Runge-Kutta-Nyström (RKN)-type methods

Wenjun Cai

School of Mathematical Sciences,
Nanjing Normal University

November 29, 2018

We consider the second-order differential equation

$$\begin{cases} y'' = f(y), \\ y(t_0) = y_0, \quad y'(t_0) = y_0', \end{cases}$$

and for simplicity, $y \in \mathbb{R}, f : \mathbb{R} \to \mathbb{R}$. Let $y' = z$ and $u = (y, z)^T$, this system can be transformed into a first-order system

$$u' = Mu + G(u), \quad u(t_0) = u_0,$$

where

$$M = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad G(u) = \begin{pmatrix} 0 \\ f(y) \end{pmatrix}, \quad u_0 = \begin{pmatrix} y_0 \\ y_0' \end{pmatrix}.$$

Variation-of-constants formula

- Solving the linear subsystem $u' = Mu$ gives $u(t) = C\exp(Mt)$.
- Replacing C to $C(t)$ and substituting it back to $u' = Mu + G(u)$ gives

$$C'(t) = \exp(-Mt)G(u(t)).$$

- Integrating both sides from t_0 to t, we have

$$C(t) = C(t_0) + \int_{t_0}^{t} \exp(-M\xi)G(u(\xi))d\xi.$$

- Solution of the original system reads

$$u(t) = \exp(Mt)C(t_0) + \int_{t_0}^{t} \exp(M(t-\xi))G(u(\xi))d\xi.$$

- Using the initial condition gives $C(t_0) = \exp(-Mt)u_0$, and

$$u(t) = \exp(M(t-t_0))u_0 + \int_{t_0}^{t} \exp(M(t-\xi))G(u(\xi))d\xi.$$

RKN

Utilizing the special form of matrix M, we have $\exp(Mt) = I + Mt$, and

$$\begin{aligned} u(t) &= \exp(M(t-t_0))u_0 + \int_{t_0}^{t} \exp(M(t-\xi))G(u(\xi))d\xi \\ &= (I + M(t-t_0))u_0 + \int_{t_0}^{t} (I + M(t-\xi))G(u(\xi))d\xi. \end{aligned}$$

RKN

Utilizing the special form of matrix M, we have $\exp(Mt) = I + Mt$, and

$$\begin{aligned} u(t) &= \exp(M(t-t_0))u_0 + \int_{t_0}^{t} \exp(M(t-\xi))G(u(\xi))d\xi \\ &= (I + M(t-t_0))u_0 + \int_{t_0}^{t} (I + M(t-\xi))G(u(\xi))d\xi. \end{aligned}$$

Let $t = t_0 + ch$ and $\xi = t_0 + \tau h$, we have

$$u(t_0 + ch) = (I + chM)u_0 + h\int_{0}^{c} (I + h(c-\tau)M)G(u(t_0 + \tau h))d\tau,$$

RKN

Utilizing the special form of matrix M, we have $\exp(Mt) = I + Mt$, and

$$
\begin{aligned}
u(t) &= \exp(M(t - t_0))u_0 + \int_{t_0}^{t} \exp(M(t - \xi))G(u(\xi))d\xi \\
&= (I + M(t - t_0))u_0 + \int_{t_0}^{t} (I + M(t - \xi))G(u(\xi))d\xi.
\end{aligned}
$$

Let $t = t_0 + ch$ and $\xi = t_0 + \tau h$, we have

$$
u(t_0 + ch) = (I + chM)u_0 + h\int_0^c (I + h(c - \tau)M)G(u(t_0 + \tau h))d\tau,
$$

which in component-wise is equivalent to

$$
\begin{cases}
y(t_0 + ch) = y_0 + chz_0 + h^2 \displaystyle\int_0^c (c - \tau) f\big(y(t_0 + \tau h)\big)d\tau, \\
z(t_0 + ch) = z_0 + h \displaystyle\int_0^c f\big(y(t_0 + \tau h)\big)d\tau.
\end{cases}
$$

Implementation of RKN

$$\begin{cases} y(t_0+ch) = y_0 + chz_0 + h^2 \int_0^c (c-\tau) f\big(y(t_0+\tau h)\big) d\tau, \\ z(t_0+ch) = z_0 + h \int_0^c f\big(y(t_0+\tau h)\big) d\tau. \end{cases}$$

