Extended RKN methods solving general second-order oscillatory systems

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1. **From RKN to ERKN**
   - The problem and numerical strategies
   - RKN, ARKN and ERKN

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4. **Practical ERKN methods and numerical illustrations**
   - Practical ERKN methods
   - Numerical experiments
Consider an IVP of the general system of second-order ODEs

\[
\begin{align*}
\begin{cases}
y''(x) + My(x) &= f(y(x), y'(x)), \quad x \in [x_0, x_{\text{end}}], \\
y(x_0) &= y_0, \quad y'(x_0) = y'_0,
\end{cases}
\end{align*}
\]

where \( y \in \mathbb{R}^d, f: \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d \), the \( d \times d \) positive semi-definite coefficient matrix \( M \) contains implicitly the frequencies of the problem and the function \( f(y, y') \) may depend on the position \( y(x) \) and the velocity \( y'(x) \) as well.
Consider an IVP of the general system of second-order ODEs

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\begin{cases}
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y(x_0) = y_0, & y'(x_0) = y'_0,
\end{cases}
\]  

(1)

where \( y \in \mathbb{R}^d, f : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d, \) the \( d \times d \) positive semi-definite coefficient matrix \( M \) contains implicitly the frequencies of the problem and the function \( f(y, y') \) may depend on the position \( y(x) \) and the velocity \( y'(x) \) as well.

**Applied fields:** classical and quantum mechanics, astronomy, chemistry, biology and engineering.
Second-order system

Traditional numerical treatment of the system (1):

* Runge-Kutta (RK) methods
* Runge-Kutta-Nyström (RKN) methods
* Linear multistep methods (LMMs)
* Two-step hybrid methods
Oscillatory system

Methods adapted to oscillatory feature of the solution of (1):
Oscillatory system

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Gaustchi-type methods (Gaustchi, 1961)
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Methods adapted to **oscillatory** feature of the solution of (1):

- **Gaustchi-type methods** (Gaustchi, 1961)
- **Bettis’ approach** (Gaustchi, 1971, 1979)
- **Trigonometrically/exponentially fitted methods**: Berghe et al. 1999, 2000, etc.
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- Wu, Wang, Xia, BIT 2012 [17]: Explicit symplectic multidimensional EF modified RKN.
- **ARKN methods**: Franco, 2002, 2006
The problem and numerical strategies

Oscillatory system

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**ARKN methods:** Franco, 2002, 2006
**Order conditions for ARKN:** Wu, You, Li. 2009
**Multidimensional ARKN:** Wu, You, Xia 2009, Wu, Wang 2010
**ERKN methods:** Yang, Wu et al. 2009
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ERKN methods: Yang, Wu et al. 2009
Multidimensional ERKN: Wu et al. 2010, 2011
RKN for $y'' + \omega^2 y = f(y, y'), \omega > 0$ (Nyström, 1925)

$$
\begin{align*}
Y_i &= y_n + c_ihy_n' + h^2 \sum_{j=1}^{s} \bar{a}_{ij}(f(Y_j, Y_j') - \omega^2 Y_j), \quad i = 1, \ldots, s, \\
    \quad i = 1, \ldots, s, \\
y_{n+1} &= y_n + hy_n' + h^2 \sum_{i=1}^{s} \bar{b}_i(f(t_n + c_i h, y_i) - \omega^2 y_i), \\
y_{n+1}' &= y_n' + h \sum_{i=1}^{s} b_i(f(t_n + c_i h, y_i) - \omega^2 y_i), \quad n = 0, 1, \ldots, N - 1, \\
\end{align*}
$$

(2)
RKN for $y'' + \omega^2 y = f(y, y')$, $\omega > 0$ (Nyström, 1925)

\[
\begin{align*}
Y_i &= y_n + c_i h y'_n + h^2 \sum_{j=1}^{s} \bar{a}_{ij}(f(Y_j, Y'_j) - \omega^2 Y_j), \quad i = 1, \ldots, s, \\
\quad i = 1, \ldots, s, \\
y_{n+1} &= y_n + h y'_n + h^2 \sum_{i=1}^{s} \bar{b}_i(f(t_n + c_i h, y_i) - \omega^2 y_i), \\
y'_{n+1} &= y'_n + h \sum_{i=1}^{s} b_i(f(t_n + c_i h, y_i) - \omega^2 y_i), \quad n = 0, 1, \ldots, N - 1,
\end{align*}
\]

(2)

where $h$: the step size,
$N$: the number of computation steps
$\bar{a}_{ij}, \bar{b}_i, b_i, i, j = 1, \ldots, s$ are constants.
ARKN for $y'' + \omega^2 y = f(y, y'), \omega > 0$ (Franco, 2002, Comput. Phy. Commu.)

$$
Y_i = y_n + c_i h y'_n + h^2 \sum_{j=1}^{s} \bar{a}_{ij} (f(Y_j, Y'_j) - \omega^2 Y_j), \quad i = 1, \ldots, s,
$$

$$
Y'_i = y'_n + h \sum_{j=1}^{s} a_{ij} (f(Y_j, Y'_j) - \omega^2 Y_j), \quad i = 1, \ldots, s,
$$

$$
y_{n+1} = \phi_0(\nu)y_n + \phi_1(\nu)h y'_n + h^2 \sum_{i=1}^{s} \bar{b}_i(\nu)f(Y_i, Y'_i),
$$

$$
y'_{n+1} = -\omega \nu \phi_1(\nu)y_n + \phi_0(\nu)y'_n + h \sum_{i=1}^{s} b_i(\nu)f(Y_i, Y'_i)
$$

where $\nu = h \omega$, $\phi_0(\nu) = \cos(\nu)$ and $\phi_1(\nu) = \sin(\nu)/\nu$. (Bettis’ functions)
From RKN to ERKN  Formulation of ERKN  The extended Nyström tree theory  Practical ERKN methods and numerical illustrations

RKN, ARKN and ERKN

**ARKN for** \(y'' + \omega^2 y = f(y, y'), \omega > 0\) (Franco, 2002, Comput. Phy. Phy. Commu.)

\[
Y_i = y_n + c_i h y_n' + h^2 \sum_{j=1}^{s} \bar{a}_{ij} (f(Y_j, Y_j') - \omega^2 Y_j), \quad i = 1, \ldots, s,
\]
\[
Y_i' = y_n' + h \sum_{j=1}^{s} a_{ij} (f(Y_j, Y_j') - \omega^2 Y_j), \quad i = 1, \ldots, s,
\]
\[
y_{n+1} = \phi_0(\nu)y_n + \phi_1(\nu)hy_n' + h^2 \sum_{i=1}^{s} \bar{b}_i(\nu)f(Y_i, Y_i'),
\]
\[
y_{n+1}' = -\omega \nu \phi_1(\nu)y_n + \phi_0(\nu)y_n' + h \sum_{i=1}^{s} b_i(\nu)f(Y_i, Y_i')
\]

where \(\nu = h\omega\), \(\phi_0(\nu) = \cos(\nu)\) and \(\phi_1(\nu) = \sin(\nu)/\nu\). (Bettis’ functions)

**Important property**: the update is exact for \(\ddot{y} + \omega^2 y = 0\).
ERKN for $y'' + \omega^2 y = f(y)$, $\omega^2$ symmetric and positive semi-definite (Yang, Wu, You, Fang, 2009, Comput. Phy. Commu.)

\begin{align*}
Y_i &= \phi_0(c_i \nu)y_n + c_i \phi_1(c_i \nu)hy_n' + h^2 \sum_{j=1}^{s} \bar{a}_{ij}(\nu)f(Y_j), \quad i = 1, \cdots, s, \\
y_{n+1} &= \phi_0(\nu)y_n + \phi_1(\nu)hy_n' + h^2 \sum_{i=1}^{s} \bar{b}_i(\nu)f(Y_i), \\
hy_{n+1}' &= -\nu^2 \phi_1(\nu)y_n + \phi_0(\nu)hy_n' + h^2 \sum_{i=1}^{s} b_i(\nu)f(Y_i),
\end{align*}

(3)

where $\bar{a}_{ij}(\nu)$, $b_i(\nu)$ and $\bar{b}_i(\nu)$, $i, j = 1, \cdots, s$, are assumed to be even functions of $\nu$. 
ERKN for $y'' + \omega^2 y = f(y)$, $\omega^2$ symmetric and positive semi-definite (Yang, Wu, You, Fang, 2009, Comput. Phy. Commu.)

\begin{align*}
Y_i &= \phi_0(c_i\nu)y_n + c_i\phi_1(c_i\nu)h y_n' + h^2 \sum_{j=1}^{s} \bar{a}_{ij}(\nu)f(Y_j), \quad i = 1, \cdots, s, \\
y_{n+1} &= \phi_0(\nu)y_n + \phi_1(\nu)h y_n' + h^2 \sum_{i=1}^{s} \bar{b}_i(\nu)f(Y_i), \\
h y_{n+1}' &= -\nu^2 \phi_1(\nu)y_n + \phi_0(\nu)h y_n' + h^2 \sum_{i=1}^{s} b_i(\nu)f(Y_i),
\end{align*}

where $\bar{a}_{ij}(\nu)$, $b_i(\nu)$ and $\bar{b}_i(\nu)$, $i, j = 1, \cdots, s$, are assumed to be even functions of $\nu$.

