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HIGHLY-ACCURATE SCHEMES FOR 3D MAXWELL EQUATIONS WITH LORENTZ MEDIA ON THE BASIS OF ALTERNATE DIRECTION IMPLICIT TIME-STEPPING ALGORITHMS

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N.A. Zaitsev, I.L. Sofronov. *Highly accurate schemes for 3D Maxwell equations with Lorentz media on the basis of alternate direction implicit time stepping algorithms.*

Abstract. An algorithm for computation of 3D unsteady diffraction problems for Maxwell equations in Lorentz media is suggested. The algorithm is based on the alternate direction implicit scheme and pseudospectral approximation of spatial derivatives. Order of approximation in time is equal to 2, 4 or 6. The Lorentz dispersion is taken into account by means of introducing additional auxiliary unknowns in the first order governing system. Computational cost of the algorithm is of order $O\left(N^3\right)\log N$ operations per time step, where N is a number of grid points in one direction.

Н.А. Зайцев, И.Л. Софронов. *Схемы высокой точности для трёхмерных уравнений Максвелла в средах Лоренца базирующиеся на неявных схемах переменных направлений.*

Аннотация. Предложен алгоритм расчета трехмерной нестационарной задачи дифракции, описываемой уравнениями Максвелла в лоренцевых средах. Алгоритм основан на неявной схеме переменных направлений с псевдоспектральной аппроксимацией пространственных производных. Порядок интегрирования по времени может составлять 2, 4, 6. Лоренцевская дисперсия учитывается путем введения вспомогательных неизвестных в исходную систему уравнений первого порядка. Вычислительная сложность алгоритма оценивается величиной $O\left(N^3\right)\log N$ операций на шаг по времени, где N — число точек сетки по одному направлению.

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Introduction

A numerical scheme for solving 3D Maxwell equations by Alternate Direction Implicit time-stepping algorithms (ADI) has been proposed in [4]. The finite-difference scheme provides unconditionally stable time stepping by using inversion of tri-diagonal operators in each direction. It includes introducing a time level n + 1/2 between the adjacent time levels n and n + 1, and has second order accuracy in both time and space.

Here we also apply the ADI scheme for 3D Maxwell equations and develop it for the case of so-called Lorentz media. Next we enhance order of integration with respect to time for ADI schemes and consider spectral approach for approximation of spatial derivatives. As a result we obtain a high-order algorithm for solution of extended equation Maxwell system in 2D with $O\left(N^3\right)\log N$ operations per time level; N is number of grid points in one direction.

§1. Central symmetric ADI for Lorentz media

This section presents the ADI method for Lorentz media. This is a central-difference time stepping scheme having the second order accuracy in time.

We consider Maxwell's equations:

$$\frac{\partial \vec{D}}{\partial t} = \nabla \times \vec{H}, \tag{1.1}$$

$$\frac{\partial \vec{B}}{\partial t} = -\nabla \times \vec{E}, \tag{1.2}$$

where

$$\vec{B} = \mu \vec{H},$$
$$\vec{D} = \varepsilon_0 \varepsilon_\infty \vec{E} + \varepsilon_0 \vec{P},$$
$$\vec{P} = \sum_{p=1}^{P} \vec{P}_p, \tag{1.3}$$
$$\vec{P}_p(t) = \int_0^\infty \vec{E}(t-s)\chi_p(s)ds,$$

$\vec{P}$ is electric polarization vector, P is the number of Lorentz pole pairs, ε is electrical permittivity, ε_0 is free-space permittivity (8.854×10^{-12} farads/meter), ε_∞ is the relative permittivity at infinite frequency (dimensionless scalar).

Lorentz media are characterized by a set of frequency-domain susceptibility functions [1]

$$\hat{\chi}_p(\omega) = (\varepsilon_s - \varepsilon_\infty)\frac{G_p\omega_p^2}{\omega_p^2 + 2i\alpha_p\omega - \omega^2}, \quad p = 1,\dots,P;$$
$$\sum_{p=1}^{P} G_p = 1. \tag{1.4}$$

The real-valued time-domain susceptibility functions $\chi_p(t)$ are obtained by the inverse Fourier transform of (1.4):

$$\chi_p(t) = \gamma_p e^{-\alpha_p t}\sin(\beta_p t), \tag{1.5}$$

where

$$\beta_p = \sqrt{\omega_p^2 - \alpha_p^2},$$
$$\gamma_p = (\varepsilon_s - \varepsilon_\infty)\frac{G_p\omega_p^2}{\beta_p}.$$

Two limitations for the time step follow from (1.5):

$$\tau < \frac{\pi}{\beta_p}, \tag{1.6}$$

and

$$\tau < \frac{1}{\alpha_p}. \tag{1.7}$$

Note that $\chi_p(t) = \mathrm{Re}\left(\tilde{\chi}_p(t)\right)$, where

$$\tilde{\chi}_p(t) = -i\gamma_p e^{(i\beta_p - \alpha_p)t}. \tag{1.8}$$

Then

$$\tilde{P}_p(t) = \int_0^\infty \vec{E}(t-s)\tilde{\chi}_p(s)ds = \int_0^\infty \vec{E}(t-s)a_p e^{b_p s}ds \tag{1.9}$$

where

$$a_p = -i\gamma_p,$$
$$b_p = -\alpha_p + i\beta_p,$$

and

$$\vec{P}_p(t) = \mathrm{Re}\left(\tilde{P}_p(t)\right),$$
$$\tilde{D} = \varepsilon_0\varepsilon_\infty\vec{E} + \varepsilon_0\tilde{P},$$
$$\vec{D} = \mathrm{Re}\left(\tilde{D}\right).$$

Let's consider the recursive convolution method for Lorentz media. Using the notation $t^n = n\tau$, where τ is the time step, $D^n = \vec{D}\left(t^n\right)$, $E^n = \vec{E}\left(t^n\right)$,

