Error Inhibiting Schemes for Initial Boundary Value Heat Equation

Adi Ditkowski

School of Mathematical Sciences, Tel Aviv University, Tel Aviv 69978, Israel

Paz Fink Shustin

School of Mathematical Sciences, Tel Aviv University, Tel Aviv 69978, Israel

Abstract

In this paper, we elaborate the analysis of some of the schemes which was presented in [2] for the heat equation with periodic boundary conditions. We adopt this methodology to derive finite-difference schemes for heat equation with Dirichlet and Neumann boundary conditions, whose convergence rates are higher than their truncation errors. We call these schemes error inhibiting schemes.

When constructing a semi-discrete approximation to a partial differential equation (PDE), a discretization of the spatial operator has to be derived. For stability, this discrete operator must be semi-bounded. Under this semi-boundness, the Lax–Ricchtmyer equivalence theorem assures that the scheme converges at most, as the order of the error will be at most of the order of the truncation error. Usually, the error is in indeed of the order of the truncation error. In this paper, we demonstrate that schemes can be constructed such that their errors are smaller than their truncation errors. This property can enable us design schemes which are more efficient than standard schemes.

Key words: Finite difference, Block finite difference, Boundary, Dirichlet, Neumann

1 Introduction

Consider the differential problem:

Email addresses: adid@tauex.tau.ac.il (Adi Ditkowski), pazfink@mail.tau.ac.il (Paz Fink Shustin).
\[ \frac{\partial u}{\partial t} = P \left( \frac{\partial}{\partial x} \right) u , \quad x \in \Omega \subset \mathbb{R}^d, t \geq 0 \quad (1) \]

\[ u(t = 0) = f(x) . \]

where \( u = (u_1, \ldots, u_m)^T \) and \( P (\partial / \partial x) \) is a linear differential operator with appropriate boundary conditions. It is assumed that this problem is well posed, in the sense that \( \exists K(t) < \infty \) such that \( ||u(t)|| \leq K(t)||f|| \), where typically \( K(t) = K e^{\alpha t} \).

Let \( Q \) be the semi-discretization of \( P (\partial / \partial x) \) where we assume:

**Assumption 1:** The discrete operator \( Q \) is based on grid points \( \{x_j\}, j = 1, \ldots, N \).

**Assumption 2:** \( Q \) is semi–bounded in some equivalent scalar product \((\cdot, \cdot)_H = (\cdot, H \cdot)_h\), i.e.
\[ (w, Qw)_H \leq \alpha (w, w)_H = \alpha \|w\|^2_H . \]

Where \( H = H^*, M I \leq H \leq MI, m, M > 0 \) and therefore this norm is equivalent to the \( L_2 \) norm.

Also, \((\cdot, \cdot)_h\) is the discrete norm product, \((u, v)_h = h \sum_j \bar{u}_j v_j\) where \( h = \text{max} h_l, h_t \) are the grid spaces.

**Assumption 3:** The local truncation error vector of \( Q \) is \( T_e \) which is defined, at each entry \( j \) by
\[ (T_e)_j = (Pw(x_j)) - (Qw)_j , \]

where \( w(x) \) is a smooth function and \( w \) is the projection of \( w(x) \) onto the grid. It is assumed that \( ||T_e|| \xrightarrow{N \to \infty} 0 \).

Consider the semi–discrete approximation:

\[ \frac{\partial v}{\partial t} = Qv , \quad t \geq 0 \quad (2) \]

\[ v(t = 0) = f . \]

