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Chapter 1
Optimized High Order Explicit Runge-Kutta-Nyström Schemes

Marc Duruflé and Mamadou N'diaye

Abstract In this paper, we are interested in solving a non-linear ordinary differential equation (ODE) of the type:

$$y'' = f(t,y).$$

For this ODE, high-order Runge-Kutta-Nyström have been proposed (see [1]). They are attractive because they are explicit, one-step methods and can be applied to a non-linear operator f. In [2], the stability condition (CFL) associated with these schemes have been studied for order 3, 4 and 5. In this paper, we extend this study for higher orders, and propose optimized coefficients with respect to the stability condition. With the obtained optimal CFL, these schemes are of practical interest for stiff problems where the stability condition is restrictive. These schemes are used for solving non-linear Maxwell's equations in 1-D:

$$\frac{\varepsilon_\infty}{c^2}\frac{\partial^2 E}{\partial t^2} + \mathrm{curl}(\mathrm{curl} E) + \frac{\gamma}{c^2}\frac{\partial^2}{\partial t^2}\left(|E|^2 E\right) \;=\; 0.$$

The non-linearity is an instantaneous Kerr effect, where γ is the non-linear susceptibility. High-order finite elements are used in space to obtain the ODE to be solved.

We are interested in the following ordinary differential equation (ODE)

$$\begin{cases} y''(t) = f(t,y(t)), & \forall t > 0, \\ y(0) = y_0, \\ y'(0) = y_0'. \end{cases}$$

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The unknown y is vectorial, its size is equal to the number of the degrees of freedom of the system, the functional f is known and describes the dynamics of the system. This kind of ordinary differential equation appears naturally in mechanical systems when the damping terms are neglected, and also in non-linear wave equation. In order to solve this kind of ODE, Runge-Kutta-Nyström schemes have been introduced by Hairer ([1]). A RKN (Runge-Kutta-Nyström) scheme is a one-step scheme, it computes a discrete sequence y_n and y'_n, which are approximations of y and y' at time $t_n = n\Delta t$. Δt is called the time step, it is assumed constant in this paper. A step of the RKN scheme is performed as follows:

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

k_i are intermediate vectors used to compute y_{n+1} and y'_{n+1}. The coefficients $\bar{a}_{i,j}, c_i, b_i, \bar{b}_i$ must satisfy the so-called order conditions such that the scheme is of order r (see [1] for a detailed description of order conditions). When it is not mentioned, the subscripts i and j vary between 0 and $s-1$ where s is the number of stages of the scheme. In this paper, only explicit schemes will be studied, the matrix $\bar{A}$ (associated with coefficients $\bar{a}_{i,j}$) is lower triangular, that is to say:

$$\bar{a}_{i,j} = 0, \text{ if } j \geq i.$$

Remark 1.1. If we consider a classical Runge-Kutta scheme of order r (with arrays A, b and c), it is sufficient to take

$$\bar{A} = A^2, \quad \bar{b} = A^T b,$$

to obtain a Runge-Kutta-Nyström scheme of order r.

1.1 Stability condition

The stability analysis is conducted for a linear functional f, which is then replaced by a matrix A:

$$f(t,y) = Ay.$$

By replacing A by its symbol $\hat{A}$ (which will be equal to an eigenvalue of A), a step of RKN scheme can be written as:

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

where $D(\Delta t^2 \hat{A})$ is a 2x2 matrix depending on coefficients $\bar{a}_{i,j}, b_i, c_i, \bar{b}_i$. Let us note:

$$z = \Delta t^2 \hat{A}.$$

The vector w_n is equal to:

$$w_n = \frac{y'_n}{\Delta t \hat{A}}.$$

The RKN scheme is equal to:

$$\begin{cases} \Delta t^2 k_i = z y_n + c_i z^2 w_n + z \sum_j \bar{a}_{i,j} \Delta t^2 k_j, \\ y_{n+1} = y_n + z w_n + \sum_i \bar{b}_i \Delta t^2 k_i, \\ w_{n+1} = w_n + \frac{1}{z} \sum_i b_i \Delta t^2 k_i. \end{cases}$$

From these relations, it can be remarked that the entries of the 2x2 matrix $D(z)$ are polynomials in z. The amplification factor $G(z)$ is defined as:

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

The stability condition is computed numerically by searching the first z such that

$$G(z) > 1.$$

The square root of this first z is defined as the CFL number:

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

1.2 Numerical method to compute the CFL

The eigenvalues of the 2×2 matrix $D(z)$ are directly computed as:

$$\lambda(D(z)) = \frac{\text{trace}(D(z)) \pm \sqrt{\text{trace}(D(z))^2 - 4 \det(D(z))}}{2}.$$

The amplification factor $G(z)$ is the maximal modulus of these two eigenvalues. From the computation of this amplification factor, the algorithm used to compute the CFL is detailed in table 1.1. The computation of local maxima z_m and of the final z such that $G(z) = 1 + \varepsilon$ is performed by using a bisection method. The first float z_0 is chosen small (we have chosen $z_0 = -10^{-5}$), this first verification is needed because it happens that the amplification factor is decreasing at the origin, ie:

$$G'(0) < 0.$$

Hence for very small negative values of z, this amplification factor will be greater than one, leading to an unstable scheme. In this case, the time scheme is therefore unconditionnally unstable. The step Δz_k is chosen in an interval (we have selected $10^{-5} \leq \Delta z_k \leq 1$) such that the intersection of the two complex conjugate eigenvalues

Table 1.1 Algorithm used to compute the CFL number of RKN schemes

If $G(z_0) > 1+\varepsilon$
    return 0
End If
$z = z_0$
While $G(z) <= 1+\varepsilon$
    Adapt Δz_k such that any intersection of roots is not missed
    If $G(z) > \max(G(z-\Delta z_k), G(z+\Delta z_{k-1}))$ Then
        Compute the local maximum z_m in the interval $[z-\Delta z_k, z+\Delta z_{k-1}]$
        If $G(z_m) > 1$
            $z = z_m$
            Terminate the main while loop
        End If
    End If
    $z = z - \Delta z_k$
End while
Compute z such that $G(z) = 1+\varepsilon$ in the interval $[z-\Delta z, z]$ by bisection method
Return z

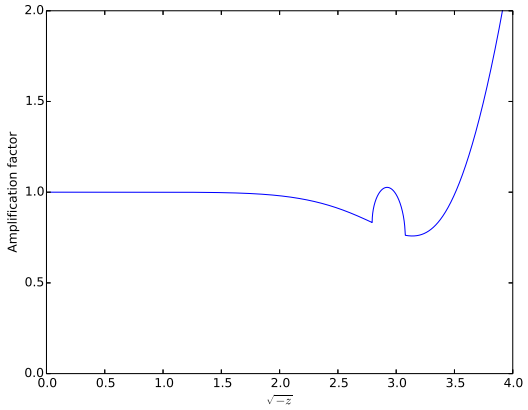

Fig. 1.1 Amplification factor $G(z)$ versus $\sqrt{-z}$ for a 6-th order RKN scheme, with the two free parameters equal to 0.0816464646464646 and 0.968757575757576.

is not missed. This intersection occurs when the two eigenvalues get close to the real axis or when they already lie in the real axis. In the figure 1.1, the amplification factor is displayed for a 6th order Runge-Kutta-Nystrom method. In this case, the CFL is equal to 2.858 because of the presence of a local maxima above 1. It has been observed that usually the first local maximum (if present) occurs around $\sqrt{-z} \approx \pi$, the second maximum would occur if present around 2π, etc. In the figure 1.2, we have displayed the trajectory of the two eigenvalues of $D(z)$ for $\sqrt{-z} \in [-4,0]$. These two eigenvalues start from the point $(1,0)$ they describe an approximate circle to reach a point close to $(-1,0)$. Then they move away from each other in the

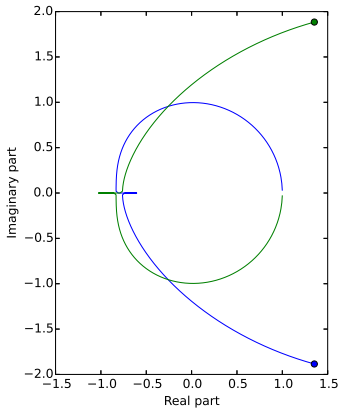

Fig. 1.2 Trajectory of the two eigenvalues of $D(z)$ for $\sqrt{-z} \in [0,4]$ for a 6-th order RKN scheme, with the two free parameters equal to 0.0816464646464646 and 0.968757575757576.

real axis, one reaches the local maximum, and the two eigenvalues get back until reaching another intersection in the real axis. Finally, they are describing a kind of hyperbole in the complex plane. With a variable Δz_k, we are able to compute quickly the CFL with a reasonable number of evaluations of the amplification factor. Finally, ε is taken equal to $2 \cdot 10^{-13}$ for a double precision computation.