$\tilde{D}^n = \tilde{D}\left(t^n\right)$, $\tilde{P}^n = \tilde{P}\left(t^n\right)$ Eq. (1.3) can be written in the time-discrete form as follows

$$\tilde{D}^n = \varepsilon_0 \varepsilon_\infty E^n + \varepsilon_0 \tilde{P}^n,$$

$$\tilde{P}^n = \sum_{p=1}^{P} \tilde{P}_p{}^n,$$

$$\tilde{P}_p{}^n = \int_0^\infty \vec{E}(t^n - s)\tilde{\chi}_p(s)ds = \sum_{m=1}^{\infty} \int_{t^{m-1}}^{t^m} \vec{E}(t^n - s)\tilde{\chi}_p(s)ds = \sum_{m=1}^{\infty} \int_{t^{m-1}}^{t^m} f(s)\tilde{\chi}_p(s)ds,$$

where $f(s) = \vec{E}(t^n - s)$. Using the piecewise-linear approximation of $f(s)$ for each m we obtain

$$f(s) \approx f(t^{m-1}) + \frac{f(t^m) - f(t^{m-1})}{\tau}(s - t^{m-1}) = C_m^0 + C_m^1 s \tag{1.10}$$

where

$$C_m^1 = \frac{f(t^m) - f(t^{m-1})}{\tau} = \frac{\vec{E}(t^n - t^m) - \vec{E}(t^n - t^{m-1})}{\tau} = \frac{E^{n-m} - E^{n-m+1}}{\tau} = \Delta^{n-m+1/2},$$

$$C_m^0 = f(t^{m-1}) - \frac{f(t^m) - f(t^{m-1})}{\tau} t^{m-1} = E^{n-m+1} - C_m^1 t^{m-1}.$$

$$\int_{t^{m-1}}^{t^m} f(s)\tilde{\chi}_p(s)ds = \int_{t^{m-1}}^{t^m} f(s) a_p e^{b_p} ds$$
$$= a_p C_m^0 \int_{t^{m-1}}^{t^m} e^{b_p} ds + a_p C_m^1 \int_{t^{m-1}}^{t^m} s e^{b_p} ds. \tag{1.11}$$

$$\int e^{bx} dx = \frac{1}{b} e^{bx}, \quad \int x e^{bx} dx = \frac{1}{b}\left[x e^{bx} - \frac{1}{b} e^{bx} \right],$$

hence

$$\int_{t^{m-1}}^{t^m} f(s)\tilde{\chi}_p(s)ds \approx a_p C_m^0 \left(\frac{1}{b_p} e^{b_p s} \right)\Bigg|_{s=t^{m-1}}^{s=t^m} + a_p C_m^1 \left(\frac{1}{b_p}\left[s e^{b_p s} - \frac{1}{b_p} e^{b_p s} \right] \right)\Bigg|_{s=t^{m-1}}^{s=t^m}$$

$$= \frac{a_p}{b_p} e^{b_p t^{m-1}} \left[E^{n-m+1} \varphi_p + \Delta^{n-m+1/2} \psi_p \right],$$

where

$$\Delta^{n-m+1/2} = \frac{E^{n-m} - E^{n-m+1}}{\tau}$$

depends on time. The values

$$\varphi_p = e^{b_p \tau} - 1$$

and

$$\psi_p = \tau e^{b_p \tau} - \frac{\varphi_p}{b_p}$$

don't depend on time. Then

$$\tilde{P}_p^{\,n} = \frac{a_p}{b_p} \sum_{m=1}^{\infty} e^{b_p t^{m-1}} \left[E^{n-m+1} \varphi_p + \Delta^{n-m+1/2} \psi_p \right], \tag{1.12}$$

$$\tilde{D}^n = \varepsilon_0 \varepsilon_\infty E^n + \varepsilon_0 \sum_{p=1}^{P} \tilde{P}_p^{\,n}.$$

For the next time level

$$\begin{aligned}\tilde{P}_p^{\,n+1} &= \frac{a_p}{b_p} \sum_{m=1}^{\infty} e^{b_p t^{m-1}} \left[E^{n+1-m+1} \varphi_p + \Delta^{n+1-m+1/2} \psi_p \right] \\ &= \frac{a_p}{b_p} \left[E^{n+1} \varphi_p + \Delta^{n+1/2} \psi_p \right] \\ &\quad + e^{b_p \tau} \frac{a_p}{b_p} \sum_{m=1}^{\infty} e^{b_p t^{m-1}} \left[E^{n-m+1} \varphi_p + \Delta^{n-m+1/2} \psi_p \right] \\ &= \frac{a_p}{b_p} \left[E^{n+1} \varphi_p + \Delta^{n+1/2} \psi_p \right] + e^{b_p \tau} \tilde{P}_p^{\,n},\end{aligned} \tag{1.13}$$

$$\tilde{D}^{n+1} = \varepsilon_0 \varepsilon_\infty E^{n+1} + \varepsilon_0 \sum_{p=1}^{P} \left[\frac{a_p}{b_p} \left(E^{n+1} \varphi_p + \Delta^{n+1/2} \psi_p \right) + e^{b_p \tau} \tilde{P}_p^{\,n} \right].$$

Substituting for the time derivative $\frac{\partial \tilde{D}}{\partial t}$ by the finite difference $\frac{\tilde{D}^{n+1} - \tilde{D}^n}{\tau}$ we obtain

$$\frac{\partial\tilde{D}}{\partial t}\to\frac{\tilde{D}^{n+1}-\tilde{D}^{n}}{\tau}=\left(\varepsilon_0\varepsilon_\infty-\frac{\varepsilon_0}{\tau}\sum_{p=1}^{P}\frac{a_p}{b_p}\psi_p\right)\frac{E^{n+1}-E^{n}}{\tau}$$
$$+\frac{1}{\tau}\left\{E^{n+1}\varepsilon_0\sum_{p=1}^{P}\frac{a_p}{b_p}\varphi_p+\varepsilon_0\sum_{p=1}^{P}\varphi_p\tilde{P}_p^{\,n}\right\}. \qquad (1.14)$$

The deferred correction method suggested in [2] uses the absence of the even derivatives in the truncation error in order to two orders of accuracy will be gained each time when the basic second order scheme is re-run. Obviously, (1.14) is not a central-difference formula. So we have to modify the recursive convolution method and to obtain a central-difference in time scheme. First we obtain the required governing equations. We take $\tilde{P}_p$ as the auxiliary functions. Using (1.13) and (1.12) we have

$$\frac{\partial\tilde{P}_p}{\partial t}=\lim_{\tau\to 0}\frac{\tilde{P}_p^{\,n+1}-\tilde{P}_p^{\,n}}{\tau}$$
$$=\lim_{\tau\to 0}\frac{1}{\tau}\left\{\frac{a_p}{b_p}\left[E^{n+1}\varphi_p+\Delta^{n+1/2}\psi_p\right]+e^{b_p\tau}\tilde{P}_p^{\,n}-\tilde{P}_p^{\,n}\right\}$$
$$=\lim_{\tau\to 0}\left\{\left(\frac{a_p}{b_p}E^{n+1}+\tilde{P}_p^{\,n}\right)\frac{\varphi_p}{\tau}+\right\}+\lim_{\tau\to 0}\left\{\frac{a_p}{b_p}\Delta^{n+1/2}\frac{\psi_p}{\tau}\right\}$$
$$=a_p\vec{E}+b_p\tilde{P}_p,$$

since

$$\lim_{\tau\to 0}\frac{\varphi_p}{\tau}=\lim_{\tau\to 0}\frac{e^{b_p\tau}-1}{\tau}=\lim_{\tau\to 0}b_p e^{b_p\tau}=b_p,$$

$$\lim_{\tau\to 0}\frac{\psi_p}{\tau}=\lim_{\tau\to 0}e^{b_p\tau}-\frac{1}{b_p}\lim_{\tau\to 0}\frac{\varphi_p}{\tau}=0.$$