**Characteristic property**: both the internal stages and the update are exact for $\ddot{y} + \omega^2 y = 0$. 
Theorem 1.1

An s-stage ERKN method for the system $y'' + \omega^2 y = f(y)$ has order $p$ if and only if

\[
\begin{cases}
    \bar{b}^T(\nu)\Phi(t) - \frac{\rho(t)!}{\gamma(t)}\phi_{\rho(t)+1}(\nu) = \mathcal{O}(h^{p-\rho(t)}), & \rho(t) = 1, 2, \ldots, p - 1, \\
    b^T(\nu)\Phi(t) - \frac{\rho(t)!}{\gamma(t)}\phi_{\rho(t)}(\nu) = \mathcal{O}(h^{p+1-\rho(t)}), & \rho(t) = 1, 2, \ldots, p,
\end{cases}
\]

where $t$ is the special extended Nyström tree (SEN-tree) of order $\rho(t)$ corresponding to an elementary differential $\mathcal{F}(y, y')$ of the function $f(y)$ at $(y_n, y'_n)$, the functions $\gamma(t)$ (signed density) and $\Phi(t)$ are defined in Yang et al. 2009 [11].
Our purposes:

- ERKN methods for the general Problem (1)

\[
\begin{align*}
    y''(x) + My(x) &= f(y(x), y'(x)), \quad x \in [x_0, x_{\text{end}}], \\
    y(x_0) &= y_0, \quad y'(x_0) = y'_0.
\end{align*}
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Our purposes:

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y''(x) + My(x) = f(y(x), y'(x)), & x \in [x_0, x_{\text{end}}], \\
y(x_0) = y_0, & y'(x_0) = y'_0. 
\end{cases}
\] (5)

frequency matrix $M$: positive semi-definite, not necessarily symmetric.
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y''(x) + My(x) = f(y(x), y'(x)), & x \in [x_0, x_{\text{end}}], \\
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frequency matrix $M$: positive semi-definite, not necessarily symmetric.

- Order conditions
Our purposes:

- ERKN methods for the general Problem (1)

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- Frequency matrix $M$: positive semi-definite, not necessarily symmetric.

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- EN tree theory:
Our purposes:

- ERKN methods for the general Problem (1)

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    y(x_0) &= y_0, & y'(x_0) &= y'_0.
\end{aligned}
\]

- frequency matrix $M$: positive semi-definite, not necessarily symmetric.
- Order conditions
- EN tree theory:

\[
y^{(3)} = (-M)y' + f_y'(-My) + f_y y' + f_y'f,
\]

- Practical ERKN methods
Our purposes:

- ERKN methods for the general Problem (1)

\[
\begin{align*}
  y''(x) + My(x) &= f(y(x), y'(x)), \quad x \in [x_0, x_{\text{end}}], \\
  y(x_0) &= y_0, \quad y'(x_0) = y'_0.
\end{align*}
\]

- Order conditions

- EN tree theory:

  \[
  y^{(3)} = (-M)y' + f_y'(-My) + f_y y' + f_y f,
  \]

- Practical ERKN methods and numerical experiments.
The matrix form of variation-of-constants formula of X. Wu et al. 2010 [12]:

\[
\begin{align*}
\text{y}(x + \lambda h) &= \phi_0(\lambda^2 V) y(x) + h \lambda \phi_1(\lambda^2 V) y'(x) + h \int_{\lambda}^{0} \phi_0((\lambda - \tau)^2 V) f(y(x + h \tau), y'(x + h \tau)) d\tau, \\
\text{y}'(x + \lambda h) &= \phi_0(\lambda^2 V) y'(x) - h \lambda M \phi_1(\lambda^2 V) y(x) + h \int_{\lambda}^{0} \phi_0((\lambda - \tau)^2 V) f(y(x + h \tau), y'(x + h \tau)) d\tau,
\end{align*}
\]

where \( V = h^2 M \), \( \phi_0(V) = \sum_{k=0}^{\infty} (-1)^k V^k (2^k k!) \) and \( \phi_1(V) = \sum_{k=0}^{\infty} (-1)^k V^k (2^k k+1)! \).
The matrix form of variation-of-constants formula of X. Wu et al. 2010 [12]: for arbitrary number $\lambda$, $h \in \mathbb{R}$, the solutions of the IVPs (1) satisfy

\begin{align*}
y(x + \lambda h) &= \phi_0(\lambda^2 V) y(x) + h\lambda \phi_1(\lambda^2 V) y'(x) \\
&\quad + h^2 \int_0^{\lambda} (\lambda - \tau) \phi_1((\lambda - \tau)^2 V) f(y(x + h\tau), y'(x + h\tau)) \, d\tau
\end{align*}

\begin{align*}
y'(x + \lambda h) &= \phi_0(\lambda^2 V) y'(x) - h\lambda M \phi_1(\lambda^2 V) y(x) \\
&\quad + h \int_0^{\lambda} \phi_0((\lambda - \tau)^2 V) f(y(x + h\tau), y'(x + h\tau)) \, d\tau,
\end{align*}

(6)
The matrix form of variation-of-constants formula of X. Wu et al. 2010 [12]: for arbitrary number $\lambda$, $h \in \mathbb{R}$, the solutions of the IVPs (1) satisfy

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y(x + \lambda h) &= \phi_0(\lambda^2 V)y(x) + h\lambda \phi_1(\lambda^2 V)y'(x) \\
&\quad + h^2 \int_{0}^{\lambda} (\lambda - \tau) \phi_1((\lambda - \tau)^2 V) f(y(x + h\tau), y'(x + h\tau)) \, d\tau \\
y'(x + \lambda h) &= \phi_0(\lambda^2 V)y'(x) - h\lambda M \phi_1(\lambda^2 V)y(x) \\
&\quad + h \int_{0}^{\lambda} \phi_0((\lambda - \tau)^2 V) f(y(x + h\tau), y'(x + h\tau)) \, d\tau,
\end{align*}

where $V = h^2 M$, $\phi_0(V) := \sum_{k=0}^{\infty} \frac{(-1)^k V^k}{(2k)!}$ and

$\phi_1(V) := \sum_{k=0}^{\infty} \frac{(-1)^k V^k}{(2k + 1)!}.$
ERKN for $y'' + M y = f(y, y')$

$$
\begin{align*}
Y_i &= \phi_0(c_i^2 V)y_n + c_i \phi_1(c_i^2 V)h y'_n + h^2 \sum_{j=1}^{s} \bar{a}_{ij}(V)f(Y_j, Y'_j), \quad i = 1, \ldots, s, \\
Y'_i &= -c_i hM \phi_1(c_i^2 V)y_n + \phi_0(c_i^2 V)y'_n + h \sum_{j=1}^{s} a_{ij}(V)f(Y_j, Y'_j), \quad i = 1, \ldots, s, \\
y_{n+1} &= \phi_0(V)y_n + \phi_1(V)h y'_n + h^2 \sum_{i=1}^{s} \bar{b}_i(V)f(Y_i, Y'_i), \\
y'_{n+1} &= -hM \phi_1(V)y_n + \phi_0(V)y'_n + h \sum_{i=1}^{s} b_i(V)f(Y_i, Y'_i),
\end{align*}
$$

(7)

where $\bar{a}_{ij}(V), a_{ij}(V), \bar{b}_i(V), b_i(V), i, j = 1, \ldots, s$ are matrix-valued functions which can be expanded into series in powers of $V = h^2 M$ with real coefficients.
### Butcher’s tableau

\[
\begin{array}{c|cc|cc}
  c & A(V) & \bar{A}(V) \\
  \hline
  b^T(V) & \bar{b}^T(V) \\
\end{array}
\]

\[
\begin{array}{cccc}
  c_1 & a_{11}(V) & \cdots & a_{1s}(V) & \bar{a}_{11}(V) & \cdots & \bar{a}_{1s}(V) \\
  \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
  c_s & a_{s1}(V) & \cdots & a_{ss}(V) & \bar{a}_{s1}(V) & \cdots & \bar{a}_{ss}(V) \\
  \hline
  b_1(V) & \cdots & b_s(V) & \bar{b}_1(V) & \cdots & \bar{b}_s(V) \\
\end{array}
\]
non-autonomous system \( y'' + M y = f(y, y') \)

\[
\begin{align*}
Y_i &= \phi_0(c_i^2 V) y_n + c_i \phi_1(c_i^2 V) h y'_n + h^2 \sum_{j=1}^{s} \bar{a}_{ij}(V) f(x_n + c_j h, Y_j, Y'_j), \\
Y'_i &= -c_i hM \phi_1(c_i^2 V) y_n + \phi_0(c_i^2 V) y'_n + h \sum_{j=1}^{s} a_{ij}(V) f(x_n + c_j h, Y_j, Y'_j) \\
y_{n+1} &= \phi_0(V) y_n + \phi_1(V) h y'_n + h^2 \sum_{i=1}^{s} \bar{b}_{i}(V) f(x_n + c_i h, Y_i, Y'_i), \\
y'_{n+1} &= -hM \phi_1(V) y_n + \phi_0(V) y'_n + h \sum_{i=1}^{s} b_{i}(V) f(x_n + c_i h, Y_i, Y'_i). \\
\end{align*}
\] (8)
An $s$-stage ERKN method (7) has order $p$, if for any smooth problem (1), the local truncation errors of the method satisfy