1.3 Optimization with a minimal number of stages

In this section, coefficients of Runge-Kutta schemes are optimized to maximize the CFL number, we consider here only schemes with a minimal number of stages (s).

1.3.1 Order 2 ($s = 1$)

For example, to obtain a second-order scheme, it is sufficient to satisfy

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

Therefore, a one-stage scheme can be obtained:

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

this scheme can be written as:

$$\begin{cases} k_0 \;=\; f\left(t^n + \dfrac{\Delta t}{2},\, y_n + \dfrac{\Delta t}{2} y'_n\right), \\ y_{n+1} \;=\; y_n + \Delta t\, y'_n + \dfrac{\Delta t^2}{2} k_0, \\ y'_{n+1} \;=\; y'_n + \Delta t\, k_0. \end{cases}$$

This scheme only needs an evaluation of f (i.e. a matrix-vector product if f is linear), its cost is equivalent to the classical second-order scheme presented in the first section. When f is linear (replaced by a matrix A), the stability condition of this scheme is:

$$\Delta t \;\leq\; \frac{2}{\sqrt{||A||_2}}.$$

This is exactly the same CFL as the classical second-order scheme:

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

Therefore, the second-order Runge-Kutta-Nyström (RKN) scheme is optimal.

1.3.2 Order 3 ($s = 2$)

A third-order RKN scheme with 2 stages is given as:

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

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

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

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

α is a free parameter, an optimal CFL of 2.498 is obtained for

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

1.3.3 Order 4 ($s = 3$)

A fourth-order RKN scheme with 3 stages is given as:

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

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

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

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

α is a free parameter an optimal CFL of 3.939 is obtained for

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

1.3.4 Order 5 ($s = 4$)

A family with two parameters is given in [3]. An optimal CFL of 2.908 is obtained for

$$\alpha = \frac{4}{11+\sqrt{16\sqrt{10}-39}}, \quad \beta = \frac{165\alpha^2-195\alpha+50-\sqrt{5\,(45\alpha^4+90\alpha^3-105\alpha^2+36\alpha-4)}}{225\alpha^2-240\alpha+60}.$$

The c_i are given as

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

For orders 3, 4, 5, we have found the same optima as in [2]. From orders 6, the optima are new and only computed numerically.

1.3.5 Order 6 ($s = 5$)

A family with one parameter is given in [3]. An optimal CFL of 3.089 is obtained for

$$\alpha \approx 0.22918326$$

The c_i are given as

$$c_0 = 0, \quad c_1 = \alpha, \quad c_2 = \frac{1}{2}, \quad c_3 = 1-\alpha, \quad c_4 = 1.$$

Another family with two parameters can also be constructed. The optimal CFL is also equal to 3.089 for this family.

1.3.6 Order 7 ($s = 7$)

A family with four free parameters is given in [3]. A nearly optimal CFL of 7.0875 is obtained with the following parameters:

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

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

The c_i are given as

$$c_0 = 0, \quad c_1 = \alpha_0, \quad c_2 = \alpha_1, \quad c_3 = \alpha_2, \quad c_4 = \alpha_3, \quad c_5 = \frac{-\frac{1}{7} + \frac{\sigma_1^c}{6} - \frac{\sigma_2^c}{5} + \frac{\sigma_3^c}{4} - \frac{\sigma_4^c}{3}}{-\frac{1}{6} + \frac{\sigma_1^c}{5} - \frac{\sigma_2^c}{4} + \frac{\sigma_3^c}{3} - \frac{\sigma_4^c}{2}}, \quad c_6 = 1.$$