Thus the desired equations read:

$$\frac{\partial\tilde{P}_p}{\partial t}=a_p\vec{E}+b_p\tilde{P}_p,\quad p=1,\ldots,P, \qquad (1.15)$$

and

$$\frac{\partial\vec{D}}{\partial t}=\varepsilon_0\varepsilon_\infty\frac{\partial\vec{E}}{\partial t}+\varepsilon_0\,\mathrm{Re}\left(\sum_{p=1}^{P}\frac{\partial\tilde{P}_p}{\partial t}\right)$$
$$=\varepsilon_0\varepsilon_\infty\frac{\partial\vec{E}}{\partial t}+\varepsilon_0\,\mathrm{Re}\left(\sum_{p=1}^{P}a_p\vec{E}+b_p\tilde{P}_p\right).$$

For the Lorentz media

$$\frac{\partial \vec{D}}{\partial t} = \varepsilon_0 \varepsilon_\infty \frac{\partial \vec{E}}{\partial t} + \varepsilon_0 \operatorname{Re}\left(\sum_{p=1}^{P} b_p \tilde{P}_p \right)$$

since $a_p = -i\gamma_p$.

Hence, the governing system is as follows

$$\frac{\partial \vec{E}}{\partial t} = \frac{1}{\varepsilon_0 \varepsilon_\infty} \nabla \times \vec{H} - \frac{1}{\varepsilon_\infty} \operatorname{Re}\left(\sum_{p=1}^{P} \left[b_p \tilde{P}_p + a_p \vec{E} \right] \right), \tag{1.16}$$

$$\frac{\partial \vec{H}}{\partial t} = -\frac{1}{\mu} \nabla \times \vec{E}, \tag{1.17}$$

$$\frac{\partial \tilde{P}_p}{\partial t} = a_p \vec{E} + b_p \tilde{P}_p, \quad p = 1, \ldots, P. \tag{1.18}$$

Note that equations (1.18) are ODEs (not PDEs).

Using the notation $\varepsilon = \varepsilon_0 \varepsilon_\infty$, the governing system (1.16) — (1.18) is written in a matrix form

$$\frac{\partial u}{\partial t} = Au + Bu \tag{1.19}$$

where

$$u = \left(E^x, \quad E^y, \quad E^z, \quad H^x, \quad H^y, \quad H^z, \quad \tilde{P}_p \right)^T,$$

$$Au = \begin{pmatrix} \dfrac{1}{\varepsilon} \dfrac{\partial H^z}{\partial y} - \dfrac{c_1}{\varepsilon_\infty} \operatorname{Re}\left(\sum_{p=1}^{P} \left[\dfrac{\partial \tilde{P}_p^x}{\partial t} \right] \right) \\ \dfrac{1}{\varepsilon} \dfrac{\partial H^x}{\partial z} - \dfrac{c_2}{\varepsilon_\infty} \operatorname{Re}\left(\sum_{p=1}^{P} \left[\dfrac{\partial \tilde{P}_p^y}{\partial t} \right] \right) \\ \dfrac{1}{\varepsilon} \dfrac{\partial H^y}{\partial x} - \dfrac{c_3}{\varepsilon_\infty} \operatorname{Re}\left(\sum_{p=1}^{P} \left[\dfrac{\partial \tilde{P}_p^z}{\partial t} \right] \right) \\ \dfrac{1}{\mu} \dfrac{\partial E^y}{\partial z} \\ \dfrac{1}{\mu} \dfrac{\partial E^z}{\partial x} \\ \dfrac{1}{\mu} \dfrac{\partial E^x}{\partial y} \\ c_4 a_p \vec{E} + c_5 b_p \tilde{P}_p \end{pmatrix}, \quad Bu = \begin{pmatrix} -\dfrac{1}{\varepsilon} \dfrac{\partial H^y}{\partial z} - \dfrac{1-c_1}{\varepsilon_\infty} \operatorname{Re}\left(\sum_{p=1}^{P} \left[\dfrac{\partial \tilde{P}_p^x}{\partial t} \right] \right) \\ -\dfrac{1}{\varepsilon} \dfrac{\partial H^z}{\partial x} - \dfrac{1-c_2}{\varepsilon_\infty} \operatorname{Re}\left(\sum_{p=1}^{P} \left[\dfrac{\partial \tilde{P}_p^y}{\partial t} \right] \right) \\ -\dfrac{1}{\varepsilon} \dfrac{\partial H^x}{\partial y} - \dfrac{1-c_3}{\varepsilon_\infty} \operatorname{Re}\left(\sum_{p=1}^{P} \left[\dfrac{\partial \tilde{P}_p^z}{\partial t} \right] \right) \\ -\dfrac{1}{\mu} \dfrac{\partial E^z}{\partial y} \\ -\dfrac{1}{\mu} \dfrac{\partial E^x}{\partial z} \\ -\dfrac{1}{\mu} \dfrac{\partial E^y}{\partial x} \\ (1-c_4) a_p \vec{E} + (1-c_5) b_p \tilde{P}_p \end{pmatrix}. \tag{1.20}$$

where $c_1,\ldots,c_5$ are arbitrary constants (some weights),

$$\left[\frac{\partial \tilde{P}_p}{\partial t}\right] = a_p\vec{E} + b_p\tilde{P}_p,$$

The equation (1.20) exactly coincides with the equation considered in [2] and hence all the techniques are applicable. So the ADI for solving (1.20) reads

$$\begin{cases} \left(1-\frac{\tau}{2}A\right)u^{n+1/2} = \left(1+\frac{\tau}{2}B\right)u^n, \\ \left(1-\frac{\tau}{2}B\right)u^{n+1} = \left(1+\frac{\tau}{2}A\right)u^{n+1/2}. \end{cases} \tag{1.21}$$

If central differences of the second order accuracy are used to approximate spatial derivatives in A and B then the ADI scheme (1.21) is absolutely stable and deals with three-diagonal matrices only. One can use central differences of the fourth order accuracy and deals with five-diagonal matrices. If a spectral method is used to approximate spatial derivatives then all matrices will be dense. The stability of the scheme is not investigated yet and must be checked at least numerically.