\[
e_{n+1} := y(x_n + h) - y_{n+1} = \mathcal{O}(h^{p+1}) \quad \text{and} \\
e_{n+1}' := y'(x_n + h) - y_{n+1}' = \mathcal{O}(h^{p+1}),
\]
An $s$-stage ERKN method (7) has order $p$, if for any smooth problem (1), the local truncation errors of the method satisfy

$$e_{n+1} := y(x_n + h) - y_{n+1} = O(h^{p+1}) \quad \text{and}$$

$$e'_{n+1} := y'(x_n + h) - y'_{n+1} = O(h^{p+1}),$$
An $s$-stage ERKN method (7) has order $p$, if for any smooth problem (1), the local truncation errors of the method satisfy

\[ e_{n+1} := y(x_n + h) - y_{n+1} = \mathcal{O}(h^{p+1}) \quad \text{and} \]

\[ e'_{n+1} := y'(x_n + h) - y'_{n+1} = \mathcal{O}(h^{p+1}), \]

Motivated by Butcher and Hairer’s idea in [13, 14] and based on the forms of the elementary differentials appeared in the expressions of the higher derivatives of $f(y(x), y'(x))$. 
Denote $M = (m_{KL})$. We can calculate the derivatives of $f^J(y(x), y'(x))$ using the relation $(y'^K)' = \sum_L (-m_{KL}y^L) + f^K$: 
Denote $M = (m_{KL})$. We can calculate the derivatives of $f^J(y(x), y'(x))$ using the relation $(y'^K)' = \sum_{L} (\!m_{KL}y^L) + f^K$:

\[
(f^J)^{(0)} = f^J. \tag{9}
\]

\[
(f^J)^{(1)} = \sum_{K} \frac{\partial f^J}{\partial y^K} y'^K + \sum_{K,L} \frac{\partial f^J}{\partial y'^K} (\!m_{KL}y^L) + \sum_{K} \frac{\partial f^J}{\partial y'^K} f^K, \tag{10}
\]
The extended Nyström tree theory

The EN-Trees and related functions

\[
(f^J)^{(2)} = \sum_{K,L} \frac{\partial^2 f^J}{\partial y^K \partial y^L} y'^K y'^L + \sum_{K,L,N} \frac{\partial^2 f^J}{\partial y^K \partial y'^L} y'^K \left( -m_{LN} y^N \right) \\
+ \sum_{K,L} \frac{\partial^2 f^J}{\partial y^K \partial y'^L} y'^K f^L + \sum_{K,L,N} \frac{\partial f^J}{\partial y^K} \frac{\partial y'^K}{\partial y'^L} \left( -m_{LN} y^N \right) + \sum_{K,L} \frac{\partial f^J}{\partial y^K} \frac{\partial y'^K}{\partial y'^L} f^L \\
+ \sum_{K,L,N} \frac{\partial^2 f^J}{\partial y'^K \partial y^L} \left( -m_{KN} y^N \right) y'^L + \sum_{K,L,N} \frac{\partial^2 f^J}{\partial y'^K \partial y^L} f^K y'^L \\
+ \sum_{K,L,N,R} \frac{\partial^2 f^J}{\partial y'^K \partial y'^L} \left( -m_{KN} y^N \right) \left( -m_{LR} y^R \right) \\
+ \sum_{K,L,N} \frac{\partial^2 f^J}{\partial y'^K \partial y'^L} \left( -m_{KN} y^N \right) f^L + \sum_{K,L} \frac{\partial f^J}{\partial y'^K} \left( -m_{KL} \right) y'^L \\
+ \sum_{K,L,N} \frac{\partial^2 f^J}{\partial y'^K \partial y'^L} f^K \left( -m_{LN} y^N \right) + \sum_{K,L} \frac{\partial^2 f^J}{\partial y'^K \partial y'^L} f^K f^L \\
+ \sum_{K,L} \frac{\partial f^J}{\partial y'^K} \cdot \frac{\partial f^K}{\partial y^L} y'^L + \sum_{K,L,N} \frac{\partial f^J}{\partial y'^K} \cdot \frac{\partial f^K}{\partial y'^L} \left( -m_{LN} y^N \right) \\
+ \sum_{K,L} \frac{\partial f^J}{\partial y'^K} \cdot \frac{\partial f^K}{\partial y'^L} f^L.
\]
The EN-Trees and related functions

\[ f^{(1)} = f_y y' + f_{yy} (-My) + f_y f. \]

\[ f^{(2)} = f_{yy} (y', y') + 2f_{yy'} (y', -My) + 2f_{yy'} (y', f) + f_y (-My) + f_y f \]
\[ + f_{yy'} (-My, -My) + 2f_{yy'} (-My, f) + f_y' (-M)y' + f_y' (f, f) \]
\[ + f_y f_y y' + f_y f_y (-My) + f_y f_y y' + f_y f_y f. \]

(12)
\[ f^{(1)} = f_y y' + f_{y'} (-My) + f_y f. \]
\[ f^{(2)} = f_{yy} (y', y') + 2f_{yy'} (y', -My) + 2f_{yy'} (y', f) + f_y (-My) + f_y f \]
\[ + f_{y'y'} (-My, -My) + 2f_{y'y'} (-My, f) + f_y' (-M)y' + f_{y'y'} (f, f) \]
\[ + f_y f_y y' + f_y f_{y'} (-My) + f_{y'} f_y y' + f_{y'} f_{y'} f. \]

\[(12)\]

The continuation of the above process, although theoretically clear, soon leads to very complicated formulae. A graphical representation of these formulas is helpful.
The extended Nyström tree theory: Practical ERKN methods and numerical illustration

The EN-Trees and related functions

\( f^{(1)} = f_y y' + f_{y'} (-My) + f_y f. \)

\( f^{(2)} = f_{yy} (y', y') + 2f_{yy'} (y', -My) + 2f_{yy'} (y', f) + f_y (-My) + fy f' 
+ f_{y'y'} (-My, -My) + 2f_{y'y'} (-My, f) + f_{y'} (-M)y' + f_{y'y'} (f, f) 
+ f_{y'} f_y y' + f_{y'} f_y (-My) + f_{y'} f_y y' + f_{y'} f_y f. \)

(12)

The continuation of the above process, although theoretically clear, soon leads to very complicated formulae. A graphical representation of these formulas is helpful. In order to distinguish the elementary differentials, we need three kinds of vertices – meagre “·”, fat black “●” and fat white “○”, denoted by letters “m”, “B” and “W”, corresponding to a derivative of \( y, y' \) and \( f \), respectively – with each of which we associate some factor of elemental differentials.
The EN-Trees and related functions

Definition 2.1

The set $ENT$ of extended Nyström trees is defined recursively as follows:

(a) The graph $\tau$, denoted by $\tau$, consisting of one fat white vertex (called the root) belongs to $ENT$, i.e., the tree “$W$” $\in$ $ENT$. 
Definition 2.1

The set $ENT$ of extended Nyström trees is defined recursively as follows:

(a) The graph $\circ$, denoted by $\tau$, consisting of one fat white vertex (called the root) belongs to $ENT$, i.e., the tree “$W$” $\in$ $ENT$.

(b) The graph “$W(Bm)^q$” ($q \geq 1$), consisting of the root “$W$” followed by a chain of $q$ (positive integer) consecutive “fat black-meagre” couples, belongs to $ENT$. 
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The set $ENT$ of extended Nyström trees is defined recursively as follows:

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"W(mB)$^q$" ($q \geq 0$), the graph consisting of the root “W” followed by a chain of $q$ consecutive “fat black-meagre” couples and then followed by a fat black ending vertex, belongs to $ENT$. 

Also "W(mB)$^q$" ($q \geq 1$) and "W(mB)$^q$m" ($q \geq 0$) belong to $ENT$. 

In summary, the extended Nyström tree theory provides a systematic way to construct and analyze hierarchical data structures, which is particularly useful in numerical analysis and scientific computing.
Definition 2.1

The set \( ENT \) of \textit{extended Nyström trees} is defined recursively as follows:

(a) The graph \( \circ \), denoted by \( \tau \), consisting of one fat white vertex (called the root) belongs to \( ENT \), i.e., the tree \( “W” \in \text{ENT} \).