Approximating the integrals by quadrature formulae

$$\begin{cases} Y_i = y_0 + c_i h z_0 + h^2 \int_0^{c_i} (c_i - \tau) \sum_{j=1}^{s} f(Y_j) l_j(\tau) d\tau \\ \quad = y_0 + c_i h z_0 + h^2 \sum_{j=1}^{s} \bar{a}_{ij} f(Y_j), \quad i = 1, \cdots, s, \end{cases}$$

Implementation of RKN

$$\begin{cases} y(t_0 + ch) = y_0 + chz_0 + h^2 \displaystyle\int_0^c (c - \tau) f\big(y(t_0 + \tau h)\big) d\tau, \\ z(t_0 + ch) = z_0 + h \displaystyle\int_0^c f\big(y(t_0 + \tau h)\big) d\tau. \end{cases}$$

Approximating the integrals by quadrature formulae

$$\begin{cases} Y_i = y_0 + c_i h z_0 + h^2 \displaystyle\int_0^{c_i} (c_i - \tau) \sum_{j=1}^{s} f(Y_j) l_j(\tau) d\tau \\ \quad = y_0 + c_i h z_0 + h^2 \displaystyle\sum_{j=1}^{s} \bar{a}_{ij} f(Y_j), \quad i = 1, \cdots, s, \\ y_1 = y_0 + chz_0 + h^2 \displaystyle\int_0^1 (1 - \tau) \sum_{j=1}^{s} f(Y_j) l_j(\tau) d\tau \\ \quad = y_0 + chz_0 + h^2 \displaystyle\sum_{i=1}^{s} \bar{b}_i f(Y_i), \end{cases}$$

Implementation of RKN

$$\begin{cases} y(t_0+ch) = y_0 + chz_0 + h^2 \int_0^c (c-\tau) f\big(y(t_0+\tau h)\big) d\tau, \\ z(t_0+ch) = z_0 + h \int_0^c f\big(y(t_0+\tau h)\big) d\tau. \end{cases}$$

Approximating the integrals by quadrature formulae

$$\begin{cases} Y_i = y_0 + c_i h z_0 + h^2 \int_0^{c_i} (c_i-\tau) \sum_{j=1}^{s} f(Y_j) l_j(\tau) d\tau \\ \quad = y_0 + c_i h z_0 + h^2 \sum_{j=1}^{s} \bar{a}_{ij} f(Y_j), \quad i = 1, \cdots, s, \\ y_1 = y_0 + chz_0 + h^2 \int_0^1 (1-\tau) \sum_{j=1}^{s} f(Y_j) l_j(\tau) d\tau \\ \quad = y_0 + chz_0 + h^2 \sum_{i=1}^{s} \bar{b}_i f(Y_i), \\ z_1 = z_0 + h \int_0^1 \sum_{j=1}^{s} f(Y_j) l_j(\tau) d\tau \\ \quad = z_0 + h \sum_{i=1}^{s} b_i f(Y_i). \end{cases}$$

ARKN : RKN adapted to perturbed oscillators

Consider the second-order initial value problem

$$\begin{cases} y'' + \omega^2 y = f(y), \quad \omega > 0, \\ y(x_0) = y_0, \quad y'(x_0) = y_0', \end{cases}$$

which can be also rewritten as

$$u' = Mu + G(u), \quad u(t_0) = u_0,$$

with $M = \begin{pmatrix} 0 & 1 \\ -\omega^2 & 0 \end{pmatrix}$ instead. Applying variation-of-constants, we have

$$u(t_0 + h) = \exp(hM)u_0 + h\int_0^1 \exp(h(1-\xi)M)G(u(t_0 + \tau h))d\tau.$$

$$u(t_0+h) = \exp(hM)u_0 + h\int_0^1 \exp(h(1-\xi)M)G(u(t_0+\tau h))d\tau.$$

Utilizing the special form of matrix M, we have

$$\exp(Mh) = \begin{pmatrix} \cos\omega h & \frac{\sin\omega h}{\omega} \\ -\omega\sin\omega h & \cos\omega h \end{pmatrix},$$