§2. The deferred correction formulas for the fourth order

Following [2] let's find the local error of the ADI scheme (1.21). To do this we have to substitute the expansions

$$u^{n+1} = u^{n+1/2} + \frac{\tau}{2}u_t^{n+1/2} + \frac{1}{2}\left(\frac{\tau}{2}\right)^2 u_{tt}^{n+1/2} + \frac{1}{3!}\left(\frac{\tau}{2}\right)^3 u_{ttt}^{n+1/2} + \frac{1}{4!}\left(\frac{\tau}{2}\right)^4 u_{tttt}^{n+1/2} + \frac{1}{5!}\left(\frac{\tau}{2}\right)^5 u_{ttttt}^{n+1/2} + \ldots$$

$$= u^{n+1/2} + \frac{\tau}{2}u_t^{n+1/2} + \frac{\tau^2}{8}u_{tt}^{n+1/2} + \frac{\tau^3}{48}u_{ttt}^{n+1/2} + \frac{\tau^4}{384}u_{tttt}^{n+1/2} + \frac{\tau^5}{3840}u_{ttttt}^{n+1/2} + \ldots$$

$$u^{n} = u^{n+1/2} - \frac{\tau}{2}u_t^{n+1/2} + \frac{1}{2}\left(\frac{\tau}{2}\right)^2 u_{tt}^{n+1/2} - \frac{1}{3!}\left(\frac{\tau}{2}\right)^3 u_{ttt}^{n+1/2} + \frac{1}{4!}\left(\frac{\tau}{2}\right)^4 u_{tttt}^{n+1/2} - \frac{1}{5!}\left(\frac{\tau}{2}\right)^5 u_{ttttt}^{n+1/2} + \ldots$$

$$= u^{n+1/2} - \frac{\tau}{2}u_t^{n+1/2} + \frac{\tau^2}{8}u_{tt}^{n+1/2} - \frac{\tau^3}{48}u_{ttt}^{n+1/2} + \frac{\tau^4}{384}u_{tttt}^{n+1/2} - \frac{\tau^5}{3840}u_{ttttt}^{n+1/2} + \ldots$$

$$u^{n+1} - u^n = \tau u_t^{n+1/2} + \frac{2\tau^3}{48}u_{ttt}^{n+1/2} + \frac{2\tau^5}{3840}u_{ttttt}^{n+1/2} + \ldots = \tau u_t^{n+1/2} + \frac{\tau^3}{24}u_{ttt}^{n+1/2} + \frac{\tau^5}{1920}u_{ttttt}^{n+1/2} + \ldots$$

$$u^{n+1} + u^n = 2u^{n+1/2} + \frac{2\tau^2}{8}u_{tt}^{n+1/2} + \frac{2\tau^4}{384}u_{tttt}^{n+1/2} + \ldots = 2u^{n+1/2} + \frac{\tau^2}{4}u_{tt}^{n+1/2} + \frac{\tau^4}{192}u_{tttt}^{n+1/2} + \ldots$$

into the one-step form of the scheme

$$\left(1-\frac{\tau}{2}A\right)\left(1-\frac{\tau}{2}B\right)u^{n+1} - \left(1+\frac{\tau}{2}A\right)\left(1+\frac{\tau}{2}B\right)u^n = 0.$$

The difference of the left hand size from 0 at a solution of the equation (1.20) gives the estimate for the local error. After some algebra we have

$$\left(1-\frac{\tau}{2}A\right)\left(1-\frac{\tau}{2}B\right)u^{n+1}-\left(1+\frac{\tau}{2}A\right)\left(1+\frac{\tau}{2}B\right)u^{n}$$

$$=\left(1-\frac{\tau}{2}A-\frac{\tau}{2}B+\frac{\tau^2}{4}AB\right)u^{n+1}-\left(1+\frac{\tau}{2}A+\frac{\tau}{2}B+\frac{\tau^2}{4}AB\right)u^{n}$$

$$=\left(1+\frac{\tau^2}{4}AB\right)\left(u^{n+1}-u^{n}\right)-\frac{\tau}{2}\left(A+B\right)\left(u^{n+1}+u^{n}\right)$$

$$=\left(1+\frac{\tau^2}{4}AB\right)\left(\tau u_t^{n+1/2}+\frac{\tau^3}{24}u_{ttt}^{n+1/2}+\frac{\tau^5}{1920}u_{ttttt}^{n+1/2}+\ldots\right)$$
$$-\frac{\tau}{2}\left(A+B\right)\left(2u^{n+1/2}+\frac{\tau^2}{4}u_{tt}^{n+1/2}+\frac{\tau^4}{192}u_{tttt}^{n+1/2}+\ldots\right)$$

$$=\tau u_t^{n+1/2}+\frac{1}{24}\tau^3 u_{ttt}^{n+1/2}+\frac{1}{1920}\tau^5 u_{ttttt}^{n+1/2}+\frac{\tau^3}{4}ABu_t^{n+1/2}+\frac{\tau^5}{96}ABu_{ttt}^{n+1/2}$$
$$-\tau\left(A+B\right)u^{n+1/2}-\frac{\tau^3}{8}\left(A+B\right)u_{tt}^{n+1/2}-\frac{\tau^5}{384}\left(A+B\right)u_{tttt}^{n+1/2}-\ldots$$

$$=\left\{u_t^{n+1/2}-\left(A+B\right)u^{n+1/2}\right\}\tau$$
$$+\left\{\frac{1}{4}ABu_t^{n+1/2}-\frac{1}{8}\left(A+B\right)u_{tt}^{n+1/2}+\frac{1}{24}u_{ttt}^{n+1/2}\right\}\tau^3$$
$$+\left\{\frac{1}{96}ABu_{ttt}^{n+1/2}-\frac{1}{384}\left(A+B\right)u_{tttt}^{n+1/2}+\frac{1}{1920}u_{ttttt}^{n+1/2}\right\}\tau^5$$
$$+\ldots$$

and obtain that the local error

$$\delta^{n+1/2} = \left\{ \frac{1}{4} ABu_t^{n+1/2} - \frac{1}{8}(A+B)u_{tt}^{n+1/2} + \frac{1}{24}u_{ttt}^{n+1/2} \right\}\tau^3$$
$$+ \left\{ \frac{1}{96} ABu_{ttt}^{n+1/2} - \frac{1}{384}(A+B)u_{tttt}^{n+1/2} + \frac{1}{1920}u_{ttttt}^{n+1/2} \right\}\tau^5 \qquad (2.1)$$
$$+ \ldots$$