1.3.7 Order 8 ($s = 8$)

A family with four free parameters is given in [3]. A nearly optimal CFL of 7.8525 is obtained with the following parameters

$$\alpha_0 = 0.135294127286225, \quad \alpha_1 = 0.24015308384744$$

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

The c_i are given as

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

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

1.3.8 Order 10 ($s = 11$)

A family is detailed in [4] with four free parameters (b_0, b_2, b_3, r_5) and a permutation (to choose among 24 permutations). r_5 is an additional free parameter that we have

recognized during the construction of the family, it is defined as

$$r_5 = \sum_{i=0}^{s-1} b_i c_i^3 \sum_{j=0}^{i-1} \bar{a}_{ij} c_j^5.$$

We denote the Gauss-Lobatto nodes $\gamma_1, \gamma_2, \gamma_3, \gamma_4$:

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

The CFL is optimal for the following permutation

$$(c_3, c_4, c_5, c_6) = (\gamma_4, \gamma_3, \gamma_1, \gamma_2).$$

The other c_i are given as

$$c_0 = 0, \quad c_2 = \frac{c_4(3c_4 - 5c_3)}{5c_4 - 10c_3}, \quad c_1 = \frac{c_2}{2}, \quad c_7 = c_3, \quad c_8 = c_2, \quad c_9 = 0, \quad c_{10} = 1.$$

For this permutation, we have obtained a nearly optimal CFL of 4.7527 with the following parameter

$$r_5 = 0.0021632268153138$$

The CFL is maximal for this permutation, it is strictly lower for other permutations. For other parameters, we can choose the values proposed by Hairer:

$$b_0 = 0, \quad b_2 = -0.1, \quad b_3 = 0,$$

since the CFL does not depend on these three parameters.

1.3.9 Efficiency

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

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

In the table 1.2, we have written the efficiency obtained for the different orders. We see here that the orders 7 and 8 are attractive since they have a correct efficiency (close to 50 %). We think that we can achieve an efficiency that tends to 100 % for high-order schemes by adding stages (the number of stages tending to the infinity).

Table 1.2 Efficiency for optimized Runge-Kutta-Nyström schemes for different orders

Order	2	3	4	5	6	7	8	10
Efficiency	100 %	62.5 %	65.7 %	36.4 %	30.9 %	50.6 %	49.1 %	21.6 %

1.3.10 Numerical results

We apply the RKN schemes for solving non-linear Maxwell's equations in 1-D, namely:

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

Here the electric field is searched as a complex field:

$$E = E_x + iE_y,$$

where E_x and E_y are x and y-components of the electric field. P_k are the polarizations, $\varepsilon_\infty, c, \gamma, \alpha_k, \omega_k$ are physical constants. We take the constants corresponding to silica:

$$\varepsilon_\infty = 1,\ c = 299792458,\ \alpha_0 = 0.6961663,\ \alpha_1 = 0.4079426,\ \alpha_2 = 0.8974794$$

$$\omega_0 = \frac{2\pi c}{0.0684043\cdot 10^{-6}},\ \omega_1 = \frac{2\pi c}{0.1162414\cdot 10^{-6}},\ \omega_2 = \frac{2\pi c}{9.896161\cdot 10^{-6}},\ \gamma = 10^{-33}.$$

The impulsion is centered at $\lambda_0 = 1.053\mu m$ with a Gaussian envelope and a circular polarization:

$$\text{Given impulsion } = E_0\, e^{-\frac{1}{2}\left(\frac{t-T\max}{\tau}\right)^2} e^{i\omega_L t}$$

where

$$\omega_L = \frac{2\pi c}{1.053\cdot 10^{-6}},\ T\max = 6\cdot 10^{-14},\ \tau = \frac{2}{2\sqrt{2\log 2}}\cdot 10^{-14},\ E_0 = 10^9.$$