(b) The graph \( “W(Bm)q” \) \( (q \geq 1) \), consisting of the root \( “W” \) followed by a chain of \( q \) (positive integer) consecutive “fat black-meagre” couples, belongs to \( ENT \). “\( W(Bm)qB” \) \( (q \geq 0) \), the graph consisting of the root \( “W” \) followed by a chain of \( q \) consecutive “fat black-meagre” couples and then followed by a fat black ending vertex, belongs to \( ENT \). Also “\( W(mB)q” \) \( (q \geq 1) \) and “\( W(mB)qm” \) \( (q \geq 0) \) belong to \( ENT \).
The extended Nyström tree theory

Figure 1: Extended Nyström trees
(c) If $t_1$ belongs to ENT, then “$W(Bm)^qB[t_1]$” ($q \geq 0$), the graph consisting of the root “W” followed by a chain of $q$ consecutive “fat black-meagre” couples, then followed by a fat black vertex with $t_1$ grafted on this fat black vertex, belongs ENT; also “$W(mB)^q[t_1]$” ($q \geq 0$) belongs to ENT.
(c) If $t_1$ belongs to $\text{ENT}$, then “$W(Bm)^qB[t_1]$” ($q \geq 0$), the graph consisting of the root “$W$” followed by a chain of $q$ consecutive “fat black-meagre” couples, then followed by a fat black vertex with $t_1$ grafted on this fat black vertex, belongs $\text{ENT}$; also “$W(mB)^q[t_1]$” ($q \geq 0$) belongs to $\text{ENT}$.

(d) If $t_1, \ldots, t_r \in \text{ENT}$, then their merging product $t = t_1 \times \ldots \times t_r$, the graph obtained by merging the roots of $t_1, \ldots, t_r$ into a new root, belongs to $\text{ENT}$. 
The rules for forming EN-trees can be described as follows:
(i) the root is always a fat white vertex “W”;
(ii) a fat black vertex “B” has at most one child and that child can not be fat black;
(iii) a meagre vertex “m” has at most one child and that child has to be a fat black vertex “B”.
The function $\rho(t)$ on the set $\text{ENT}$, the order, is defined recursively by

(a) $\rho(W) = 1$.

(b) $\rho(W(Bm)^q) = \rho(W(mb)^q) = 2q + 1$ ($q \geq 1$), $\rho(W(Bm)^qB) = \rho(W(mb)^qm) = 2q + 2$ ($q \geq 0$).

(c) $\rho(W(Bm)^qB[t_1]) = \rho(t_1) + 2q + 2$, $\rho(W(mb)^q[t_1]) = \rho(t_1) + 2q + 1$ ($q \geq 0$).

(d) If $t = t_1 \times \ldots \times t_r$,

$$\rho(t) = 1 + \sum_{i=1}^{r} (\rho(t_i) - 1).$$
Definition 2.2

The function $\rho(t)$ on the set $\text{ENT}$, the order, is defined recursively by

(a) $\rho(W) = 1$.
(b) $\rho(W(Bm)^q) = \rho(W(mB)^q) = 2q + 1$ ($q \geq 1$),
$\rho(W(Bm)^q B) = \rho(W(mB)^qm) = 2q + 2$ ($q \geq 0$).
(c) $\rho(W(Bm)^q B[t_1]) = \rho(t_1) + 2q + 2$, $\rho(W(mB)^q[t_1]) = \rho(t_1) + 2q + 1$ ($q \geq 0$).
(d) If $t = t_1 \times \ldots \times t_r$,

$$\rho(t) = 1 + \sum_{i=1}^{r} (\rho(t_i) - 1).$$

For a specific EN-tree $t$, the order $\rho(t)$ is the number of vertices of $t$. The set of all the EN-trees of order $q$ is denoted by $\text{ENT}_q$. 
The integer coefficients in the expressions (12) can be defined in the following.

**Definition 2.3**

The function \( \alpha \) on the set \( \text{ENT} \) is defined recursively by

(a) \( \alpha(W) = 1 \).

(b) \( \alpha(W(Bm)^q) = \alpha(W(mB)^q) = 1 \) \( (q \geq 1) \),
\[ \alpha(W(Bm)^q B) = \alpha(W(mB)^q m) = 1 \] \( (q \geq 0) \).

(c) \( \alpha(W(Bm)^q B[t_1]) = \alpha(W(mB)^q [t_1]) = \alpha(t_1) \) \( (q \geq 0) \).

(d) If \( t = t_1^{\lambda_1} \times \ldots \times t_r^{\lambda_r} \),

\[
\alpha(t) = (\rho(t) - 1)! \prod_{i=1}^{r} \frac{1}{\lambda_i!} \left( \frac{\alpha(t_i)}{(\rho(t_i) - 1)!} \right)^{\lambda_i},
\]

where \( \lambda_i \) is the multiplicity of the tree \( t_i, i = 1, \ldots, r \).
The integer coefficients in the expressions (12) can be defined in the following.

**Definition 2.3**

The function $\alpha$ on the set ENT is defined recursively by

(a) $\alpha(W) = 1$.
(b) $\alpha(W(Bm)^q) = \alpha(W(mb)^q) = 1 \ (q \geq 1)$,
$c$ $\alpha(W(Bm)^qB) = \alpha(W(mb)^qm) = 1 \ (q \geq 0)$.
(c) $\alpha(W(Bm)^qB[t_1]) = \alpha(W(mb)^q[t_1]) = \alpha(t_1) \ (q \geq 0)$.
(d) If $t = t_1^{\lambda_1} \times \ldots \times t_r^{\lambda_r}$,

$$
\alpha(t) = (\rho(t) - 1)! \prod_{i=1}^{r} \frac{1}{\lambda_i!} \left( \frac{\alpha(t_i)}{(\rho(t_i) - 1)!} \right)^{\lambda_i},
$$

where $\lambda_i$ is the multiplicity of the tree $t_i$, $i = 1, \ldots, r$.

An EN-tree can be labelled monotonically by indices $j, k, l, \ldots$.

$\alpha(t)$ is the number of different monotonic labellings of $t$. 
Definition 2.4

For a labelled EN-tree \( t \), we denote by \( \mathcal{F}^J(t)(y, y') \) the expression which is a sum over all its indices except “\( j \)”, the index of the root. The general term of this sum is a product of expressions

\[
\frac{\partial^r f^K}{\partial y^L \ldots \partial y'^N \ldots}
\]

for the fat white vertex \( k \) that is connected with the fat black vertices \( l, \ldots \) and with the fat white or meagre vertices \( n, \ldots \); and \( f^K \) for the ending fat white vertex \( k \);
Definition 2.4

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for the fat white vertex \( k \) that is connected with the fat black vertices \( l, \ldots \) and with the fat white or meagre vertices \( n, \ldots \); and \( f^K \) for the ending fat white vertex \( k \);

(b) \( \delta_{KL} \), the Kronecker function, for the fat black vertex \( k \) that has the fat white vertex \( l \) as its child; and \( y'^K \) for the ending fat black vertex \( k \);
The EN-Trees and related functions

**Definition 2.4**

For a labelled EN-tree $t$, we denote by $\mathcal{F}^J(t)(y, y')$ the expression which is a sum over all its indices except “$j$”, the index of the root. The general term of this sum is a product of expressions

\[
\frac{\partial^r f^K}{\partial y^L \ldots \partial y'^N \ldots}
\]

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(b) $\delta_{KL}$, the Kronecker function, for the fat black vertex $k$ that has the fat white vertex $l$ as its child; and $y'^K$ for the ending fat black vertex $k$;

(c) $-m_{KL}$ for the meagre vertex $k$ that has the fat black vertex $l$ as its child; $-\sum_N m_{KN} y^N$ for the ending meagre vertex $k$. 
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$$\frac{\partial^r f^K}{\partial y^L \ldots \partial y'^N \ldots}$$

for the fat white vertex $k$ that is connected with the fat black vertices $l, \ldots$ and with the fat white or meagre vertices $n, \ldots$; and $f^K$ for the ending fat white vertex $k$;

(b) $\delta_{KL}$, the Kronecker function, for the fat black vertex $k$ that has the fat white vertex $l$ as its child; and $y'^K$ for the ending fat black vertex $k$;

(c) $-m_{KL}$ for the meagre vertex $k$ that has the fat black vertex $l$ as its child; $-\sum_N m_{KN} y^N$ for the ending meagre vertex $k$.