To get a fourth order accurate in time ADI algorithm, we would approximate $\delta^{n+1/2}$ by means of the second order accurate central differences:

$$u_t^{n+1/2} \approx \frac{u^{n+1} - u^n}{\tau};$$

$$u_{tt}^{n+1/2} \approx \frac{1}{2\tau}\left(u_t^{n+3/2} - u_t^{n-1/2}\right) = \frac{1}{2\tau}\left(\frac{u^{n+2} - u^{n+1}}{\tau} - \frac{u^n - u^{n-1}}{\tau} \right)$$
$$= \frac{u^{n+2} - u^{n+1} - u^n + u^{n-1}}{2\tau^2}; \qquad (2.2)$$

$$u_{ttt}^{n+1/2} \approx \frac{1}{\tau}\left(u_{tt}^{n+1} - u_{tt}^{n}\right) = \frac{1}{\tau}\left(\frac{u^{n+2} - 2u^{n+1} + u^n}{\tau^2} - \frac{u^{n+1} - 2u^n + u^{n-1}}{\tau^2} \right)$$
$$= \frac{u^{n+2} - 3u^{n+1} + 3u^n - u^{n-1}}{\tau^3};$$

Then we have

$$\tilde{\delta}^{n+1/2} = \left\{ \frac{1}{4} ABu_t^{n+1/2} - \frac{1}{8}(A+B)u_{tt}^{n+1/2} + \frac{1}{24}u_{ttt}^{n+1/2} \right\}\tau^3$$
$$= \left\{ \frac{1}{4} AB\frac{u^{n+1} - u^n}{\tau} - \frac{1}{8}(A+B)\frac{u^{n+2} - u^{n+1} - u^n + u^{n-1}}{2\tau^2} \right.$$
$$\left. + \frac{1}{24}\frac{u^{n+2} - 3u^{n+1} + 3u^n - u^{n-1}}{\tau^3} \right\}\tau^3$$

or

$$\tilde{\delta}^{n+1/2} = \frac{\tau^2}{4}AB\left(u^{n+1} - u^n\right) - \frac{\tau}{16}(A+B)\left(u^{n+2} - u^{n+1} - u^n + u^{n-1}\right)$$
$$+ \frac{1}{24}\left(u^{n+2} - 3u^{n+1} + 3u^n - u^{n-1}\right). \qquad (2.3)$$

The procedure to increase the temporal order of accuracy from 2 to 4 consists of the following steps:

- Step the ADI scheme over some time interval $[0,T]$.

- Using the numerical values from this solution, evaluate the approximation (2.3) of the local truncation error $\tilde{\delta}^{n+1/2}$ at each time level.
- Re-run the ADI scheme over the time $[0,T]$, with $\tilde{\delta}^{n+1/2}$ as a RHS to the equation.

Thus at the third stage we have to solve the following system:

$$\begin{cases} \left(1-\frac{\tau}{2}A\right)u^{n+1/2} = \left(1+\frac{\tau}{2}B\right)u^n + \frac{1}{2}\delta^{n+1/2}, \\ \left(1-\frac{\tau}{2}B\right)u^{n+1} = \left(1+\frac{\tau}{2}A\right)u^{n+1/2} + \frac{1}{2}\delta^{n+1/2} \end{cases} \tag{2.4}$$

where $\delta^{n+1/2} = \tilde{\delta}^{n+1/2}$.

A natural question is what to do at the vicinities of the ends of the interval $[0,T]$?

First of all, the approximation (2.3) uses points u^{n+2} and u^{n-1}. So we have to use other approximations of (2.1) at points $t=\tau/2$ and $t=T-\tau/2$. Let's derive unilateral approximation of the second order for $t=T-\tau/2$. After some calculations

$$u_t^{n+1/2} \approx \frac{u^{n+1}-u^n}{\tau};$$

$$u_t^{n+1} \approx \frac{3u^{n+1}-4u^n+u^{n-1}}{2\tau};$$

$$u_{tt}^{n+1/2} \approx \frac{1}{\tau}\left(u_t^{n+1}-u_t^n\right) = \frac{1}{\tau}\left(\frac{3u^{n+1}-4u^n+u^{n-1}}{2\tau} - \frac{3u^n-4u^{n-1}+u^{n-2}}{2\tau}\right)$$

$$= \frac{3u^{n+1}-7u^n+5u^{n-1}-u^{n-2}}{2\tau^2};$$

Let

$$u_{ttt}^{n+1/2} \approx a_1u^{n+1} + a_0u^n + a_{-1}u^{n-1} + a_{-2}u^{n-2} + a_{-3}u^{n-3}.$$

Using

$$u^{n+1} \approx u^{n+1/2} + \frac{\tau}{2}u_t^{n+1/2} + \frac{1}{2}\left(\frac{\tau}{2}\right)^2 u_{tt}^{n+1/2} + \frac{1}{3!}\left(\frac{\tau}{2}\right)^3 u_{ttt}^{n+1/2} + \frac{1}{4!}\left(\frac{\tau}{2}\right)^4 u_{tttt}^{n+1/2}$$

$$u^{n} \approx u^{n+1/2} - \frac{\tau}{2}u_t^{n+1/2} + \frac{1}{2}\left(\frac{\tau}{2}\right)^2 u_{tt}^{n+1/2} - \frac{1}{3!}\left(\frac{\tau}{2}\right)^3 u_{ttt}^{n+1/2} + \frac{1}{4!}\left(\frac{\tau}{2}\right)^4 u_{tttt}^{n+1/2}$$

$$u^{n-1} \approx u^{n+1/2} - \frac{3\tau}{2}u_t^{n+1/2} + \frac{1}{2}\left(\frac{3\tau}{2}\right)^2 u_{tt}^{n+1/2} - \frac{1}{3!}\left(\frac{3\tau}{2}\right)^3 u_{ttt}^{n+1/2} + \frac{1}{4!}\left(\frac{3\tau}{2}\right)^4 u_{tttt}^{n+1/2}$$

$$u^{n-2} \approx u^{n+1/2} - \frac{5\tau}{2} u_t^{n+1/2} + \frac{1}{2}\left(\frac{5\tau}{2}\right)^2 u_{tt}^{n+1/2} - \frac{1}{3!}\left(\frac{5\tau}{2}\right)^3 u_{ttt}^{n+1/2} + \frac{1}{4!}\left(\frac{5\tau}{2}\right)^4 u_{tttt}^{n+1/2}$$

$$u^{n-3} \approx u^{n+1/2} - \frac{7\tau}{2} u_t^{n+1/2} + \frac{1}{2}\left(\frac{7\tau}{2}\right)^2 u_{tt}^{n+1/2} - \frac{1}{3!}\left(\frac{7\tau}{2}\right)^3 u_{ttt}^{n+1/2} + \frac{1}{4!}\left(\frac{7\tau}{2}\right)^4 u_{tttt}^{n+1/2}$$

