quadrature formula \((b_i, c_i)_{i=1}^{s}\), we denote \(c = (c_1, \cdots, c_s)^T\), \(\mathbb{B} = \text{diag}(b_1, \cdots, b_s)\), \(W = (P_0(c), P_1(c), \cdots, P_{k-1}(c)) \in \mathbb{R}^{s \times k}\), and define \(A = W \bar{X} W^T \mathbb{B}\) with \(\bar{X} = (\bar{X}_{ij}) \in \mathbb{R}^{k \times k}\). Then, for the \(s\)-stage RK method with coefficient matrix \(A\),

1. it is symplectic if \(\bar{X}_{11} = \frac{1}{2}\) and \(\bar{X}_{ij} = -\bar{X}_{ji}\) when \(i + j \neq 2\);
2. it is symmetric if \(\bar{X}_{11} = \frac{1}{2}\) and \(\bar{X}_{ij} = 0\) when \(i + j(\neq 2)\) is even, in the case that \(b_{s+1-i} = b_i\) and \(c_{s+1-i} = 1 - c_i\), \(i = 1, \cdots, s\).

\[
\begin{array}{c|ccc}
 & \mathbb{B} & \mathbb{B} & \mathbb{B} \\
\hline
c & W \bar{X} W^T & b^T \\
\end{array}
\]

\(c, b \in \mathbb{R}^s, W \in \mathbb{R}^{s \times k}\).

- We have slightly extended the classical results of Chan 1990 and Sun 1993.
- Symplectic \(\alpha\)-RK methods (EQUIP methods, Brugnano et al 2012);
- Low rank symplectic RK for stochastic Hamiltonian systems (Burrage 2012).
Introduction of conjugate-symplectic integrators

Definition

Two numerical methods $\Phi_h$ and $\Psi_h$ are called mutually conjugate, if there exists a global change of coordinates $\chi_h$, such that

$$\Phi_h = \chi_h^{-1} \circ \Psi_h \circ \chi_h.$$ 

Definition

A method $\Phi_h(y)$ of order $p$ is called conjugate-symplectic up to order $p + r$ (with $r \geq 0$), if there exists a change of coordinates $z = \chi_h(y) = y + O(h^p)$, such that $\Psi_h = \chi_h \circ \Phi_h \circ \chi_h^{-1}$ satisfies

$$\Psi'_h(z)^T J \Psi'_h(z) = J + O(h^{p+r+1}).$$

- Conjugate-symplectic integrators share the similar long-time behavior of symplectic integrators;
- The modified equation is $\dot{\tilde{y}} = (\chi'_h(\tilde{y})^T J \chi'_h(\tilde{y}))^{-1} \nabla \tilde{H}(\chi_h(\tilde{y}))$ when the conj. symp. order is up to $\infty$;
- Pseudo-conj.-symp. implies $H(y_n) - H(y_0) = O(h^p) + O(t_nh^{p+r});$
New conjugate-symplectic integrators

We have constructed the following two families of 2-order RK methods with conjugate symplecticity **up to order** $\infty$ by composition approach.

\begin{align*}
\begin{array}{c|ccc}
\gamma - \frac{1}{2} & \gamma - \frac{1}{2} & \frac{1}{2} \\
\gamma + \frac{1}{2} & \gamma & 1 - \gamma \\
\hline
\end{array}
\end{align*}

(\gamma \neq 0, 1)

(1)

\begin{align*}
\begin{array}{c|ccc}
\gamma + \frac{\omega-1}{2} & \gamma + \frac{\omega-1}{2} & \\
\gamma + \frac{\omega+1}{2} & \gamma + \omega & \frac{1-\omega}{2} \\
\hline
\gamma & \omega & 1 - \gamma - \omega \\
\end{array}
\end{align*}

(\omega \neq 0, 1, \gamma \neq 0, \gamma + \omega \neq 1)

(2)

Both of them are irreducible, non-symplectic and diagonally implicit. In tableau (1), when $\gamma = \frac{1}{2}$, we retrieve the trapezoidal rule.
Lemma (Hairer & Zbinden 2012)

Consider a symmetric B-series integrator of order \( p = 2s \) \((s \geq 1)\) that satisfies the simplifying assumptions \( C(s) \) and \( D(s - 1) \).

- It is always conjugate-symplectic up to order \( 2s + 2 \).
- For \( s \geq 1 \), it is conjugate-symplectic up to order \( 2s + 4 \) iff

\[
(s + 2)(s + 1)a(\tau_s, [\tau_1, \tau_{s+1}]) = (s + 1)a(\tau_s, \tau_{s+3}) + (s + 2)a(\tau_s, [\tau_{s+2}]),
\]

\[
(s + 2)(s + 1)a(\tau_{s+1}, [\tau_{s+1}]) = (s + 2)a(\tau_{s+1}, \tau_{s+2}) + s(s + 2)a(\tau_s, [\tau_{s+2}]) - sa(\tau_s, \tau_{s+3}).
\]

Theorem

Consider the energy-preserving CSRK method with

\[
A_{\tau, \sigma} = \sum_{i=0}^{\infty} \omega_i \int_0^\tau P_i(x) \, dx \, P_i(\sigma), \quad 0 < k := \min\{i \in \mathbb{Z} : \omega_i \neq 1\} < \infty,
\]

then the method is of order \( 2k \), symmetric and conjugate-symplectic up to order \( 2k + 2 \), and it is conjugate-symplectic up to order \( 2k + 4 \) iff

\[
\frac{\omega_k}{2k-1} - \frac{\omega_{k+1}}{2k+1} = \frac{2}{4k^2 - 1}.
\]
### Overview on conjugate-symplecticity order