The vector $\mathcal{F}(t)(y, y') = (\mathcal{F}^1(t)(y, y'), \ldots, \mathcal{F}^d(t)(y, y'))^T$ is called the elementary differential associated with the EN-tree $t$. 
The extended Nyström tree theory

Practical ERKN methods and numerical illustrations

The EN-Trees and related functions

Table 1: Trees in ENT<sub>m</sub>, m ≤ 3

<table>
<thead>
<tr>
<th>Graph of EN-tree</th>
<th>ρ</th>
<th>α</th>
<th>˜γ</th>
<th>Φ&lt;sub&gt;j&lt;/sub&gt;</th>
<th>F</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>I</td>
<td>f</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1</td>
<td>2</td>
<td>c&lt;sub&gt;j&lt;/sub&gt;I</td>
<td>f&lt;sub&gt;y&lt;/sub&gt;y'</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1</td>
<td>2</td>
<td>c&lt;sub&gt;j&lt;/sub&gt;I</td>
<td>f&lt;sub&gt;y&lt;/sub&gt;(−M&lt;sub&gt;y&lt;/sub&gt;)</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1</td>
<td>2</td>
<td>∑&lt;sub&gt;k&lt;/sub&gt;a&lt;sub&gt;jk&lt;/sub&gt;(0)</td>
<td>f&lt;sub&gt;y&lt;/sub&gt;f</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>1</td>
<td>3</td>
<td>c&lt;sub&gt;j&lt;/sub&gt;²I</td>
<td>f&lt;sub&gt;yy&lt;/sub&gt;(y', y')</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>1</td>
<td>3</td>
<td>c&lt;sub&gt;j&lt;/sub&gt;²I</td>
<td>f&lt;sub&gt;y&lt;/sub&gt;(−M&lt;sub&gt;y&lt;/sub&gt;)</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>1</td>
<td>6</td>
<td>∑&lt;sub&gt;k&lt;/sub&gt;a&lt;sub&gt;jk&lt;/sub&gt;(0)</td>
<td>f&lt;sub&gt;y&lt;/sub&gt;f</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>2</td>
<td>3</td>
<td>c&lt;sub&gt;j&lt;/sub&gt;∑&lt;sub&gt;l&lt;/sub&gt;a&lt;sub&gt;jl&lt;/sub&gt;(0)</td>
<td>f&lt;sub&gt;yy&lt;/sub&gt;(y', f)</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>1</td>
<td>3</td>
<td>c&lt;sub&gt;j&lt;/sub&gt;²I</td>
<td>f&lt;sub&gt;y'y'(-M&lt;sub&gt;y&lt;/sub&gt;,−M&lt;sub&gt;y&lt;/sub&gt;)</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>2</td>
<td>3</td>
<td>c&lt;sub&gt;j&lt;/sub&gt;∑&lt;sub&gt;l&lt;/sub&gt;a&lt;sub&gt;jl&lt;/sub&gt;(0)</td>
<td>f&lt;sub&gt;y'y'(-M&lt;sub&gt;y&lt;/sub&gt;, f)</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>1</td>
<td>3</td>
<td>c&lt;sub&gt;j&lt;/sub&gt;²I</td>
<td>f&lt;sub&gt;y'y'(-M&lt;sub&gt;y&lt;/sub), y')</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>1</td>
<td>3</td>
<td>∑&lt;sub&gt;k,l&lt;/sub&gt;a&lt;sub&gt;jk&lt;/sub&gt;(0)a&lt;sub&gt;jl&lt;/sub&gt;(0)</td>
<td>f&lt;sub&gt;y'y'(f, f)</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>1</td>
<td>3</td>
<td>c&lt;sub&gt;j&lt;/sub&gt;²I</td>
<td>f&lt;sub&gt;y'(-M)y'</td>
</tr>
</tbody>
</table>

ρ, α, ˜γ, Φ<sub>j</sub>, F represent the structures and functions of the EN-Trees.
### The EN-Trees and related functions

<table>
<thead>
<tr>
<th>Tree</th>
<th>Rank</th>
<th>Type</th>
<th>Function</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Tree" /></td>
<td>3 1 3</td>
<td></td>
<td>$c_j^2 I$</td>
<td>( f_y(-My) )</td>
</tr>
<tr>
<td><img src="image" alt="Tree" /></td>
<td>3 1 6</td>
<td></td>
<td>( \sum_k a_{jk}(0) )</td>
<td>( f_yf )</td>
</tr>
<tr>
<td><img src="image" alt="Tree" /></td>
<td>3 2 3</td>
<td></td>
<td>$c_j^2 I$</td>
<td>( f_{yy'}(y', -My) )</td>
</tr>
<tr>
<td><img src="image" alt="Tree" /></td>
<td>3 2 3</td>
<td></td>
<td>$c_j \sum_l a_{jl}(0)$</td>
<td>( f_{yy'}(y', f) )</td>
</tr>
<tr>
<td><img src="image" alt="Tree" /></td>
<td>3 1 3</td>
<td></td>
<td>$c_j^2 I$</td>
<td>( f_{yy'}(-My, -My) )</td>
</tr>
<tr>
<td><img src="image" alt="Tree" /></td>
<td>3 2 3</td>
<td></td>
<td>$c_j \sum_l a_{jl}(0)$</td>
<td>( f_{yy'}(-My, f) )</td>
</tr>
<tr>
<td><img src="image" alt="Tree" /></td>
<td>3 1 3</td>
<td></td>
<td>$\sum_{k,l} a_{jk}(0)a_{jl}(0)$</td>
<td>( f_{yy'}(f, f) )</td>
</tr>
<tr>
<td><img src="image" alt="Tree" /></td>
<td>3 1 3</td>
<td></td>
<td>$c_j^2 I$</td>
<td>( f_{y'y'}(-My)y' )</td>
</tr>
<tr>
<td><img src="image" alt="Tree" /></td>
<td>3 1 6</td>
<td></td>
<td>( \sum_k a_{jk}(0)c_k )</td>
<td>( f_yf_{yy'} )</td>
</tr>
<tr>
<td><img src="image" alt="Tree" /></td>
<td>3 1 6</td>
<td></td>
<td>( \sum_{k,l} a_{jk}(0)a_{kl}(0) )</td>
<td>( f_yf_{yy}' )</td>
</tr>
<tr>
<td><img src="image" alt="Tree" /></td>
<td>3 1 6</td>
<td></td>
<td>( \sum_k a_{jk}(0)c_k )</td>
<td>( f_yf_{y'y'}(-My) )</td>
</tr>
</tbody>
</table>
Table 2. Trees in $ENT_4$

<table>
<thead>
<tr>
<th>Graph of EN-trees of order 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>![Tree Diagram]</td>
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<tr>
<td>![Tree Diagram]</td>
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<tr>
<td>![Tree Diagram]</td>
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<tr>
<td>![Tree Diagram]</td>
</tr>
<tr>
<td>![Tree Diagram]</td>
</tr>
</tbody>
</table>

The EN-Trees and related functions
Theorem 2.1

The \( q \)-th derivative of \( f(y, y') \) is given by

\[
(f(y, y'))^{(q)} = \sum_{t \in ENT_{q+1}} \alpha(t) F(t)(y, y'), \quad q \geq 1,
\]
Theorem 2.1

The $q$-th derivative of $f(y, y')$ is given by

$$
(f(y, y'))^{(q)} = \sum_{t \in \text{ENT}_{q+1}} \alpha(t) F(t)(y, y'), \quad q \geq 1, \tag{13}
$$

Proof by induction.
Definition 2.5

With an EN-tree $t$, we associated an expression $\Phi_j(t)$ related to the coefficients of the $j$-th internal stage of the ERKN method (7). The expression is a sum over all its indices except “$j$”, the index of the root. The general term of this sum is a product of
Definition 2.5

With an EN-tree \( t \), we associated an expression \( \Phi_j(t) \) related to the coefficients of the \( j \)-th internal stage of the ERKN method (7). The expression is a sum over all its indices except “\( j \)”, the index of the root. The general term of this sum is a product of

(a) \( a^{(q)}_{kl}(0) \) if the fat white vertex “\( k \)” is connected upwards via a chain of \( q \) “mB” couples (\( q \geq 0 \)) with a fat white vertex “\( l \)”;

(b) \( \bar{a}^{(q)}_{kl}(0) \) if the fat white vertex “\( k \)” is connected upwards via a chain of \( q \) “Bm” couples (\( q \geq 0 \)) with a fat black vertex and then with a fat white vertex “\( l \)”;

(c) \( \delta_{kl}c_{l}I \) if the fat white vertex “\( k \)” has the fat black vertex “\( l \)” or the meagre vertex “\( l \)” as its child and has no other fat white vertex as its descendant, where \( I \) is the \( d \times d \) identity matrix.
Definition 2.5

With an EN-tree $t$, we associated an expression $\Phi_j(t)$ related to the coefficients of the $j$-th internal stage of the ERKN method (7). The expression is a sum over all its indices except “$j$”, the index of the root. The general term of this sum is a product of

(a) $a_{kl}^{(q)}(0)$ if the fat white vertex “$k$” is connected upwards via a chain of $q$ “mB” couples ($q \geq 0$) with a fat white vertex “$l$”; 

(b) $\tilde{a}_{kl}^{(q)}(0)$ if the fat white vertex “$k$” is connected upwards via a chain of $q$ “Bm” couples ($q \geq 0$) with a fat black vertex and then with a fat white vertex “$l$”;
Derivatives of $f(Y_i, Y'_i)$

**Definition 2.5**

With an EN-tree $t$, we associated an expression $\Phi_j(t)$ related to the coefficients of the $j$-th internal stage of the ERKN method (7). The expression is a sum over all its indices except "j", the index of the root. The general term of this sum is a product of

(a) $a^{(q)}_{kl}(0)$ if the fat white vertex "k" is connected upwards via a chain of $q$ “mB” couples ($q \geq 0$) with a fat white vertex “l”;

(b) $\bar{a}^{(q)}_{kl}(0)$ if the fat white vertex "k" is connected upwards via a chain of $q$ “Bm” couples ($q \geq 0$) with a fat black vertex and then with a fat white vertex “l”;

(c) $\delta_{kl}c_lI$ if the fat white vertex $k$ has the fat black vertex $l$ or the meagre vertex $l$ as its child and has no other fat white vertex as its descendant, where $I$ is the $d \times d$ identity matrix.
Definition 2.6

The signed density, denoted by $\tilde{\gamma}(t)$, of an EN-tree $t$, is recursively defined as follows.