we obtain

$$\begin{aligned} u_{ttt}^{n+1/2} \approx a_1 &\left\{u^{n+1/2} + \frac{1}{2}\tau u_t^{n+1/2} + \frac{1}{8}\tau^2 u_{tt}^{n+1/2} + \frac{1}{48}\tau^3 u_{ttt}^{n+1/2} + \frac{1}{384}\tau^4 u_{tttt}^{n+1/2}\right\} \\ +a_0 &\left\{u^{n+1/2} - \frac{1}{2}\tau u_t^{n+1/2} + \frac{1}{8}\tau^2 u_{tt}^{n+1/2} - \frac{1}{48}\tau^3 u_{ttt}^{n+1/2} + \frac{1}{384}\tau^4 u_{tttt}^{n+1/2}\right\} \\ +a_{-1} &\left\{u^{n+1/2} - \frac{3}{2}\tau u_t^{n+1/2} + \frac{9}{8}\tau^2 u_{tt}^{n+1/2} - \frac{27}{48}\tau^3 u_{ttt}^{n+1/2} + \frac{81}{384}\tau^4 u_{tttt}^{n+1/2}\right\} \\ +a_{-2} &\left\{u^{n+1/2} - \frac{5}{2}\tau u_t^{n+1/2} + \frac{25}{8}\tau^2 u_{tt}^{n+1/2} - \frac{125}{48}\tau^3 u_{ttt}^{n+1/2} + \frac{625}{384}\tau^4 u_{tttt}^{n+1/2}\right\} \\ +a_{-3} &\left\{u^{n+1/2} - \frac{7}{2}\tau u_t^{n+1/2} + \frac{49}{8}\tau^2 u_{tt}^{n+1/2} - \frac{343}{48}\tau^3 u_{ttt}^{n+1/2} + \frac{2401}{384}\tau^4 u_{tttt}^{n+1/2}\right\} \end{aligned}$$

where

$$a_1 = \frac{2}{\tau^3}, \quad a_0 = \frac{-7}{\tau^3}, \quad a_{-1} = \frac{9}{\tau^3}, \quad a_{-2} = \frac{-5}{\tau^3}, \quad a_{-3} = \frac{1}{\tau^3}$$

or

$$u_{ttt}^{n+1/2} \approx \frac{2u^{n+1} - 7u^n + 9u^{n-1} - 5u^{n-2} + u^{n-3}}{\tau^3}.$$

Let us collect the results:

$$u_t^{n+1/2} \approx \frac{u^{n+1} - u^n}{\tau};$$

$$u_{tt}^{n+1/2} \approx \frac{3u^{n+1} - 7u^n + 5u^{n-1} - u^{n-2}}{2\tau^2}; \qquad (2.5)$$

$$u_{ttt}^{n+1/2} \approx \frac{2u^{n+1} - 7u^n + 9u^{n-1} - 5u^{n-2} + u^{n-3}}{\tau^3}.$$

and

$$\tilde{\delta}^{n+1/2} = \frac{\tau^2}{4} AB\left(u^{n+1} - u^n\right) - \frac{\tau}{16}\left(A+B\right)\left(3u^{n+1} - 7u^n + 5u^{n-1} - u^{n-2}\right) + \frac{1}{24}\left(2u^{n+1} - 7u^n + 9u^{n-1} - 5u^{n-2} + u^{n-3}\right) \quad (2.6)$$

For the time moment $t = \tau / 2$ we can use u^{n-1} obtained in the previous time interval.

Formula (2.6) is acceptable if we want to get the fourth order of accuracy only. But the six and higher orders are unavailable because the truncation error of (2.6) is asymmetric.

Another way of operating is the over stepping. It means the following. Let $T = N\tau$. Then to obtain fourth order accuracy we have to rerun ADI after each N time steps. Field u^0 for the current time interval is given, because it coincides with u^N of the previous interval. Field u^1 we can calculate using information from the previous interval. Levels u^n for $n = 2,..., N-1$ are calculated by the natural way. But for calculating u^N we need u^{N+1}. So we have to calculate it in advance, to use it during the second run and to forget about it. The next time interval starts from u^N. This way has some extra cost at each time interval (u^{N+1} of the first run), but it allows to use RHS in the form (2.3) only. Such RHS has only the odd degrees in the truncation error, and hence, admits to increase of the order of accuracy.

The formal description of the both algorithms is as follows.

The first variant.

0) u^0 and u^{-1} are given.

1) Compute u^n for $n = 1,..., N$ of the current time interval $\left[t^0, t^N\right]$ using the standard ADI scheme (1.21).

2) Compute $\tilde{\delta}^{n+1/2}$ for $n = 0,..., N-2$ by (2.3).

3) Compute $\tilde{\delta}^{n+1/2}$ for $n = N-1$ by (2.6).

4) Re-compute u^n for $n = 1,..., N$ by means of the ADI scheme (2.4) using the computed $\tilde{\delta}^{n+1/2}$ as the RHS.

The second variant.

0) u^0 and u^{-1} are given.

1) Compute u^n for $n = 1,..., N+1$ of the current time interval $\left[t^0, t^N\right]$ using the standard ADI scheme (1.21).

2) Compute $\tilde{\delta}^{n+1/2}$ for $n = 0,..., N-1$ by (2.3).

3) Re-compute u^n for $n = 1,..., N$ by means of the ADI scheme (2.4) using the computed $\tilde{\delta}^{n+1/2}$ as the RHS.

The objection of the first variant is the inability to get the sixth order of accuracy. The objection of the second variant is the necessity to compute of one extra step at each time interval of the length T. However, even for fourth order scheme the second variant could be more effective (in the sense of CPU time) because the stencil in (2.6) is wider then in (2.3) and hence in spite of the same order of accuracy has bigger coefficient of truncation error. On the other hand in the first variant $N=1$ is applicable (i.e. only the (2.6) approximation is used), and hence both runs of ADI can be done simultaneously. This leads to extremely small request for memory: one needs to keep only 5 time levels in memory. (If we do so for the second variant extra pay will be very big.)

§3. The deferred correction formulas for the sixth order

It was obtained in the previous section that the truncation error of ADI (1.21) is defined by (2.1). For deriving the sixth order scheme we must approximate $\delta^{n+1/2}$ with 4th order finite differences for the time derivatives of the first term (the factor of τ^3) and with 2nd order finite differences for time derivatives of the second term (the factor of τ^5). In [2] the numerical values from ADI are suggested to be used to compute the first term in the RHS of (2.1). But probably the accuracy of the data is insufficient because the data contain an error of order τ^2. Thus the numerical values from the forth order scheme are more preferable in our opinion. Besides, in the last case we don't need to keep the numerical values from ADI.