<table>
<thead>
<tr>
<th>Methods</th>
<th>Order</th>
<th>Sympl. or not</th>
<th>Conj. sympl. order</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>Symplectic (RK) methods</em></td>
<td>any order</td>
<td>yes</td>
<td>$\infty$</td>
</tr>
<tr>
<td>Radau IA, $k \geq 1$</td>
<td>$2k - 1$</td>
<td>no</td>
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<td>$2k - 1$</td>
<td>no</td>
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</tr>
<tr>
<td>Lobatto IIIA, $k \geq 3$</td>
<td>$2k - 2$</td>
<td>no</td>
<td>$2k$</td>
</tr>
<tr>
<td>Lobatto IIIB, $k \geq 3$</td>
<td>$2k - 2$</td>
<td>no</td>
<td>$2k - 2$</td>
</tr>
<tr>
<td>Lobatto IIIC, $k \geq 2$</td>
<td>$2k - 2$</td>
<td>no</td>
<td>$2k - 2$</td>
</tr>
<tr>
<td>Trapezoidal rule</td>
<td>$2$</td>
<td>no</td>
<td>$\infty$</td>
</tr>
<tr>
<td>DIRK methods by us</td>
<td>$2$</td>
<td>no</td>
<td>$\infty$</td>
</tr>
<tr>
<td>Symmetric LMMs</td>
<td>even order</td>
<td>no</td>
<td>$\infty$</td>
</tr>
<tr>
<td>AVF method</td>
<td>$2$</td>
<td>no</td>
<td>4</td>
</tr>
<tr>
<td>EP colloc.(C-TFEM)</td>
<td>$2k$</td>
<td>no</td>
<td>$2k + 2$</td>
</tr>
<tr>
<td>EP methods by us</td>
<td>$2k$</td>
<td>no</td>
<td>$2k + 4$</td>
</tr>
</tbody>
</table>

### Remark

Though **SLMMs** are conjugate-symplectic up to order $\infty$ in the sense of step-transition operator (Feng), they are **not recommended** for the long-time integration of Hamiltonian systems. The parasitic solution components have to be got under control (Hairer 2008).
Outlook & Challenge

Theorem (Chartier, Faou & Murua 2006)

A symplectic B-series integrator is formally conjugate to a B-series with exact energy-preservation.

Challenge

Find a computational method that exactly preserves the energy and at the same time it is conjugate-symplectic up to order \( \infty \).
Examples for numerical tests

1. The mathematical pendulum problem

\[
\begin{aligned}
\dot{p} &= -\sin(q), \quad p, q \in \mathbb{R} \\
\dot{q} &= p,
\end{aligned}
\]

with \( H(p, q) = \frac{1}{2}p^2 - \cos(q) \). The initial conditions are \((p_0, q_0) = (0, \frac{\pi}{4})\).

2. The Kepler problem

\[
\begin{aligned}
\dot{p}_1 &= -q_1/(q_1^2 + q_2^2)^{3/2} \\
\dot{p}_2 &= -q_2/(q_1^2 + q_2^2)^{3/2} \\
\dot{q}_1 &= p_1 \\
\dot{q}_2 &= p_2
\end{aligned}
\]

with \( H(p_1, p_2, q_1, q_2) = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}} \) and the initial conditions \( p_1(0) = 0, p_2(0) = 2, q_1(0) = 0.4, q_2(0) = 0 \). The angular momentum \( L(p_1, p_2, q_1, q_2) = q_1p_2 - q_2p_1 \) is a quadratic invariant.
New EP integrators \((k = 1, \theta = 0.5)\) for mathematical pendulum with \(h = 0.6, 500\) steps.

![Log10 of energy error vs. time](image)
EP method ($k = 2, \theta = 0$) for Kepler problem with $h = 0.02$, 10,000 steps.
Conj. sympl. DIRK method in tableau (1) for Kepler problem with $h = 0.02$, 2,000 steps.

![Log10 of energy error over time graph]

- Log10 of energy error
- Time
- Log|$H - H_0$|

Legend:
- conj.-sympl. meth. (gamma=1.5)
- conj.-sympl. meth. (gamma=0.7)
- trapezoidal rule (gamma=0.5)
- conj.-sympl. meth. (gamma=0.1)
- implicit midpoint rule (gamma=0)

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Conj. sympl. DIRK method in tableau (1) for Kepler problem with $h = 0.02$, 2,000 steps.

Log10 of angular momentum error

-2
-4
-6
-8
-10
-12
-14
-16

0 5 10 15 20 25 30 35 40

$\log|L - L_0|$
Concluding remarks

We study the construction of four kinds of geometric numerical integrators based on CSRK. The key tool is the orthogonal polynomial expansion and simplifying assumptions, which allows us to

1. construct new classes of RK type methods and extend the W-transformation;
2. develop new time integration especially for geometric integration (such as EP, symplectic, symmetric and conjugate-symplectic integrators);
3. understand the time integration in a unified way:
   - Time finite element methods including continuous and discontinuous cases;
   - EP methods such as AVF method, HBVMs, EP collocation methods;
   - Symplectic $\alpha$-RK methods (EQUIP methods, Brugnano et al 2012);
   - Low rank symplectic RK for stochastic Hamiltonian systems.
4. easily extend to the partitioned Runge-Kutta case.

Thank you very much for your attention!
References