(a) $\tilde{\gamma}("W")=1$.

(b) For $t="W(Bm)^q", "W(Bm)^qB", "W(mB)^q"$ or $"W(mB)^q m"$, $\tilde{\gamma}(t) = \rho(t)$.

(c) For $t="W(mB)^q[t_1]"$,

$$
\tilde{\gamma}(t) = \frac{(-1)^q \rho(t)(\rho(t) - 1) \ldots (\rho(t) - 2q)}{(2q)!} \tilde{\gamma}(t_1),
$$

and for $t="W(Bm)^qB[t_1]"$,

$$
\tilde{\gamma}(t) = \frac{(-1)^q \rho(t)(\rho(t) - 1) \ldots (\rho(t) - 2q - 1)}{(2q)!} \tilde{\gamma}(t_1).
$$
Definition 2.6

(d) For $t = t_1 \times \ldots \times t_r$, 

$$\tilde{\gamma}(t) = \rho(t) \prod_{i=1}^{r} \frac{\tilde{\gamma}(t_i)}{\rho(t_i)}.$$
Derivatives of $f(Y_i, Y'_i)$

$\tilde{\gamma}(t_1) = 4, \tilde{\gamma}(t_2) = -12$

$t_1 = \{ , t_2 = \}$
Table 3. EN-trees of up to order four without redundancy (i)

<table>
<thead>
<tr>
<th>EN-tree</th>
<th>$\rho$</th>
<th>$\alpha$</th>
<th>$\tilde{\gamma}$</th>
<th>$\Phi_j$</th>
<th>$\mathcal{F}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\circ$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>$I$</td>
<td>$f$</td>
</tr>
<tr>
<td>$\circ$</td>
<td>2</td>
<td>1</td>
<td>2</td>
<td>$c_j I$</td>
<td>$f_y y'$</td>
</tr>
<tr>
<td>$\circ$</td>
<td>2</td>
<td>1</td>
<td>2</td>
<td>$\sum_k a_{jk}(0)$</td>
<td>$f_y' f$</td>
</tr>
<tr>
<td>$\circ$</td>
<td>3</td>
<td>1</td>
<td>3</td>
<td>$c_j^2 I$</td>
<td>$f_{yy}(y', y')$</td>
</tr>
<tr>
<td>$\circ$</td>
<td>3</td>
<td>1</td>
<td>6</td>
<td>$\sum_k \bar{a}_{jk}(0)$</td>
<td>$f_y f$</td>
</tr>
<tr>
<td>$\circ$</td>
<td>3</td>
<td>2</td>
<td>3</td>
<td>$c_j \sum_l a_{jl}(0)$</td>
<td>$f_{yy'}(y', f)$</td>
</tr>
<tr>
<td>$\circ$</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>$\sum_{k,l} a_{jk}(0) a_{jl}(0)$</td>
<td>$f_{y'y'}(f, f)$</td>
</tr>
<tr>
<td>$\circ$</td>
<td>3</td>
<td>1</td>
<td>6</td>
<td>$\sum_k a_{jk}(0) c_k$</td>
<td>$f_y f_y y'$</td>
</tr>
<tr>
<td>$\circ$</td>
<td>3</td>
<td>1</td>
<td>6</td>
<td>$\sum_{k,l} a_{jk}(0) a_{kl}(0)$</td>
<td>$f_y f_y f$</td>
</tr>
<tr>
<td>$\circ$</td>
<td>4</td>
<td>1</td>
<td>4</td>
<td>$c_j^3 I$</td>
<td>$f_{yyy}(y', y', y')$</td>
</tr>
<tr>
<td>$\circ$</td>
<td>4</td>
<td>1</td>
<td>4</td>
<td>$\sum_{k,l,n} a_{jk}(0) a_{jl}(0) a_{kn}(0)$</td>
<td>$f_{y'y'y'}(f, f, f)$</td>
</tr>
<tr>
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<td>4</td>
<td>$c_j^3 \sum_k a_{jk}(0)$</td>
<td>$f_{yyy}(y', y', f)$</td>
</tr>
<tr>
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<td>4</td>
<td>$c_j \sum_{k,l} a_{jk}(0) a_{kl}(0)$</td>
<td>$f_{y'y'y'}(y', f, f)$</td>
</tr>
<tr>
<td>EN-tree</td>
<td>ρ</td>
<td>α</td>
<td>˜γ</td>
<td>Φ</td>
<td>j</td>
</tr>
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<td>---</td>
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<td>2</td>
<td>3</td>
<td>1</td>
<td>6</td>
<td>1</td>
<td>2</td>
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<td>8</td>
<td>2</td>
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<tr>
<td>5</td>
<td>4</td>
<td>3</td>
<td>8</td>
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<td>1</td>
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<tr>
<td>6</td>
<td>4</td>
<td>3</td>
<td>8</td>
<td>2</td>
<td>1</td>
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</table>

Derivatives of \( f(Y_i, Y_i') \)

<table>
<thead>
<tr>
<th>EN-tree</th>
<th>ρ</th>
<th>α</th>
<th>˜γ</th>
<th>Φ</th>
<th>j</th>
<th>F</th>
</tr>
</thead>
<tbody>
<tr>
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<td>1</td>
<td>4</td>
<td>1</td>
<td>2</td>
<td>2</td>
</tr>
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<td>4</td>
<td>1</td>
<td>4</td>
<td>1</td>
<td>2</td>
<td>2</td>
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<td>4</td>
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<tr>
<td>7</td>
<td>4</td>
<td>3</td>
<td>8</td>
<td>2</td>
<td>1</td>
<td>2</td>
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</tbody>
</table>

Table 3. EN-trees of up to order four without redundancy (i)
Table 4. EN-trees of up to order four without redundancy (ii)

<table>
<thead>
<tr>
<th>j</th>
<th>4 3 8</th>
<th>( c_j \sum_{k,l} a_{jk}(0) a_{kl}(0) )</th>
<th>( f_{y'y'}(f_y, f_y) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>j</td>
<td>4 3 8</td>
<td>( \sum_{k,l} a_{jk}(0) a_{jl}(0) c_l )</td>
<td>( f_{y'y'}(f_y y', f) )</td>
</tr>
<tr>
<td>j</td>
<td>4 3 8</td>
<td>( \sum_{k,l,n} a_{jk}(0) a_{jl}(0) a_{ln}(0) )</td>
<td>( f_{y'y'}(f_y f, f) )</td>
</tr>
<tr>
<td>j</td>
<td>4 1 12</td>
<td>( \sum_{k} a_{jk}(0) c_k^2 )</td>
<td>( f_{y'y'}(y', f) )</td>
</tr>
<tr>
<td>j</td>
<td>4 1 12</td>
<td>( \sum_{k,l,n} a_{jk}(0) a_{kl}(0) a_{kn}(0) )</td>
<td>( f_{y'y'}(f, f) )</td>
</tr>
<tr>
<td>j</td>
<td>4 2 12</td>
<td>( \sum_{k,l} a_{jk}(0) a_{kl}(0) c_k a_{kl}(0) )</td>
<td>( f_{y'y'}(y', f) )</td>
</tr>
<tr>
<td>j</td>
<td>4 1 24</td>
<td>( \sum_{k} \tilde{a}_{jk}(0) c_k )</td>
<td>( f_y f_{y'} )</td>
</tr>
<tr>
<td>j</td>
<td>4 1 24</td>
<td>( \sum_{k,l} \tilde{a}<em>{jk}(0) a</em>{kl}(0) )</td>
<td>( f_y f_{y'} f )</td>
</tr>
<tr>
<td>j</td>
<td>4 1 -12</td>
<td>( \sum_{k} a_{jk}^{(1)}(0) )</td>
<td>( f_{y'}(-M) f )</td>
</tr>
<tr>
<td>j</td>
<td>4 1 24</td>
<td>( \sum_{k,l} a_{jk}(0) \tilde{a}_{kl}(0) )</td>
<td>( f_{y'y'} f )</td>
</tr>
</tbody>
</table>
## Derivatives of \( f(Y_i, Y'_i) \)