Anyway we have the approximation formulas

$$u^{n+3} \approx u^{n+1/2} + \frac{5\tau}{2}u_t^{n+1/2} + \frac{1}{2}\left(\frac{5\tau}{2}\right)^2 u_{tt}^{n+1/2} + \frac{1}{3!}\left(\frac{5\tau}{2}\right)^3 u_{ttt}^{n+1/2} + \frac{1}{4!}\left(\frac{5\tau}{2}\right)^4 u_{tttt}^{n+1/2} + \frac{1}{5!}\left(\frac{5\tau}{2}\right)^5 u_{ttttt}^{n+1/2}$$

$$u^{n+2} \approx u^{n+1/2} + \frac{3\tau}{2}u_t^{n+1/2} + \frac{1}{2}\left(\frac{3\tau}{2}\right)^2 u_{tt}^{n+1/2} + \frac{1}{3!}\left(\frac{3\tau}{2}\right)^3 u_{ttt}^{n+1/2} + \frac{1}{4!}\left(\frac{3\tau}{2}\right)^4 u_{tttt}^{n+1/2} + \frac{1}{5!}\left(\frac{3\tau}{2}\right)^5 u_{ttttt}^{n+1/2}$$

$$u^{n+1} \approx u^{n+1/2} + \frac{\tau}{2}u_t^{n+1/2} + \frac{1}{2}\left(\frac{\tau}{2}\right)^2 u_{tt}^{n+1/2} + \frac{1}{3!}\left(\frac{\tau}{2}\right)^3 u_{ttt}^{n+1/2} + \frac{1}{4!}\left(\frac{\tau}{2}\right)^4 u_{tttt}^{n+1/2} + \frac{1}{5!}\left(\frac{\tau}{2}\right)^5 u_{ttttt}^{n+1/2}$$

$$u^{n} \approx u^{n+1/2} - \frac{\tau}{2}u_t^{n+1/2} + \frac{1}{2}\left(\frac{\tau}{2}\right)^2 u_{tt}^{n+1/2} - \frac{1}{3!}\left(\frac{\tau}{2}\right)^3 u_{ttt}^{n+1/2} + \frac{1}{4!}\left(\frac{\tau}{2}\right)^4 u_{tttt}^{n+1/2} - \frac{1}{5!}\left(\frac{\tau}{2}\right)^5 u_{ttttt}^{n+1/2}$$

$$u^{n-1} \approx u^{n+1/2} - \frac{3\tau}{2}u_t^{n+1/2} + \frac{1}{2}\left(\frac{3\tau}{2}\right)^2 u_{tt}^{n+1/2} - \frac{1}{3!}\left(\frac{3\tau}{2}\right)^3 u_{ttt}^{n+1/2} + \frac{1}{4!}\left(\frac{3\tau}{2}\right)^4 u_{tttt}^{n+1/2} - \frac{1}{5!}\left(\frac{3\tau}{2}\right)^5 u_{ttttt}^{n+1/2}$$

$$u^{n-2} \approx u^{n+1/2} - \frac{5\tau}{2}u_t^{n+1/2} + \frac{1}{2}\left(\frac{5\tau}{2}\right)^2 u_{tt}^{n+1/2} - \frac{1}{3!}\left(\frac{5\tau}{2}\right)^3 u_{ttt}^{n+1/2} + \frac{1}{4!}\left(\frac{5\tau}{2}\right)^4 u_{tttt}^{n+1/2} - \frac{1}{5!}\left(\frac{5\tau}{2}\right)^5 u_{ttttt}^{n+1/2}$$

Let

$$u_t^{n+1/2} \approx a_2 u^{n+2} + a_1 u^{n+1} + a_0 u^n + a_{-1} u^{n-1}.$$

Then we obtain

$$a_2 = -\frac{1}{24\tau}, \quad a_1 = \frac{9}{8\tau}, \quad a_0 = -\frac{9}{8\tau}, \quad a_{-1} = \frac{1}{24\tau},$$

or

$$u_t^{n+1/2} \approx \frac{-u^{n+2} + 27u^{n+1} - 27u^n + u^{n-1}}{24\tau}. \tag{3.1}$$

Similarly, let

$$u_{tt}^{n+1/2} \approx s_3 u^{n+3} + s_2 u^{n+2} + s_1 u^{n+1} + s_0 u^n + s_{-1} u^{n-1} + s_{-2} u^{n-2}$$

and we obtain

$$u_{tt}^{n+1/2} \approx \frac{-5u^{n+3} + 39u^{n+2} - 34u^{n+1} - 34u^n + 39u^{n-1} - 5u^{n-2}}{48\tau^2}. \tag{3.2}$$

$$u_{ttt}^{n+1/2} \approx \frac{-u^{n+3} + 13u^{n+2} - 34u^{n+1} + 34u^n - 13u^{n-1} + u^{n-2}}{8\tau^3} \tag{3.3}$$

for the fourth order approximation of the first group of derivatives in (2.1).
The second group of derivatives in (2.1) must be approximated at least with the second order of approximation. We get finally:

$$\begin{aligned} u_{ttt}^{n+1/2} &\approx \frac{u^{n+2} - 3u^{n+1} + 3u^n - u^{n-1}}{\tau^3}; \\ u_{tttt}^{n+1/2} &\approx \frac{u^{n+3} - 3u^{n+2} + 2u^{n+1} + 2u^n - 3u^{n-1} + u^{n-2}}{2\tau^4}; \\ u_{ttttt}^{n+1/2} &\approx \frac{u^{n+3} - 5u^{n+2} + 10u^{n+1} - 10u^n + 5u^{n-1} - u^{n-2}}{\tau^5}. \end{aligned} \tag{3.4}$$

Thus substituting (3.1)- (3.4) into (2.1) we estimate

$$\begin{aligned} \tilde{\tilde{\delta}}^{n+1/2} = {} & \frac{\tau^2}{96} AB\left(-u^{n+2} + 27u^{n+1} - 27u^n + u^{n-1}\right) \\ & - \frac{\tau}{384}\left(A+B\right)\left(-5u^{n+3} + 39u^{n+2} - 34u^{n+1} - 34u^n + 39u^{n-1} - 5u^{n-2}\right) \\ & \frac{1}{192}\left(-u^{n+3} + 13u^{n+2} - 34u^{n+1} + 34u^n - 13u^{n-1} + u^{n-2}\right) \\ & + \frac{\tau^2}{96} AB\left(u^{n+2} - 3u^{n+1} + 3u^n - u^{n-1}\right) \\ & - \frac{\tau}{768}\left(A+B\right)\left(u^{n+3} - 3u^{n+2} + 2u^{n+1} + 2u^n - 3u^{n-1} + u^{n-2}\right) \\ & + \frac{1}{1920}\left(u^{n+3} - 5u^{n+2} + 10u^{n+1} - 10u^n + 5u^{n-1} - u^{n-2}\right). \end{aligned} \tag{3.5}$$

The formal description of the sixth order approximation computations is as follows.
0) u^0, u^{-1} and u^{-2} are given.
1) Compute u^n for $n=1,...,N+2$ of the current time interval $\left[t^0,t^N\right]$ using the standard ADI scheme (1.21).
2) Compute $\tilde{\delta}^{n+1/2}$ for $n=0,...,N+1$ using (2.3).
3) Re-compute u^n for $n=1,...,N+2$ by means of the forth-order scheme (ADI scheme with RHS (2.4) using the computed $\tilde{\delta}^{n+1/2}$ as the RHS).
4) Compute $\tilde{\tilde{\delta}}^{n+1/2}$ for $n=0,...,N+1$ using (3.5).
5) Re-compute u^n for $n=1,...,N$ by means of ADI scheme with RHS (2.4) using the computed $\tilde{\tilde{\delta}}^{n+1/2}$ as the RHS.

