Optimized High Order Explicit Runge-Kutta-Nyström Schemes

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Bibliography and motivation

- Runge-Kutta-Nyström methods well adapted to solve $y'' = f(t, y)$
- Proposed methods (by Hairer, Dormand Prince, etc) have been optimized for non-stiff problems
- Stability condition (CFL) optimized by Chawla and Sharma for order 3, 4, 5
- Numerical optimization for orders 6, 7, 8 and 10
- Application to stiff problems (non-linear Maxwell's equations)

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Runge-Kutta Nyström schemes

- One-step schemes that solve $y'' = f(t, y)$
- y_{n+1} and y'_{n+1} are computed from y_n and y'_n.
- Defined through coefficients c_i, b_i, $\bar{b}_i$ and $\bar{a}_{i,j}$, that must satisfy order conditions to obtain a scheme of order p
- If a Runge-Kutta scheme is known, a Runge-Kutta-Nyström (RKN) scheme can be obtained by setting $\bar{A} = A^2, \bar{b} = A^T b$

Runge-Kutta Nyström schemes

Initial conditions : y_0, y'_0

$$\begin{cases} k_i = f\Big(t_n + c_i\,\Delta t, \quad y_n + c_i\,\Delta t\,y'_n + \Delta t^2 \sum_j \bar{a}_{i,j}\,k_j\Big) \\ y_{n+1} = y_n + \Delta t\,y'_n + \Delta t^2 \sum_j \bar{b}_j\,k_j \\ y'_{n+1} = y'_n + \Delta t \sum_j b_j\,k_j \end{cases}$$

Second-order scheme (p=2)

Order conditions to satisfy to obtain a second-order scheme:

$$\sum_i b_i = 1, \quad \sum_i b_i c_i = \frac{1}{2}, \quad \sum_i \bar{b}_i = \frac{1}{2}$$

A one-stage scheme satisfies these conditions:

$$\bar{A} = (0), \quad c = \left(\frac{1}{2}\right), \quad b = (1), \quad \bar{b} = \left(\frac{1}{2}\right)$$

Second-order scheme (p=2)

$$\left\{ \begin{array}{rcl} k_0 & = & f\left(t_n + \frac{\Delta t}{2},\ y_n + \frac{\Delta t}{2} y'_n\right) \\ y_{n+1} & = & y_n + \Delta t\, y'_n + \frac{\Delta t^2}{2} k_0 \\ y'_{n+1} & = & y'_n + \Delta t\, k_0 \end{array} \right.$$

- Conservative scheme
- Stability condition : $\Delta t \leq \dfrac{2}{\sqrt{||A||_2}}$ (for f linear and replaced by a matrix A)

Second-order scheme (p=2)

Compared to the usual second-order two-step scheme:

$$\frac{y_{n+1} - 2y_n + y_{n-1}}{\Delta t^2} = f(t_n, y_n)$$

Similar properties:

$$\Rightarrow \text{ Conservative scheme}$$

$$\Rightarrow \text{ Same stability condition : } \Delta t \leq \frac{2}{\sqrt{||A||_2}}$$

$\Rightarrow$ these two schemes are optimal with respect to this stability condition

Stability condition

Linear case : $f(t, y) = A\,y$
$\widehat{A}$ being the symbol of A (an eigenvalue), we have:

$$\begin{bmatrix} y_{n+1} \\ w_{n+1} \end{bmatrix} = D(\Delta t^2 \widehat{A}) \begin{bmatrix} y_n \\ w_n \end{bmatrix}$$

Let us note

$$z = \Delta t^2 \widehat{A}$$

$D(z)$ is a 2x2 matrix whose entries are polynomials in z, the coefficients of the polynomials depend on $b_i, c_i, \bar{b}_i$ and $\bar{a}_{i,j}$.