<table>
<thead>
<tr>
<th>EN-tree</th>
<th>4 1 12</th>
<th>4 2 12</th>
<th>4 1 24</th>
<th>4 1 24</th>
<th>4 1 24</th>
<th>4 1 24</th>
<th>4 1 24</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \sum_{k,l,n} a_{jk}(0) a_{kl}(0) a_{kn}(0) )</td>
<td>( f_y f_y' (f, f) )</td>
<td>( f_y f_y' (y', f) )</td>
<td>( \sum_k \tilde{a}_{jk}(0) c_k )</td>
<td>( f_y f_y' )</td>
<td>( \sum_{k,l} \tilde{a}<em>{jk}(0) a</em>{kl}(0) )</td>
<td>( f_y f_y' f )</td>
<td>( \sum_{k,l} a_{jk}(0) a_{kl}(0) c_l )</td>
</tr>
<tr>
<td>( \sum_{k,l} \bar{a}<em>{jk}(0) c</em>{kl} )</td>
<td>( \sum_{k,l,n} a_{jk}(0) a_{kl}(0) a_{kn}(0) )</td>
<td>( f_y f_y' (f, f) )</td>
<td>( \sum_{k,l} a_{jk}(0) \bar{a}_{kl}(0) )</td>
<td>( f_y f_y f )</td>
<td>( \sum_{k,l,n} a_{jk}(0) a_{kl}(0) a_{kn}(0) )</td>
<td>( f_y f_y f_y f )</td>
<td></td>
</tr>
<tr>
<td>( \sum_{k} a_{jk}(0) c_k )</td>
<td>( \sum_{k,l} a_{jk}(0) a_{kl}(0) )</td>
<td>( f_y f_y' (y', f) )</td>
<td>( \sum_{k,l,n} \bar{a}<em>{jk}(0) a</em>{kl}(0) a_{kn}(0) )</td>
<td>( f_y f_y f_y' )</td>
<td>( \sum_{k,l} a_{jk}(0) \bar{a}_{kl}(0) )</td>
<td>( f_y f_y' f )</td>
<td></td>
</tr>
</tbody>
</table>
Derivatives of $f(Y_i, Y'_i)$

**Theorem 2.2**

The $q$-th derivative of $f(Y_j, Y'_j)$ at $h = 0$ can be expressed in terms of EN-trees of order $q + 1$ as

$$
(f(Y_j, Y'_j))^{(q)}igg|_{h=0} = \frac{1}{q + 1} \sum_{t \in \text{ENT}_{q+1}} \Phi_j(t) \tilde{\gamma}(t) \alpha(t) \mathcal{F}(t)(y_n, y'_n), \quad q \geq 0.
$$

Proof. An argument by induction proves the theorem using the Faà di Bruno’s formula.
Theorem 2.2

The $q$-th derivative of $f(Y_j, Y'_j)$ at $h = 0$ can be expressed in terms of EN-trees of order $q + 1$ as

$$
(f(Y_j, Y'_j))^{(q)} \bigg|_{h=0} = \frac{1}{q + 1} \sum_{t \in ENT_{q+1}} \Phi_j(t)\tilde{\gamma}(t)\alpha(t)F(t)(y_n, y'_n), \quad q \geq 0.
$$

Proof. An argument by induction proves the theorem using the Faà di Bruno’s formula.
Theorem 2.3

The scheme (7) is of order $p$ if and only if

$$
\sum_{i=1}^{s} \bar{b}_i(V)\Phi_i(t) = \frac{\rho(t)!}{\tilde{\gamma}(t)} \phi_{\rho(t)+1}(V) + O(h^{p-\rho(t)}), \quad t \in ENT, \quad \rho(t) \leq p - 1
$$

and

$$
\sum_{i=1}^{s} b_i(V)\Phi_i(t) = \frac{\rho(t)!}{\tilde{\gamma}(t)} \phi_{\rho(t)}(V) + O(h^{p-\rho(t)+1}), \quad t \in ENT, \quad \rho(t) \leq p.
$$

(14)
Practical ERKN methods

**ERKN2: order 2**

<table>
<thead>
<tr>
<th>0</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>$\phi_1(V) - \frac{3}{2} \phi_2(V)$</td>
<td>$\frac{3}{2} \phi_2(V)$</td>
<td>$\phi_2(V) - \frac{3}{2} \phi_3(V)$</td>
</tr>
</tbody>
</table>

(15)
ERKN3: order 3

\[
\begin{array}{c|ccc|ccc}
0 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 \\
2 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 \\
\hline
b_1(V) & b_2(V) & b_3(V) & \bar{b}_1(V) & \bar{b}_2(V) & \bar{b}_3(V)
\end{array}
\]

(16)

with

\[
\begin{align*}
b_1(V) &= \phi_1(V) - 3\phi_2(V) + 4\phi_3(V), & b_2(V) &= 4\phi_2(V) - 8\phi_3(V), \\
b_3(V) &= -\phi_2(V) + 4\phi_3(V), & \bar{b}_1(V) &= \phi_2(V) - 2\phi_3(V), & \bar{b}_2(V) &= 2\phi_3(V), & \bar{b}_3(V) &= 0.
\end{align*}
\]
## ERKN4: order 4

<table>
<thead>
<tr>
<th></th>
<th>( a_{21}(V) )</th>
<th>( a_{31}(V) )</th>
<th>( a_{32}(V) )</th>
<th>( a_{41}(V) )</th>
<th>( a_{42}(V) )</th>
<th>( a_{43}(V) )</th>
<th>( \bar{a}_{31}(V) )</th>
<th>( \bar{a}_{41}(V) )</th>
<th>( \bar{a}_{42}(V) )</th>
<th>( \bar{b}_{1}(V) )</th>
<th>( \bar{b}_{2}(V) )</th>
<th>( \bar{b}_{3}(V) )</th>
<th>( \bar{b}_{4}(V) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
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<td></td>
</tr>
<tr>
<td>( c_2 )</td>
<td></td>
<td>( a_{21}(V) )</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( c_3 )</td>
<td>( a_{31}(V) )</td>
<td>( a_{32}(V) )</td>
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<td></td>
</tr>
<tr>
<td>( c_4 )</td>
<td>( a_{41}(V) )</td>
<td>( a_{42}(V) )</td>
<td>( a_{43}(V) )</td>
<td>( \bar{a}_{31}(V) )</td>
<td>( \bar{a}_{41}(V) )</td>
<td>( \bar{a}_{42}(V) )</td>
<td>( \bar{b}_{1}(V) )</td>
<td>( \bar{b}_{2}(V) )</td>
<td>( \bar{b}_{3}(V) )</td>
<td>( \bar{b}_{4}(V) )</td>
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<td></td>
</tr>
<tr>
<td></td>
<td>( b_1(V) )</td>
<td>( b_2(V) )</td>
<td>( b_3(V) )</td>
<td>( b_4(V) )</td>
<td>( \bar{b}_1(V) )</td>
<td>( \bar{b}_2(V) )</td>
<td>( \bar{b}_3(V) )</td>
<td>( \bar{b}_4(V) )</td>
<td></td>
<td></td>
<td></td>
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</tr>
</tbody>
</table>

where

\[
\begin{align*}
c_2 &= \frac{1}{5}, \quad c_3 = \frac{2}{3}, \quad c_4 = 1, \\
a_{31}(V) &= -\frac{17}{27} I, \quad a_{42}(V) = -\frac{22}{7} I, \\
a_{41}(V) &= \frac{13}{5} I,
\end{align*}
\]
Practical ERKN methods

ERKN4: order 4

\[
a_{21}(V) = \frac{1}{2} c_2 \left( \phi_0(c_2^2 V) + \phi_1(c_2^2 V) \right),
\]
\[
a_{32}(V) = \frac{1}{2} \left( -2a_{31}(V) + c_3 \left( \phi_0(c_3^2 V) + \phi_1(c_3^2 V) \right) \right) (\phi_0(c_2^2 V))^{-1},
\]
\[
a_{43}(V) = \frac{1}{2} \left( -2a_{41}(V) - 2a_{42}(V)\phi_0(c_2^2 V) + c_4 \left( \phi_0(c_4^2 V) + \phi_1(c_4^2 V) \right) \right)
\]

(17)
Practical ERKN methods

ERKN4: order 4

\[
\bar{b}_1(V) = \phi_2(V) + (\beta_1 \phi_3(V) + \gamma_1 \phi_4(V)) M_1^{-1},
\]
\[
\bar{b}_2(V) = (\beta_2 \phi_3(V) + \gamma_2 \phi_4(V)) M_2^{-1},
\]
\[
\bar{b}_3(V) = (\beta_3 \phi_3(V) + \gamma_3 \phi_4(V)) M_3^{-1},
\]
\[
\bar{b}_4(V) = (\beta_4 \phi_3(V) + \gamma_4 \phi_4(V)) M_4^{-1},
\]

where
From RKN to ERKN  Formulation of ERKN  The extended Nyström tree theory  Practical ERKN methods and numerical illustrations