The computational domain is the 1-D interval $\Omega = [0, 1.5\cdot 10^{-4}]$, a Neumann boundary condition is set on the right extremity. 1-D finite elements are used to discretize these equations:

$$E \in V_h = \left\{ u \in H^1(\Omega) \text{ such that } u|_{[z_i, z_{i+1}]} \in \mathbb{Q}_{10} \right\}$$

where $(z_i)_{0 \leq i \leq 250}$ are a regular subdivision of the computational domain Ω. The mesh contains 250 elements (i.e. 2501 degrees of freedom), the numerical error due to the space discretization is around 10^{-6} (the domain contains more than 200 wavelengths). After space discretization, the system can be written in the form

$$y'' = f(t, y)$$

by using the displacement as unknown

$$D = \varepsilon_\infty E + \left(\sum_k P_k \right) + \gamma |E|^2 E.$$

The electric field E is recovered from D by solving the non-linear equation written above for each degree of freedom. This equation is solved with a Newton's method, two or three iterations are sufficient to get machine precision accuracy. Gauss-Lobatto points are used both for interpolation (for the discretization of V_h) and quadrature, leading to a diagonal mass matrix. As a result the computation of $f(t, y)$ is explicit, it does not involve any solution of a linear system. The electric field is propagated from $t = 0$ until $t = 5 \cdot 10^{-11}$, in the figure 1.3, the solution is plotted at two different times. The solution at the final time $t = 5 \cdot 10^{-11}$ is compared with a reference solution computed with a small time step (with tenth order RKN scheme). We try to reach an error of 0.01 % for each scheme in order to compare the efficiency. In the table 1.3, the computational time needed to obtain this accuracy is

Table 1.3 Computational time needed to reach an accuracy of 0.01% for different orders of RKN schemes.

Order	3	4	5	6	7	8	10
Time	730s	144s	60.9s	70.8s	43.2s	44.8s	103s
Error	$1.0 \cdot 10^{-4}$	$1.0 \cdot 10^{-4}$	$1.5 \cdot 10^{-6}$	$7.3 \cdot 10^{-7}$	$6.5 \cdot 10^{-7}$	$1.1 \cdot 10^{-7}$	$2.0 \cdot 10^{-10}$

given for each optimized RKN scheme. The simulations are performed in parallel on 20 cores on an Intel-Xeon (2 Dodeca-core Haswell E5-2680, 2.5 Ghz). From order 5, we are using the maximal time step allowed (the CFL becomes quite restrictive), that's why the error is below 0.01 % from these orders. We see that RKN schemes of order 7 or 8 are the most efficient for this problem while order 10 is not very efficient because of its small CFL.

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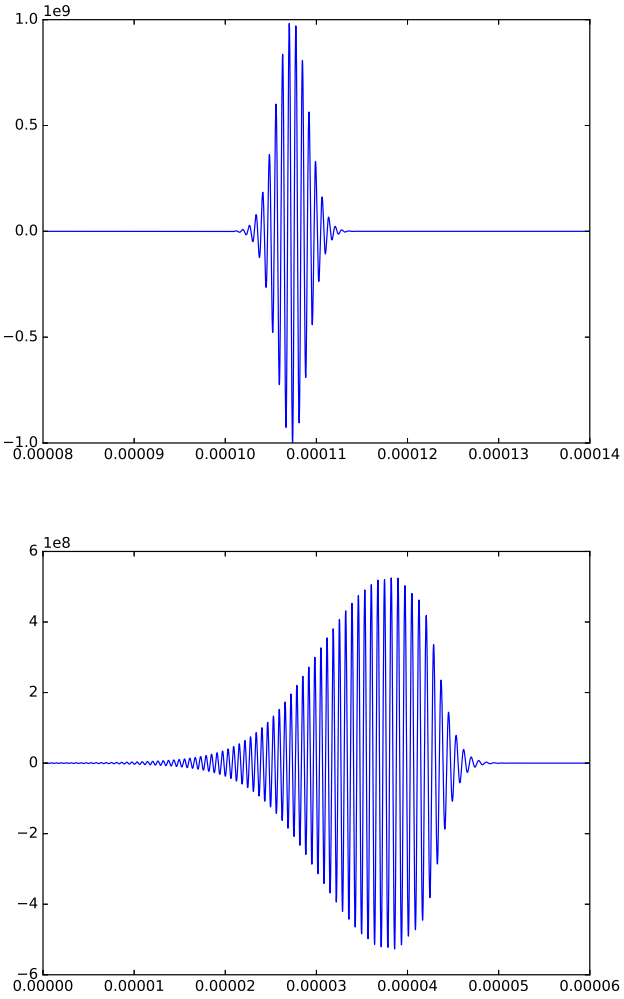

Fig. 1.3 Electric field E_x for $t = 10^{-12}$ and $t = 5 \cdot 10^{-11}$

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