Stability condition

Matrix D(z) for order 2

$$D(z) = \begin{pmatrix} 1 + \dfrac{z}{2} & z + \dfrac{z^2}{4} \\ 1 & 1 + \dfrac{z}{2} \end{pmatrix}$$

Stability condition

Matrix D(z) for order 3

$$D(z) = \begin{pmatrix} 1 + \frac{z}{2} + \beta_0 z^2 & z + \frac{z^2}{6} + \beta_1 z^3 \\ 1 + \frac{z}{6} & 1 + \frac{z}{2} + \beta_2 z^2 \end{pmatrix}$$

Coefficients β_i depend on $b_i, c_i, \bar{b}_i$ and $\bar{a}_{i,j}$

Stability condition

Matrix D(z) for order 4

$$D(z) = \begin{pmatrix} 1 + \frac{z}{2} + \frac{z^2}{24} + \beta_0 z^3 & z + \frac{z^2}{6} + \beta_1 z^3 + \beta_2 z^4 \\ 1 + \frac{z}{6} + \beta_3 z^2 & 1 + \frac{z}{2} + \frac{z^2}{24} + \beta_4 z^3 \end{pmatrix}$$

Coefficients β_i depend on b_i, c_i, $\bar{b}_i$ and $\bar{a}_{i,j}$

Stability condition

Matrix D(z) for order 5

$$D(z) = \begin{pmatrix} 1 + \frac{z}{2} + \frac{z^2}{24} + \beta_0 z^3 + \beta_1 z^4 & z + \frac{z^2}{6} + \frac{z^3}{120} + \beta_2 z^4 + \beta_3 z^5 \\ 1 + \frac{z}{6} + \frac{z^2}{120} + \beta_4 z^3 & 1 + \frac{z}{2} + \frac{z^2}{24} + \beta_5 z^3 + \beta_6 z^4 \end{pmatrix}$$

$\Rightarrow$ Taylor expansion of $\cos\left(\sqrt{-z}\right)$ and $\sin\left(\sqrt{-z}\right)$

Stability condition

Amplification factor

$$G(z) \;=\; \text{Spectral radius of } D(z)$$

CFL number is defined as the first time when $G(z) > 1$:

$$\text{CFL number} \;=\; \min_{z \leq 0} \{ \sqrt{-z} \;\text{ such that } G(z) > 1 \}$$

Stability condition is then given as:

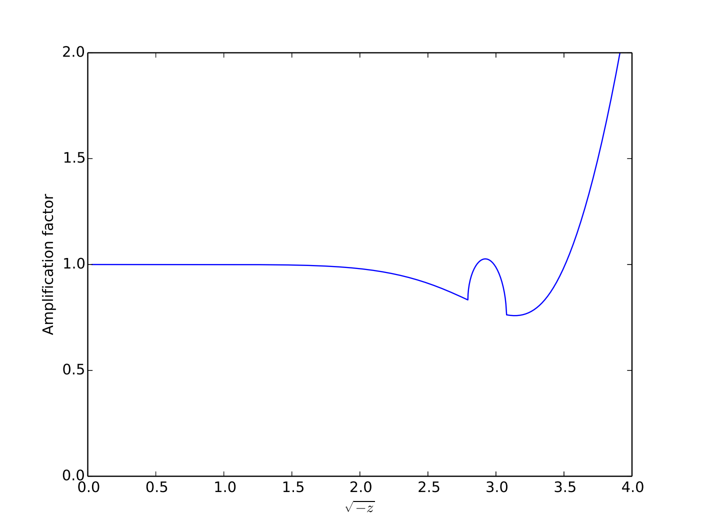
$$\Delta t \;\leq\; \frac{\text{CFL number}}{\sqrt{||A||_2}}$$

For $p = 2$, we have obtained

$$\text{CFL number} = 2$$

Numerical computation of the CFL

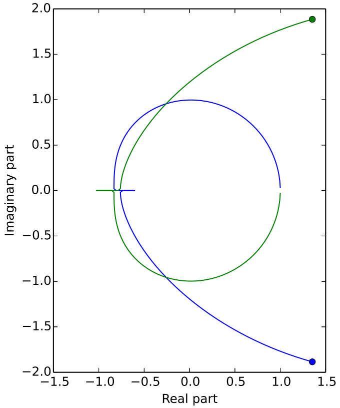
Amplification factor $G(z)$ versus $\sqrt{-z}$ for a 6-th order RKN scheme