**Proposition:** Under Assumptions 1–3 the semi–discrete approximation converges.

**Proof:** Let \( u \) is the projection of \( u(x, t) \) onto the grid. Then, from assumption 3,
\[ \frac{\partial u}{\partial t} = Pu = Qu + T_e \quad (3) \]
Let $\mathbf{E} = \mathbf{u} - \mathbf{v}$ then by subtracting (2) from (3) one obtains the equation for $\mathbf{E}$, namely
\[
\frac{\partial \mathbf{E}}{\partial t} = Q\mathbf{E} + \mathbf{T}_e.
\] (4)
Next, by taking the $H$ scalar product with $\mathbf{E}$, using assumption 2 and the Schwartz inequality the following estimate can be derived
\[
\left(\mathbf{E}, \frac{\partial \mathbf{E}}{\partial t}\right)_H = \frac{1}{2} \frac{\partial}{\partial t} \left(\mathbf{E}, \mathbf{E}\right)_H = \left\|\mathbf{E}\right\|_H \frac{\partial}{\partial t} \left\|\mathbf{E}\right\|_H
\]
\[
= (\mathbf{E}, Q\mathbf{E})_H + (\mathbf{E}, \mathbf{T}_e)_H
\]
\[
\leq \alpha (\mathbf{E}, \mathbf{E})_H + \left\|\mathbf{E}\right\|_H \left\|\mathbf{T}_e\right\|_H.
\]
Thus
\[
\frac{\partial}{\partial t} \left\|\mathbf{E}\right\|_H \leq \alpha \left\|\mathbf{E}\right\|_H + \left\|\mathbf{T}_e\right\|_H.
\] (5)
Therefore:
\[
\left\|\mathbf{E}\right\|_H(t) \leq \left\|\mathbf{E}\right\|_H(t = 0)e^{\alpha t} + \frac{e^{\alpha t} - 1}{\alpha} \max_{0 \leq \tau \leq t} \left\|\mathbf{T}_e\right\|_H \xrightarrow{N \to \infty} 0.
\] (6)
Here we assumed that $\left\|\mathbf{E}\right\|_H(t = 0)$ is either 0, or at least of the order of machine accuracy. Equation (6) establishes the fact that if the scheme is stable and consistent, the numerical solution $\mathbf{v}$ converges to the projection of the exact solution onto the grid, $\mathbf{u}$. Furthermore, it assures that the error will be at most in the truncation error $\left\|\mathbf{T}_e\right\|_H$. This is one part of the landmark Lax–Richtmyer equivalence theorem for semi-discrete approximation. See e.g. [5].

Typically the error and the truncation error are of the same order. This can be seen in [5]. Notice that (4) is an equality and (6) is an estimate for the error norm. We would like to investigate this phenomenon where the order of the error is higher than the truncation error.

In [6] Nodal-basis DG schemes were presented. If we consider them as FD schemes, then the truncation error is of first order but the convergence order is two.

In [2], several schemes for which the convergence orders are more accurate in two orders than their truncation errors.

Here we would like to exploit the algebraic structure of FD schemes in a purpose to inhibit the error. Since we do not let the error develop, we call them Error Inhibiting schemes (EIS).
For IBVP, the major difficulty in using high-order schemes is due to the presence of boundary conditions. Next to the boundaries we do not usually have enough discrete points to apply the high-order scheme, therefore we cannot use the inner scheme which is usually central. At these nodes we must consider one sided approximations, which also contain the boundary conditions, or creating ghost points outside of the computational domain. These boundary stencils should be developed so that the scheme is stable and maintaining the accuracy. The higher the order, the more difficult the problem is. It is well known that the scheme next to the boundaries can be of a lower accuracy order and preserve the accuracy. See e.g. [1], [3], and [4].

This paper is constructed as follows; description of the scheme for periodic heat equation, convergence proofs are presented in section 2. In section 3, the method to impose boundary conditionns for the IBVP is presented, 3th-order and 5th-order accurate schemes are developed. Numerical simulation results supporting the theory are shown. In Appendix an alternative method for deriving initial Dirichlet problem??.

2 Two-Point Block Finite Difference Scheme for Heat Equation with Periodic Boundary Conditions

As was pointed out in the introduction, this scheme was first presented in [2]. Here we present the complete analysis of this scheme.

2.1 Second and Third order Scheme for Heat Equation with Periodic Boundary Conditions

Consider the heat equation

\[ \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + F(x, t), \quad x \in [0, 2\pi), \quad t \geq 0, \quad F(x, t) = F(x + 2\pi, t) \]

\[ u(x, t = 0) = f(x), \quad f(x) = f(x + 2\pi) \]

with periodic boundary conditions. Let the grid be:

\[ x_j = jh, \quad h = 2\pi/(N + 1) \text{ and } x_{j+1/2} = x_j + h/2, \quad j = 0, \ldots N. \]

Altogether there are \(2(N + 1)\) points with spacing of \(h/2\). For simplicity, we assume that \(N\) is even. See Figure [1].
Using a grid of two-point blocks in FD is motivated by the DG-FE methods as described in [6], where the elements of the FE method are translated to a FD method with a grid of blocks. Thus the interval \([x_0 = 0, x_{N+1} = 2\pi]\) can be viewed as division into \(N + 1\) blocks of size \(h\) \([x_j, x_{j+1}]\), each one of which has a central node denoted by \(x_{j+1/2}\) for \(j = 0, \ldots, N\). Two points \(x_j, x_{j+1/2}\) are taken from each block for the scheme.