§4. Spatial discretization

We describe here pseudospectral approximation for spatial derivatives

4.1 Periodic case

Suppose we need to solve an L-periodic problem: $u(s+L)=u(s)$. Then we choose the equidistant grid

$$s_j = s_0 + \Delta s \cdot j, \quad j=-N/2,...,N/2-1 \qquad (N \text{ is even})$$

where N is the number of grid steps per period, s_0 is the center of the interval of interest,

$$\Delta s = L/N$$

is the grid step. The linear transformation

$$x=\frac{2\pi}{L}\left(s-s_0\right)$$

maps our spatial domain onto the fundamental domain $[-\pi,\pi)$ with the equidistant grid $x_j = jh$ where

$$h=\frac{2\pi}{N}.$$

The derivative

$$\frac{du}{ds}=\frac{du}{dx}\frac{2\pi}{L}.$$

Denote $u_j=u\left(x_j\right)$. In order to compute the first derivative $\frac{du}{dx}$ in the same points we have to

(1) Compute the discrete Fourier transform

$$\hat{u}_\xi = \left(\mathrm{F}_N u\right)_\xi = h \sum_{j=-N/2}^{N/2-1} e^{-i\xi jh} u_j \,;$$

(2) Multiply $\hat{u}_\xi$ by $i\xi$, except that $\hat{u}_{-N/2}$ is multiplied by 0:

$$\hat{v}_\xi = \begin{cases} 0, & \xi = -N/2, \\ i\xi\hat{u}_\xi, & \text{othervise} \end{cases}$$

(3) Compute the inverse transform and assign

$$\frac{du(x_k)}{dx} := \left(\mathrm{F}_N^{-1}\hat{v}\right)_k = \frac{1}{2\pi} \sum_{\xi=-N/2}^{N/2-1} e^{i\xi kh} \hat{v}_\xi \,.$$

The same result can be obtained by multiplication of vector $\{u_j\}$ by a skew-symmetric Toeplitz $N \times N$ matrix $D^{(N)}$ of elements

$$D_{k,j}^{(N)} = \frac{i}{N} \sum_{\xi=-N/2+1}^{N/2-1} \xi e^{i\xi 2\pi(k-j)/N} = \begin{cases} 0 & \text{if} \quad k = j, \\ \dfrac{1}{2}(-1)^{k+j} \cot\left(\pi \dfrac{k-j}{N}\right) & \text{if} \quad k \neq j \end{cases}$$

see [3], i.e.

$$\left(\mathrm{F}_N^{-1}\hat{v}\right)_k = \sum_{j=-N/2}^{N/2-1} D_{k,j}^{(N)} u_j$$

Remark 1. Values x_j are never used.

Remark 2. From the practical point of view it is better to use indexes $j = 1, \ldots, N$ instead of $j = -N/2, \ldots, N/2 - 1$.

Remark 3. The discrete Fourier transform can be computed with great efficiency by the fast Fourier transform (FFT) algorithm.

4.2. Non-periodic case

For non-periodic case the best approximation is given by the Chebyshev points,

$$x_j = \cos(j\pi / N), \quad j = 0, 1, \ldots, N \,.$$

In order to map the interval of interest $\left[s_{left}, s_{right}\right]$ onto the fundamental interval $\left[-1, 1\right]$ we use the following linear transformation:

$$x = \frac{2}{L}\left(s_{left} - s_{right}\right) - 1.$$

Then

$$\frac{du}{ds} = \frac{du}{dx}\frac{2}{L}.$$

To obtain the vector of derivatives $\frac{du}{dx}$ one can multiply the vector u by $(N+1)\times(N+1)$ matrix, which we shall denote by $D^{(N)}$:

$$\frac{du}{dx} = D^{(N)}u$$

where

$$D_{i,j}^{(N)} = \begin{cases} \frac{2N^2+1}{6} & \text{for} \quad i=j=0 \\ -\frac{2N^2+1}{6} & \text{for} \quad i=j=N \\ \frac{-x_j}{2\left(1-x_j^2\right)} & \text{for} \quad 0<i=j<N \\ \frac{c_i}{c_j}\frac{(-1)^{i+j}}{x_i-x_j} & \text{for} \quad i \neq j \end{cases}$$

and

$$c_i = \begin{cases} 2 & \text{for} \quad i=0 \text{ or } N, \\ 1 & \text{for} \quad 0<i<N \end{cases}$$

see [3].
On the other hand for given data $\{u_j\}$ defined at the Chebyshev points $\{x_j\}$, $0 \le j \le N$, one can think of the same data as being defined at the equally spaced points $\{\theta_j\}$ in $[0,\pi]$:

$$\theta_j = \frac{j\pi}{N}, \quad x = \cos\theta.$$

Then

$$\frac{du}{dx} = \frac{du}{d\theta}\left(\frac{dx}{d\theta}\right)^{-1} = \frac{-1}{\sin\theta}\frac{du}{d\theta} = -\frac{1}{\sqrt{1-x^2}}\frac{du}{d\theta}.$$

To calculate $\frac{du}{d\theta}$ one can use the FFT: the cos-FFT and the inverse sin-FFT.

$$u(\theta)=\sum_{n=0}^{N} a_n \cos n\theta,$$

$$\frac{du}{d\theta}=-\sum_{n=0}^{N} na_n \sin n\theta,$$

At $x=\pm 1$, i.e. $\theta=0,\pi$, L'Hopital's rule gives the special values

$$\frac{du}{dx}=\frac{-1}{\sqrt{1-x^2}}\frac{du}{d\theta}=\sum_{n=0}^{N}\frac{na_n \sin n\theta}{\sqrt{1-x^2}}=\sum_{n=0}^{N}\frac{na_n \sin n\theta}{\sin\theta}\rightarrow\sum_{n=0}^{N}\left(\pm 1\right)^n n^2 a_n$$

as $x\rightarrow\pm 1$.

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