Presence of a local maximum

Numerical computation of the CFL

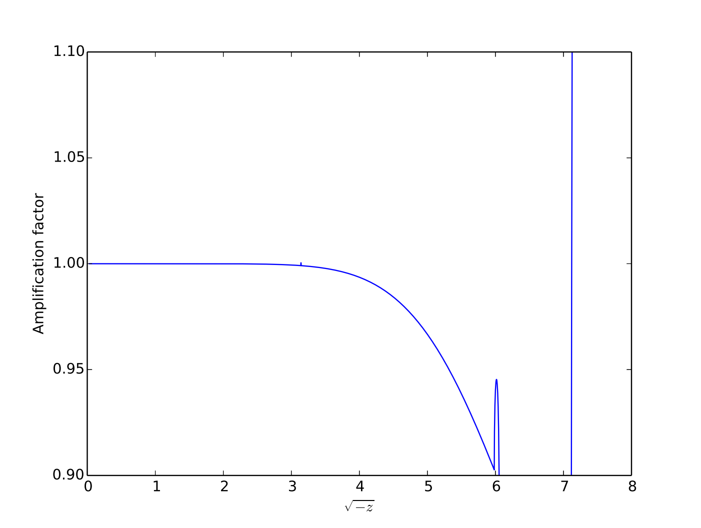
Trajectory of the two eigenvalues of $D(z)$



The local maximum occurs when the two eigenvalues of $D(z)$ are real

Numerical computation of the CFL

Amplification factor $G(z)$ versus $\sqrt{-z}$ for a 7-th order RKN scheme



Numerical computation of the CFL

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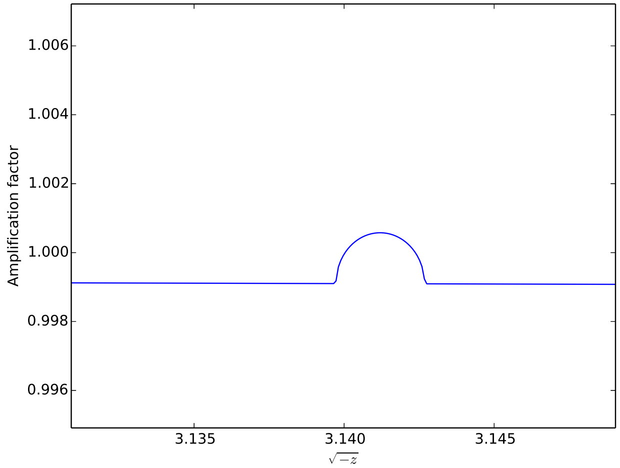


Numerical computation of the CFL

Main elements of the algorithm used to compute the CFL:

- Check that $G(-10^{-5}) <= 1$
- Decrease z by a variable step size Δz_k to capture the intersection of eigenvalues
- Compute a local maximum if we find z such that $G(z) > \max(G(z - \Delta z_k), G(z + \Delta z_{k-1}))$
- The final CFL number is found by bisection method when we have found z_0 and z_1 such that $G(z_0) \leq 1$ and $G(z_1) > 1$

Optimization with a minimal number of stages

- For order 3, 4, 5, 6, 7, 8, we are optimizing the families proposed in *Méthodes de Nyström pour l'équation différentielle y" = f(x, y)*, E. Hairer
- For order 10, we are optimizing the family proposed in *A one-step method of order 10 for y" = f(x, y)*, E. Hairer
- These families achieve the desired order with a minimal number of stages
- A large number of values for free parameters are tested, an optimization (the simplex method by Nelder and Mead) is performed for the best candidates

Order 3 (two stages)

$$c_0 = \alpha, \quad c_1 = \frac{2 - 3\alpha}{3 - 6\alpha}$$

$$b_0 = \frac{\frac{c_1}{2} - \frac{1}{3}}{c_0(c_1 - c_0)}, \quad b_1 = 1 - b_0$$

$$\bar{b}_0 = \frac{\frac{c_1}{2} - \frac{1}{6}}{c_1 - c_0}, \quad \bar{b}_1 = \frac{1}{2} - \bar{b}_0$$

$$\bar{a}_{1,0} = \frac{1}{6 b_1}$$

Order 3 (two stages)