In each block \(\frac{\partial^2 u}{\partial x^2}\) is approximated by:

\[
\frac{d^2}{dx^2} u_j \approx \frac{1}{(h/2)^2} \left[ (u_{j-1/2} - 2u_j + u_{j+1/2}) + c (-u_{j-1/2} + 3u_j - 3u_{j+1/2} + u_{j+1}) \right]
\]

\[
\frac{d^2}{dx^2} u_{j+1/2} \approx \frac{1}{(h/2)^2} \left[ (u_j - 2u_{j+1/2} + u_{j+1}) + c (u_{j-1/2} - 3u_j + 3u_{j+1/2} - u_{j+1}) \right]
\]

The local truncation errors for this approximation are:

\[
(T_e)_j = \frac{1}{12} \left( \frac{h}{2} \right)^2 \frac{\partial^4 u_j}{\partial x^4} + c \left[ \left( \frac{h}{2} \right) \frac{\partial^3 u_j}{\partial x^3} + \frac{1}{2} \left( \frac{h}{2} \right)^2 \frac{\partial^4 u_j}{\partial x^4} + \frac{1}{4} \left( \frac{h}{2} \right)^3 \frac{\partial^5 u_j}{\partial x^5} \right] + O(h^4) = O(h)
\]

\[
(T_e)_{j+1/2} = \frac{1}{12} \left( \frac{h}{2} \right)^2 \frac{\partial^4 u_{j+1/2}}{\partial x^4} + \frac{c}{2} \left[ \left( \frac{h}{2} \right) \frac{\partial^3 u_{j+1/2}}{\partial x^3} + \frac{1}{2} \left( \frac{h}{2} \right)^2 \frac{\partial^4 u_{j+1/2}}{\partial x^4} - \frac{1}{4} \left( \frac{h}{2} \right)^3 \frac{\partial^5 u_{j+1/2}}{\partial x^5} \right] + O(h^4) = O(h)
\]

### 2.1.1 Analysis

The approximation (7) can be written in a matrix form and thus the scheme gets the form of non homogeneous (2), namely
\[
\frac{\partial \mathbf{v}}{\partial t} = Q \mathbf{v} + \mathbf{F}(t) , \quad t \geq 0
\]
\[
\mathbf{v}(t = 0) = \mathbf{f} ,
\]
where \( \mathbf{v} \) is the numerical approximation, \( \mathbf{F}(t) \) and \( \mathbf{f} \) are the projections of \( F(x, t) \) and \( f(x) \) onto the grid respectively. It is assumed the non-homogeneous term is smooth enough. Since it does not affect on stability, as can be shown using Duhamel’s principle, the analysis is done for the homogeneous problem.

We would like to diagonalize \( Q \), but \( Q \) is not diagonalizable by discrete Fourier transform. Therefore, for the analysis we first split the Fourier spectrum into low and high frequency modes as follows; let \( \omega \in \{-N/2, \ldots, N/2\} \) and

\[
\nu = \nu(\omega) = \begin{cases} 
\omega - (N + 1) & \omega > 0 \\
\omega + (N + 1) & \omega \leq 0
\end{cases}
\]

Such that they satisfy

\[
e^{i\omega x_j} = e^{i\nu x_j} \quad \text{and} \quad e^{i\omega x_j + 1/2} = -e^{i\nu x_j + 1/2} .
\]

We denote the vectors \( e^{i\omega x} \) and \( e^{i\nu x} \) by

\[
e^{i\omega x} = \begin{pmatrix} 
\vdots \\
e^{i\omega x_j} \\
\vdots \\
e^{i\omega x_{j+1/2}} \\
\vdots 
\end{pmatrix} , \quad e^{i\nu x} = \begin{pmatrix} 
\vdots \\
e^{i\nu x_j} \\
\vdots \\
e^{i\nu x_{j+1/2}} \\
\vdots 
\end{pmatrix}
\]