which can be used to simplify the solution as

$$\begin{cases} y(t_0+h) = \phi_0(\nu)y_0 + h\phi_1(\nu)z_0 + h^2\int_0^1 (1-\tau)\phi_1\big((1-\tau)\nu\big)f\big(y(t_0+\tau h)\big)d\tau, \\ z(t_0+h) = -h\omega^2\phi_1(\nu)y_0 + \phi_0(\nu)z_0 + h\int_0^1 \phi_0\big((1-\tau)\nu\big)f\big(y(t_0+\tau h)\big)d\tau, \end{cases}$$

where

$$\phi_0(\nu) = \cos\nu, \quad \phi_1(\nu) = \frac{\sin\nu}{\nu}, \quad \nu = h\omega.$$

Implementation of ARKN

$$
\begin{cases}
y(t_0+h) = \phi_0(\nu)y_0 + h\phi_1(\nu)z_0 + h^2\displaystyle\int_0^1 (1-\tau)\phi_1\big((1-\tau)\nu\big)f\big(y(t_0+\tau h)\big)d\tau, \\
z(t_0+h) = -h\omega^2\phi_1(\nu)y_0 + \phi_0(\nu)z_0 + h\displaystyle\int_0^1 \phi_0\big((1-\tau)\nu\big)f\big(y(t_0+\tau h)\big)d\tau,
\end{cases}
$$

Approximating the integrals by quadrature formulae

$$
\begin{cases}
Y_i = y_0 + c_i h z_0 + h^2 \displaystyle\sum_{j=1}^{s} \bar{a}_{ij}\Big(f(Y_j) - \omega Y_j\Big), \quad i = 1, \cdots, s,
\end{cases}
$$

Implementation of ARKN

$$
\begin{cases}
y(t_0+h) = \phi_0(\nu)y_0 + h\phi_1(\nu)z_0 + h^2\displaystyle\int_0^1 (1-\tau)\phi_1\big((1-\tau)\nu\big)f\big(y(t_0+\tau h)\big)d\tau, \\
z(t_0+h) = -h\omega^2\phi_1(\nu)y_0 + \phi_0(\nu)z_0 + h\displaystyle\int_0^1 \phi_0\big((1-\tau)\nu\big)f\big(y(t_0+\tau h)\big)d\tau,
\end{cases}
$$

Approximating the integrals by quadrature formulae

$$
\begin{cases}
Y_i = y_0 + c_i h z_0 + h^2\displaystyle\sum_{j=1}^{s}\bar{a}_{ij}\Big(f(Y_j) - \omega Y_j\Big), \quad i = 1, \cdots, s, \\
y_1 = \phi_0(\nu)y_0 + h\phi_1(\nu)z_0 + h^2\displaystyle\int_0^1 (1-\tau)\phi_1\big((1-\tau)\nu\big)\sum_{j=1}^{s} f(Y_j)l_j(\tau)d\tau, \\
\quad = \phi_0(\nu)y_0 + h\phi_1(\nu)z_0 + h^2\displaystyle\sum_{j=1}^{s}\bar{b}_i(\nu)f(Y_j)
\end{cases}
$$

Implementation of ARKN

$$\begin{cases} y(t_0+h) = \phi_0(\nu)y_0 + h\phi_1(\nu)z_0 + h^2\displaystyle\int_0^1 (1-\tau)\phi_1\big((1-\tau)\nu\big)f\big(y(t_0+\tau h)\big)d\tau, \\ z(t_0+h) = -h\omega^2\phi_1(\nu)y_0 + \phi_0(\nu)z_0 + h\displaystyle\int_0^1 \phi_0\big((1-\tau)\nu\big)f\big(y(t_0+\tau h)\big)d\tau, \end{cases}$$