α is a free parameter

$$c_0 = \alpha, \quad c_1 = \frac{2 - 3\alpha}{3 - 6\alpha}$$

An optimal CFL of 2.498 is obtained for

$$\alpha = \frac{3 - \sqrt{3}}{6}$$

Order 4 (three stages)

$$c_0 = \alpha, \quad c_1 = \frac{1}{2}, \quad c_2 = 1 - \alpha$$

$$b_0 = \frac{1}{6(1-2\alpha)^2}, \quad b_1 = 1 - 2b_0, \quad b_2 = b_0$$

$$\bar{b}_0 = b_0(1 - c_0), \quad \bar{b}_1 = b_1(1 - c_1), \quad \bar{b}_2 = b_2(1 - c_2)$$

$$\bar{a}_{1,0} = \frac{(1-4\alpha)(1-2\alpha)}{8(6\alpha(\alpha-1)+1)},$$

$$\bar{a}_{2,0} = 2\alpha(1-2\alpha), \quad \bar{a}_{2,1} = \frac{(1-2\alpha)(1-4\alpha)}{2}$$

Order 4 (three stages)

α is a free parameter

$$c_0 = \alpha, \quad c_1 = \frac{1}{2}, \quad c_2 = 1 - \alpha$$

An optimal CFL of 3.939 is obtained for

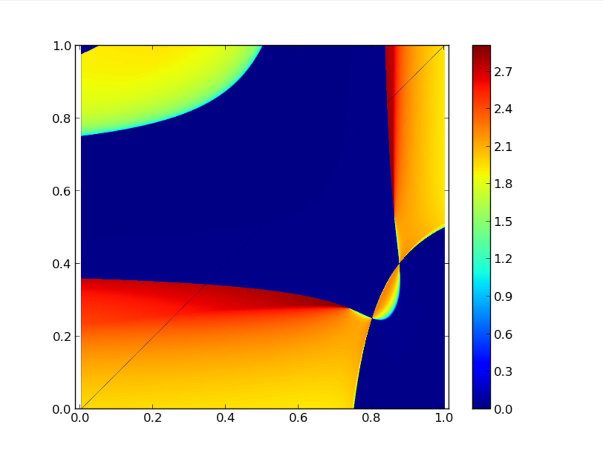
$$\alpha = \frac{1}{4\left(1 + \cos(\frac{\pi}{9})\right)}$$

Order 5 (four stages)

α and β are free parameters

$$c_0 = 0, \quad c_1 = \alpha, \quad c_3 = \beta, \quad c_2 = \frac{12 - 15(\alpha+\beta) + 20\alpha\beta}{15 - 20(\alpha+\beta) + 30\alpha\beta}$$

CFL number versus these two parameters:



Order 5 (four stages)

α and β are free parameters

$$c_0 = 0, \quad c_1 = \alpha, \quad c_3 = \beta, \quad c_2 = \frac{12 - 15(\alpha + \beta) + 20\alpha\beta}{15 - 20(\alpha + \beta) + 30\alpha\beta}$$

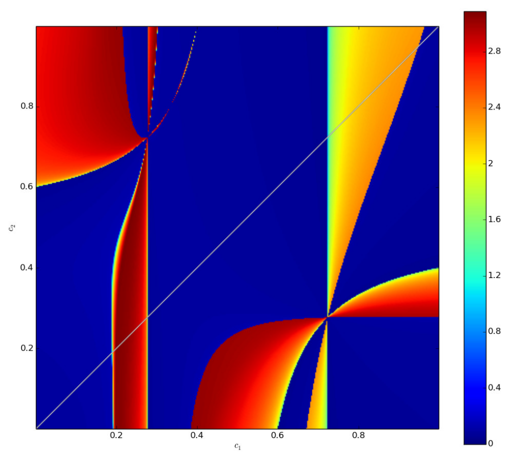
An optimal CFL of 2.908 is obtained for

$$\alpha = \frac{4}{11 - \sqrt{16\sqrt{10} - 39}},$$

$$\beta = \frac{165\alpha^2 - 195\alpha + 50 + \sqrt{5\,(45\alpha^4 + 90\alpha^3 - 105\alpha^2 + 36\alpha - 4)}}{225\alpha^2 - 240\alpha + 60}$$

Order 6 (5 stages)

c_1 and c_2 are free parameters
CFL number vs these parameters:



Order 6 (5 stages)

c_1 and c_2 are free parameters

$$c_0 = 0, \quad c_4 = 1$$

$$c_3 = \frac{\frac{1}{30} - \frac{1}{20}(c_1 + c_2) + \frac{1}{12}c_1 c_2}{\frac{1}{20} - \frac{1}{12}(c_1 + c_2) + \frac{1}{6}c_1 c_2}.$$

An optimal CFL of 3.089 is obtained for

$$c_1 \approx 0.22918326, \quad c_2 \approx 0.5$$

Order 7 (7 stages)

$\alpha_0, \alpha_1, \alpha_2, \alpha_3$ are four free parameters

$$c_0 = 0, \quad c_1 = \alpha_0, \quad c_2 = \alpha_1, \quad c_3 = \alpha_2, \quad c_4 = \alpha_3$$

$$c_5 = \frac{-\frac{1}{7} + \frac{\sigma_1^c}{6} - \frac{\sigma_2^c}{5} + \frac{\sigma_3^c}{4} - \frac{\sigma_4^c}{3}}{-\frac{1}{6} + \frac{\sigma_1^c}{5} - \frac{\sigma_2^c}{4} + \frac{\sigma_3^c}{3} - \frac{\sigma_4^c}{2}}, \quad c_6 = 1$$

An optimal CFL of 7.0875 is obtained for:

$$\alpha_0 = 0.110451398065702, \quad \alpha_1 = 0.173816271367107$$

$$\alpha_2 = 0.459433163929695, \quad \alpha_3 = 0.652002232653235$$

Order 8 (8 stages)

$\alpha_0, \alpha_1, \alpha_2, \alpha_3$ are four free parameters

$$c_0 = 0, \quad c_1 = \frac{\alpha_0}{2}, \quad c_2 = \alpha_0, \quad c_3 = \alpha_1, \quad c_4 = \alpha_2, \quad c_5 = \alpha_3$$

$$c_6 = \frac{-\frac{1}{8} + \frac{\sigma_1^c}{7} - \frac{\sigma_2^c}{6} + \frac{\sigma_3^c}{5} - \frac{\sigma_4^c}{4} + \frac{\sigma_5^c}{3}}{-\frac{1}{7} + \frac{\sigma_1^c}{6} - \frac{\sigma_2^c}{5} + \frac{\sigma_3^c}{4} - \frac{\sigma_4^c}{3} + \frac{\sigma_5^c}{2}}, \quad c_7 = 1$$

An optimal CFL of 7.8525 is obtained for:

$$\alpha_0 = 0.135294127286225, \quad \alpha_1 = 0.240153083847448$$

$$\alpha_2 = 0.453046953126355, \quad \alpha_3 = 0.695039606659698$$

Order 10 (11 stages)

There are four free parameters (b_1, b_3, b_4, r_5) and a permutation. r_5 defined as

$$\sum_{i=1}^{s-1} b_i c_i^k \sum_{j=1}^{i-1} \bar{a}_{i,j}\, c_j^5 = r_5$$

Gauss-Lobatto nodes defined as:

$$\begin{cases} \gamma_1 = \dfrac{1}{2}\left(1 - \sqrt{\dfrac{7+2\sqrt{7}}{21}}\right), \quad \gamma_4 = 1 - \gamma_1 \\ \gamma_2 = \dfrac{1}{2}\left(1 - \sqrt{\dfrac{7-2\sqrt{7}}{21}}\right), \quad \gamma_3 = 1 - \gamma_2 \end{cases}$$

c_4, c_5, c_6, c_7 to choose among these four Gauss-Lobatto nodes (24 permutations possible)

Order 10 (11 stages)

There are four free parameters (b_1, b_3, b_4, r_5) and a permutation. An optimal CFL of 4.7527 is obtained for

$$(c_4, c_5, c_6, c_7) = (\gamma_4, \gamma_3, \gamma_1, \gamma_2) \, .$$

$$r_5 = 0.0021632268153138$$

and does not depend on b_1, b_3, b_4 that can be chosen as:

$$b_1 = 0, \quad b_3 = -0.1, \quad b_4 = 0$$

Efficiency of the optimized schemes

s being the number of stages, the efficiency is given as:

$$\text{Efficiency} = \frac{\text{CFL number}}{2s}$$

Efficiency obtained for the different orders:

Order	2	3	4
Efficiency	100 %	62.5 %	65.7 %

Order	5	6	7	8	10
Efficiency	36.4 %	30.9 %	50.6 %	49.1 %	21.6 %

Non-linear Maxwell's equations

$$
\begin{cases}
\dfrac{\varepsilon_\infty}{c^2}\dfrac{\partial^2 E}{\partial t^2} + \dfrac{1}{c^2}\dfrac{\partial^2}{\partial t^2}\left(\sum_k P_k\right) + \text{curl}(\text{curl}E) + \dfrac{\gamma}{c^2}\dfrac{\partial^2}{\partial t^2}\left(|E|^2 E\right) \; = \; 0 \\
\dfrac{1}{{\omega_k}^2}\dfrac{\partial^2 P_k}{\partial t^2} + P_k \; = \; \alpha_k \, E \\
E(x,y,z,t=0) = \dfrac{\partial E}{\partial t}(x,y,z,t=0) = 0 \\
E(x,y,z=0,t) = \text{ Given impulsion}
\end{cases}
$$

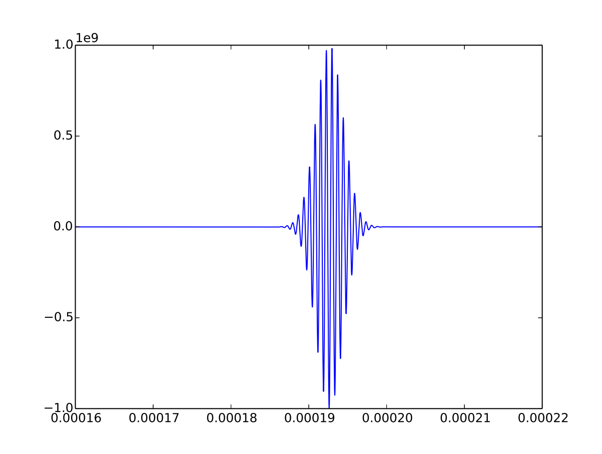
$\varepsilon_\infty, c, \gamma, \alpha_k, \omega_k$ physical constants (silica is chosen)

Simulation parameters

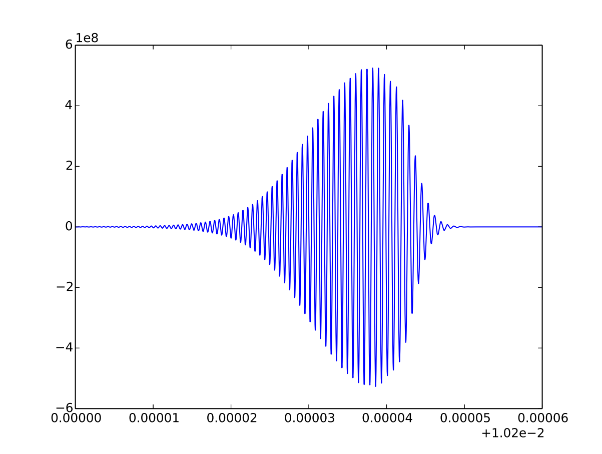
- 1-D finite elements $\mathbb{Q}_{10}$
- Domain $[0, 1.5 \cdot 10^{-4}]$ (more than 200 wavelengths) with 250 cells
- Circular polarization, $\lambda_0 = 1.053 \mu m$
- Optical period $T_0 = 3.5 \cdot 10^{-15} s$
- Final time $T_{\text{max}} = 5 \cdot 10^{-11} s$
- Gaussian impulsion of width $60 \cdot 10^{-15} s$

Simulation parameters

Solution at $t = 10^{-12}s$



Solution at the final time $t = 5 \cdot 10^{-11} s$



Numerical results

Computation time needed to reach an error of 1 % :

Order	2	3	4	5	6	7	8	10
Time	1 240 s	186s	**41s**	54s	63s	44s	47s	106s

For orders $\geq$ 5, the error is below 10^{-5}, the CFL is reached.

Numerical results

Computation time needed to reach an error of 10^{-4} :

Order	2	3	4	5	6	7	8	10
Time	14 164s	647s	129s	54s	63s	**44s**	47s	106s

For orders ≥ 5, the error is below 10^{-5}, the CFL is reached.

Prospects

- Optimization with additional stages
- Continuous interpolants

Thanks for your attention