It follows from (7) that

\[
Q e^{i\omega x} = \text{diag} (\mu_1, \mu_2, \mu_1, \mu_2, \ldots, \mu_1, \mu_2) e^{i\omega x}
\]
\[
Q e^{i\nu x} = \text{diag} (\sigma_1, \sigma_2, \sigma_1, \sigma_2, \ldots, \sigma_1, \sigma_2) e^{i\nu x}
\]

where \( Q \) is defined in (7) and \( \mu_1, \mu_2, \sigma_1, \sigma_2 \) are:
\[ \mu_1 = -4 \sin^2 \left( \frac{\omega h}{4} \right) \frac{(h/2)^2}{(h/2)^2} - \frac{8 i c e^{i \omega h/4} \sin \left( \frac{\omega h}{4} \right)}{(h/2)^2} \]

\[ \mu_2 = -4 \sin^2 \left( \frac{\omega h}{4} \right) \frac{(h/2)^2}{(h/2)^2} + \frac{8 i c e^{-i \omega h/4} \sin \left( \frac{\omega h}{4} \right)}{(h/2)^2} \]

\[ \sigma_1 = -4 \sin^2 \left( \frac{\nu h}{4} \right) \frac{(h/2)^2}{(h/2)^2} - \frac{8 i c e^{i \nu h/4} \sin \left( \frac{\nu h}{4} \right)}{(h/2)^2} \]

\[ \sigma_2 = -4 \sin^2 \left( \frac{\nu h}{4} \right) \frac{(h/2)^2}{(h/2)^2} + \frac{8 i c e^{-i \nu h/4} \sin \left( \frac{\nu h}{4} \right)}{(h/2)^2} \]

We look for eigenvectors in the form of:

\[ \psi_k(\omega) = \frac{\alpha_k}{\sqrt{2\pi}} e^{i \omega x} + \frac{\beta_k}{\sqrt{2\pi}} e^{i \nu x} \]  

(10)

where, for normalization, it is required that \(|\alpha_k|^2 + |\beta_k|^2 = 1, k = 1, 2\).

Note that these eigenvectors are for \(\omega \neq 0\). In the case of \(\omega = 0\) the eigenvectors are \(e^{i0x}, e^{i(N+1)x}\) which denoted by \(\psi_1(0), \psi_2(0)\) respectively.

In order to find the coefficients \(\alpha_k, \beta_k\) and the eigenvalues (symbols) \(\hat{Q}_k\) for \(\omega \neq 0\), we look at a certain \(x_j\) and solve the system of equations:

\[ \mu_1 \frac{\alpha_k}{\sqrt{2\pi}} e^{i \omega x_j} + \sigma_1 \frac{\beta_k}{\sqrt{2\pi}} e^{i \nu x_j} = \hat{Q}_k \left( \frac{\alpha_k}{\sqrt{2\pi}} e^{i \omega x_j} + \frac{\beta_k}{\sqrt{2\pi}} e^{i \nu x_j} \right) \]

\[ \mu_2 \frac{\alpha_k}{\sqrt{2\pi}} e^{i \omega x_{j+1/2}} + \sigma_2 \frac{\beta_k}{\sqrt{2\pi}} e^{i \nu x_{j+1/2}} = \hat{Q}_k \left( \frac{\alpha_k}{\sqrt{2\pi}} e^{i \omega x_{j+1/2}} + \frac{\beta_k}{\sqrt{2\pi}} e^{i \nu x_{j+1/2}} \right) \]

We denote \(r_k = \beta_k/\alpha_k\) and use the relations (9) to obtain:

\[ \mu_1 + \sigma_1 r_k = \hat{Q}_k (1 + r_k) \]  

(11)

\[ \mu_2 - \sigma_2 r_k = \hat{Q}_k (1 - r_k) \]

Thus for \(\omega \neq 0\), \(r_k\) and the eigenvalues (symbols) \(\hat{Q}_k\) are:

\[ r_{1,2} = \frac{(4 - 8c) \cos(\omega(h/2)) \pm \Delta}{2c(2 \sin(\omega(h/2)) + \sin(2\omega(h/2)))} i \]
\[
\hat{Q}_{1,2}(\omega) = \frac{-4 + 2c\cos(2(h/2)\omega) + 3 \pm \Delta}{2(h/2)^2}
\]  
(12)

where

\[
\Delta = \sqrt{2c^2 \cos(4(h/2)\omega) + 38c^2 + 8(c - 1)(3c - 1) \cos(2(h/2)\omega) - 32c + 8}
\]

It can be verified that for all \( c < 1/2 \), \( r_{1,2} \) are imaginary and \( \hat{Q}_{1,2} \) are real and negative. Therefore the scheme is von Neumann stable.