Approximating the integrals by quadrature formulae

$$\begin{cases} Y_i = y_0 + c_i h z_0 + h^2 \displaystyle\sum_{j=1}^{s} \bar{a}_{ij}\Big(f(Y_j) - \omega Y_j\Big), \quad i = 1, \cdots, s, \\ y_1 = \phi_0(\nu)y_0 + h\phi_1(\nu)z_0 + h^2\displaystyle\int_0^1 (1-\tau)\phi_1\big((1-\tau)\nu\big)\sum_{j=1}^{s} f(Y_j)l_j(\tau)d\tau, \\ \quad = \phi_0(\nu)y_0 + h\phi_1(\nu)z_0 + h^2\displaystyle\sum_{j=1}^{s}\bar{b}_i(\nu)f(Y_j) \\ z_1 = -h\omega^2\phi_1(\nu)y_0 + \phi_0(\nu)z_0 + h\displaystyle\int_0^1 \phi_0\big((1-\tau)\nu\big)\sum_{j=1}^{s} f(Y_j)l_j(\tau)d\tau, \\ \quad = -h\omega^2\phi_1(\nu)y_0 + \phi_0(\nu)z_0 + h\displaystyle\sum_{j=1}^{s} b_i(\nu)f(Y_j). \end{cases}$$

(Multidimensional) ERKN

$$\begin{cases} y(t_0+h) = \phi_0(\nu)y_0 + h\phi_1(\nu)z_0 + h^2\displaystyle\int_0^1 (1-\tau)\phi_1\big((1-\tau)\nu\big)f\big(y(t_0+\tau h)\big)d\tau, \\ z(t_0+h) = -h\omega^2\phi_1(\nu)y_0 + \phi_0(\nu)z_0 + h\displaystyle\int_0^1 \phi_0\big((1-\tau)\nu\big)f\big(y(t_0+\tau h)\big)d\tau, \end{cases}$$

Approximating the integrals by quadrature formulae

$$\begin{cases} Y_i = \phi_0(c_i\nu)y_0 + c_ih\phi_1(c_i\nu)z_0 + h^2\displaystyle\int_0^{c_i} (c_i-\tau)\phi_1\big((c_i-\tau)\nu\big)f\big(y(t_0+\tau h)\big)d\tau, \\ \quad = \phi_0(c_i\nu)y_0 + c_ih\phi_1(c_i\nu)z_0 + h^2\tilde{a}_{ij}f(Y_j), \quad i=1,\cdots,s, \\ y_1 = \phi_0(\nu)y_0 + h\phi_1(\nu)z_0 + h^2\displaystyle\sum_{j=1}^{s}\bar{b}_i(\nu)f(Y_j) \\ z_1 = -h\omega^2\phi_1(\nu)y_0 + \phi_0(\nu)z_0 + h\displaystyle\sum_{j=1}^{s}b_i(\nu)f(Y_j). \end{cases}$$

AAVF : AVF adapted to perturbed oscillators

$$\begin{cases} q(t_0+h) = \phi_0(\nu)q_0 + h\phi_1(\nu)p_0 - h^2 \displaystyle\int_0^1 (1-\tau)\phi_1\big((1-\tau)\nu\big)\nabla U\big(q(t_0+\tau h)\big)d\tau, \\ p(t_0+h) = -h\omega^2\phi_1(\nu)q_0 + \phi_0(\nu)p_0 - h\displaystyle\int_0^1 \phi_0\big((1-\tau)\nu\big)\nabla U\big(q(t_0+\tau h)\big)d\tau, \end{cases}$$

Let

$$\phi_2(\nu) = \int_0^1 (1-\tau)\phi_1\big((1-\tau)\nu\big)d\tau = \nu^{-2}(1-\cos\nu),$$

and notice that

$$\phi_1 = \int_0^1 \phi_0\big((1-\tau)\nu\big)d\tau,$$

we obtain the so-called AAVF method

$$\begin{cases} q_1 = \phi_0(\nu)q_0 + h\phi_1(\nu)p_0 - h^2\phi_2(\nu)\displaystyle\int_0^1 \nabla U\big((1-\tau)q_0+\tau q_1\big)d\tau, \\ p_1 = -h\omega^2\phi_1(\nu)q_0 + \phi_0(\nu)p_0 - h\phi_1(\nu)\displaystyle\int_0^1 \nabla U\big((1-\tau)q_0+\tau q_1\big)d\tau. \end{cases}$$