Practical ERKN methods

**ERKN4: order 4**

\[\beta_1 = - (a_{42}(V)c_2 + a_{43}(V)c_3)(c_2^2 - c_3^2) + a_{32}(V)c_2(c_2^2 - c_4^2),\]

\[\gamma_1 = -2a_{32}(V)c_2(c_2 - c_4) + (c_2 - c_3)(2a_{42}(V)c_2 + 2a_{43}(V)c_3 - (c_2 - c_4)(c_3 - c_4)I),\]

\[M_1 = a_{42}(V)c_2^2 c_3(c_2 - c_3) + a_{43}(V)c_2 c_3^2(c_2 - c_3) - a_{32}(V)c_2^2 c_4(c_2 - c_4),\]

\[\beta_2 = -a_{42}(V)c_2 c_3^2 - a_{43}(V)c_3^3 + a_{32}(V)c_2 c_4^2,\]

\[\gamma_2 = 2a_{42}(V)c_2 c_3 + 2a_{43}(V)c_3^2 + c_4(-2a_{32}(V)c_2 + c_3^2I - c_3 c_4I),\]

\[M_2 = c_2(a_{42}c_2(c_2 - c_3)c_3 + a_{43}(c_2 - c_3)c_3^2 + a_{32}c_2 c_4(-c_2 + c_4)),\]

\[\beta_3 = -c_2(a_{42}(V)c_2 + a_{43}(V)c_3),\]

\[\gamma_3 = 2a_{42}(V)c_2 + 2a_{43}(V)c_3 + (c_2 - c_4)c_4I,\]

\[M_3 = a_{42}(V)c_2 c_3(-c_2 + c_3) + a_{43}(V)c_3^2(-c_2 + c_3) + a_{32}(V)c_2(c_2 - c_4)c_4,\]

\[\beta_4 = a_{32}(V)c_2^2, \quad \gamma_4 = -2a_{32}(V)c_2 + c_3(-c_2 + c_3)I,\]

\[M_4 = a_{42}(V)c_2 c_3(-c_2 + c_3) + a_{43}(V)c_3^2(-c_2 + c_3) + a_{32}(V)c_2(c_2 - c_4)c_4.\]
ERKN2;
ERKN3;
ERKN4;
ARKNGV4: The matrix form of the four-stage ARKN method of order four for the general perturbed problems (1) given by Franco in [3] and by A.B. González et al. in [16].
ARKNGV5: The matrix form of the six-stage ARKN method of order five for the general perturbed problems (1) given by Franco in [3].
RKN5: limit method of ARKNGV5;
RKN4: II.14 of [13], pp. 284.
Problem 1. We first consider the famous van de Pol equation

\[ y'' + y = \delta(1 - y^2)y' \]

with the initial values

\[ y(0) = 2 + \frac{1}{96}\delta^2 + \frac{1033}{552960}\delta^4 + \frac{1019689}{55738368000}\delta^6, \quad y'(0) = 0. \]

Here we take \( \delta = 0.8 \times 10^{-4} \).
Problem 1. We first consider the famous van de Pol equation

\[
y'' + y = \delta(1 - y^2)y'
\]

with the initial values

\[
y(0) = 2 + \frac{1}{96} \delta^2 + \frac{1033}{552960} \delta^4 + \frac{1019689}{55738368000} \delta^6, \quad y'(0) = 0.
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Here we take \( \delta = 0.8 \times 10^{-4} \). The principal frequency is \( \omega = 1 \).

Integration interval: \([0, 100]\)
Stepsizes: \( h = 1/2^j, j = 1, 2, 3, 4 \) for the four-stage methods ERKN4, ARKNGV4 and RKN4, \( h/2 \) for the two-stage method ERKN2, \( 3h/4 \) for the three-stage method ERKN3 and \( 3h/2 \) for the six-stage method ARKNGV5 and RKN5.
Numerical experiments

Figure: Problem 1 integrated on [0, 100]
**Problem 2.** Consider the linear initial value problem in the form

\[ y''(x) + My(x) = Ky'(x), \]
\[ y(0) = \left( -\frac{1}{2}, \frac{1}{6}, -\frac{1}{6} \right)^T, \quad y'(0) = (1, 2, 1)^T, \]

where

\[
M = \begin{pmatrix}
1 & -\frac{9}{40} & \frac{27}{40} \\
\frac{9}{2} & 0 & \frac{3}{2} \\
0 & \frac{3}{8} & \frac{63}{8}
\end{pmatrix}, \quad K = \begin{pmatrix}
0 & \frac{21}{40} & \frac{3}{10} \\
0 & \frac{1}{2} & 1 \\
0 & \frac{1}{8} & \frac{1}{2}
\end{pmatrix}.
\]
The analytic solution to this problem is

\[ y(x) = \begin{pmatrix} \sin(x) - \cos(2x)/2 \\ \sin(2x) + \cos(2x)/2 - \cos(3x)/3 \\ \sin(3x)/3 - \cos(2x)/2 + \cos(3x)/3 \end{pmatrix}. \]

We integrate the problem in the interval \([0, 20]\). The step sizes for the four-stage methods are \( h = 1/2^j, j = 2, 3, 4, 5 \). 
Numerical experiments

Problem 2: Efficiency curves

- ERKN4
- ERKN3
- ERKN2
- ARKNV5
- ARKNV4
- RKN5
- RKN4

Figure: Problem 2 integrated on \([0, 20]\)
Problem 3. Consider the initial value problem

\[ y''(x) + \begin{pmatrix} 13 & -12 \\ -12 & 13 \end{pmatrix} y(t) = \frac{12\varepsilon}{5} \begin{pmatrix} 3 & 2 \\ -2 & -3 \end{pmatrix} y'(t) + \varepsilon^2 \begin{pmatrix} f_1(x) \\ f_2(x) \end{pmatrix} \]

\[ y(0) = (\varepsilon, \varepsilon), \quad y'(0) = (-4, 6), \]

with

\[ f_1(x) = \frac{36}{5} \sin(x) + 24 \sin(5x), \]

\[ f_2(x) = -\frac{24}{5} \sin(x) - 36 \sin(5x), \]
Analytic solution is

\[
y(x) = \begin{pmatrix} 
\sin(x) - \sin(5x) + \varepsilon \cos(x) \\
\sin(x) + \sin(5x) + \varepsilon \cos(5x)
\end{pmatrix}.
\]
Analytic solution is

$$y(x) = \begin{pmatrix} \sin(x) - \sin(5x) + \varepsilon \cos(x) \\ \sin(x) + \sin(5x) + \varepsilon \cos(5x) \end{pmatrix}.$$

We choose the parameter value $\varepsilon = 10^{-3}$ and integrate the problem in the interval $[0, 20]$. The step sizes for the four-stage methods are $h = 1/2^j$, $j = 3, 4, 5, 6$. 
Numerical experiments

Problem 3: Efficiency curves

![Efficiency curves graph](image)

The graph shows the efficiency curves for various methods, including ERKN4, ERKN3, ERKN2, ARKN4, ARKN5, RKN4, and RKN5. The x-axis represents the number of function evaluations on a logarithmic scale, while the y-axis represents the logarithm of the mean global error (MGE) on another logarithmic scale.
Problem 4. Consider the damped wave equation with periodic boundary conditions (wave propagation in a medium, see Weinberger [?])

\[
\begin{aligned}
\frac{\partial^2 u}{\partial t^2} + \delta \frac{\partial u}{\partial t} &= \frac{\partial^2 u}{\partial x^2} + f(u), \quad -1 < x < 1, \quad t > 0, \\
u(-1, t) &= u(1, t).
\end{aligned}
\]
\[ \ddot{U} + MU = F(U, \dot{U}), \quad 0 < t \leq t_{\text{end}} , \]

where \( U(t) = (u_1(t), \cdots, u_N(t))^T \) with
\( u_i(t) \approx u(x_i, t), \quad i = 1, \cdots, N, \)

\[ M = \frac{1}{\Delta x^2} \begin{pmatrix} 2 & -1 & & & -1 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ -1 & & & -1 & 2 \end{pmatrix} \]

with \( \Delta x = 2/N \) and \( x_i = -1 + i \Delta x \), and
\( F(U, \dot{U}) = (f(u_1) - \delta \dot{u}_1, \cdots, f(u_N) - \delta \dot{u}_N)^T . \)
In this experiment, we consider the damped sine Gordon equation with \( f(u) = -\sin u \) and \( \delta = 1 \). Following the paper [4], we take the initial conditions as

\[
U(0) = (\pi)^N_{i=1}, \quad U_t(0) = \sqrt{N}(0.01 + \sin(\frac{2\pi i}{N}))^N_{i=1},
\]

with \( N = 64 \) and integrate the problem in the interval \([0, 40]\) with the step sizes \( h = 1/2^j, j = 4, 5, 6, 7 \) for the four-stage methods.
Numerical experiments

Problem 4: Efficiency curves

- ERKN4
- ERKN3
- ERKN2
- ARKNGV5
- ARKNGV4
- RKN5
- RKN4

Figure: Problem 4 integrated on [0, 40]
Summary

- ERKN methods for \( y''(x) + M y(x) = f(y(x), y'(x)) \);
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- Extended Nyström tree (EN) theory;
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Summary

- ERKN methods for $y''(x) + My(x) = f(y(x), y'(x))$;
- Extended Nyström tree (EN) theory;
- Order conditions for ERKN methods;
- Practical ERKN methods: ERKN3, ERKN4;
- Numerical conclusion: ERKN methods outperform existing codes of RKN type.
Further topics

- Higher order, embedded, two-step ERKN;
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- Structure-preserving properties of ERKN methods: symplecticity, symmetry, energy preservation,...;
- Applications: oscillatory genetic regulatory networks ...
Numerical experiments


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THANK YOU