Let $V=\int_0^1 \nabla U\big((1-\tau)q_0+\tau q_1\big)d\tau$ and omit the variable ν in ϕ_0, ϕ_1 and ϕ_2 for short, we have

$$\begin{cases} q_1 = \phi_0 q_0 + h\phi_1 p_0 + h^2\phi_2 V, \\ p_1 = -h\omega^2\phi_1 q_0 + \phi_0 p_0 + h\phi_1 V. \end{cases}$$

$$\begin{aligned} p_1p_1+\omega^2q_1q_1 &= p_0p_0+\omega^2q_0q_0+V^2\frac{2-2\cos(h\omega)}{\omega^2}+(2\cos(h\omega)-2)q_0V+\frac{2\sin(h\omega)}{\omega}p_0V \\ &= p_0p_0+\omega^2q_0q_0+2V\Big(V\frac{1-\cos(h\omega)}{\omega^2}+(\cos(h\omega)-1)q_0+\frac{\sin(h\omega)}{\omega}p_0\Big) \\ &= p_0p_0+\omega^2q_0q_0+2V\Big(\phi_0q_0+h\phi_1p_0+h^2\phi_2V-q_0\Big) \\ &= p_0p_0+\omega^2q_0q_0+2V\Big(q_1-q_0\Big) \\ &= p_0p_0+\omega^2q_0q_0+2\Big(-\nabla U(q_1)+\nabla U(q_0)\Big) \end{aligned}$$

Therefore, we obtain the discrete energy conservation law

$$H_1 = H_0, \quad \text{with} \quad H_0=\frac{1}{2}p_0p_0+\frac{1}{2}\omega^2q_0q_0+U(q_0).$$

$$
\begin{aligned}
q' &= p, \\
p' &= -Mq - \nabla U(q)
\end{aligned}
$$

$$
\begin{aligned}
q_{n+2} - q_n &= 2hp_{n+1}, \\
p_{n+1} - p_n &= -h\Big(Mq_{n+1/2} + \int_0^1 \nabla U(\xi q_{n+1} + (1-\xi)q_n)d\xi\Big)
\end{aligned}
$$

$$
\begin{aligned}
q_{n+2} &= q_n + 2hp_n - 2h^2\Big(Mq_{n+1/2} + \int_0^1 \nabla U(\xi q_{n+1} + (1-\xi)q_n)d\xi\Big), \\
p_{n+1} &= p_n - h\Big(Mq_{n+1/2} + \int_0^1 \nabla U(\xi q_{n+1} + (1-\xi)q_n)d\xi\Big)
\end{aligned}
$$

$$u(t_0+2h)=\exp(2hM)u_0+\int_{t_0}^{t_0+2h}\exp(M(t_0+2h-\xi))G(u(\xi))d\xi$$

$$u(t_0+2h)=\exp(2hM)u_0+\int_0^1\exp(2h(1-\tau)M)G(u(t_0+2\tau h))d\tau$$

$\nu=h\omega$, $\xi=t_0+2\tau h$

$$\begin{cases} q_{n+2}=\phi_0(2\nu)q_n+2h\phi_1(2\nu)p_n+2h^2\int_0^1(1-\tau)\phi_1\big((1-\tau)2\nu\big)f\big(q(t_n+\tau h)\big)d\tau,\\ p_{n+1}=-h\omega^2\phi_1(\nu)q_n+\phi_0(\nu)p_n+h\int_0^1\phi_0\big((1-\tau)\nu\big)f\big(q(t_n+\tau h)\big)d\tau, \end{cases}$$

$$\begin{cases} q_{n+2}=\phi_0(2\nu)q_n+2h\phi_1(2\nu)p_n+2h^2R,\\ p_{n+1}=-h\omega^2\phi_1(\nu)q_n+\phi_0(\nu)p_n+hS, \end{cases}$$

$$H_{n+1}=H_n,\quad \text{with}\quad H_n=\frac{1}{2}\frac{q_{n+1}-q_n}{h}\frac{q_n-q_{n-1}}{h}+\frac{1}{2}q_nq_n+U(q_n)$$

$$\frac{1}{2}\frac{q_{n+2}-q_{n+1}}{h}\frac{q_{n+1}-q_n}{h}$$