Using the normalization condition \(|\alpha_k|^2 + |\beta_k|^2 = 1\) we choose the coefficients \( \alpha_k, \beta_k \) to be

\[
\alpha_1 = \frac{1}{\sqrt{1 + |r_1|^2}}, \quad \beta_1 = \frac{r_1}{\sqrt{1 + |r_1|^2}}
\]

and

\[
\alpha_2 = \frac{|r_2|/r_2}{\sqrt{1 + |r_2|^2}}, \quad \beta_2 = \frac{|r_2|}{\sqrt{1 + |r_2|^2}}
\]

In order to find the eigenvalues (symbols) for \( \omega = 0 \), we again look at a certain \( x_j \) and solve the corresponding two systems. Here \( \mu_1 = \mu_2 = 0, \sigma_1 = \sigma_2 = \frac{-4 + 8c}{(h/2)^2} \).

The system for the eigenvector \( \psi_1(0) \) is:

\[
\mu_1 e^{i0x_j} = \hat{Q}_1 e^{i0x_j}
\]

\[
\mu_1 e^{i0x_{j+1/2}} = \hat{Q}_1 e^{i0x_{j+1/2}}
\]

whose solution is \( \hat{Q}_1(0) = 0 \).

The system for the eigenvector \( \psi_2(0) \) is:

\[
\sigma_1 e^{i(N+1)x_j} = \hat{Q}_2 e^{i(N+1)x_j}
\]

\[
\sigma_1 e^{i(N+1)x_{j+1/2}} = \hat{Q}_2 e^{i(N+1)x_{j+1/2}}
\]

which has a solution \( \hat{Q}_2(0) = \frac{-4 + 8c}{(h/2)^2} \).
2.1.2 Stability of The Scheme

Unlike the Fourier mode $e^{i\omega x}/\sqrt{2\pi}$, the $\psi_k(\omega)$ are not orthogonal, since
\[ \langle \psi_1(\omega), \psi_2(\omega) \rangle_{h/2} = \sum_j \frac{h}{2} \psi_1(\omega)_j \psi_2(\omega)_j \neq 0, \]
where the inner product $\langle \cdot, \cdot \rangle_{h/2}$ is the scalar inner product normalized by $\frac{h}{2}$. It is necessary to show that the norms of $\Psi, \Psi^{-1}$ are bounded, where

\[
\Psi = \begin{pmatrix}
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\psi_1\left(-\frac{N}{2}\right) & \psi_2\left(-\frac{N}{2}\right) & \psi_1\left(-\frac{N}{2} + 1\right) & \psi_2\left(-\frac{N}{2} + 1\right) & \cdots & \psi_1\left(\frac{N}{2}\right) & \psi_2\left(\frac{N}{2}\right) \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\end{pmatrix}
\]

This condition assures the stability as shown below. Note that the norm which is being used is the induced norm $||\cdot||_{h/2} := \langle \cdot, \cdot \rangle_{h/2}$.

At this point $||\Psi||_{h/2}$ and $||\Psi^{-1}||$ should be evaluated. Let us denote by $F^{-1}$ the matrix

\[
F^{-1} = \begin{pmatrix}
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
e^{i\left(-\frac{N}{2}\right)x} & e^{i\left(-\frac{N}{2} + (N+1)x\right)} & \cdots & e^{i\left(\frac{N}{2}\right)x} & e^{i\left(\frac{N}{2} - (N+1)x\right)} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\end{pmatrix}
\]

Since the columns of $F^{-1}$ are orthonormal in the $\langle \cdot, \cdot \rangle_{h/2}$ inner product, i.e. the columns of $\sqrt{\frac{h}{2}}F^{-1}$ are orthonormal in the euclidean inner product, the matrix $\sqrt{\frac{h}{2}}F^{-1}$ is unitary. Therefore $\sqrt{\frac{h}{2}}F = \left(\sqrt{\frac{h}{2}}F^{-1}\right)^{-1} = \sqrt{\frac{k}{2}}(F^{-1})^*$ is unitary as well, therefore preserve norms. We denote by $A$ the coefficient matrix

\[
A = \begin{pmatrix}
\alpha_1\left(-\frac{N}{2}\right) & \alpha_2\left(-\frac{N}{2}\right) \\
\beta_1\left(-\frac{N}{2}\right) & \beta_2\left(-\frac{N}{2}\right) \\
\vdots & \vdots & \ddots & \ddots \\
\alpha_1\left(\frac{N}{2}\right) & \alpha_2\left(\frac{N}{2}\right) \\
\beta_1\left(\frac{N}{2}\right) & \beta_2\left(\frac{N}{2}\right) \\
\end{pmatrix}
\]

Then

\[
\Psi = F^{-1}A
\]
In order to bound $||\Psi||_{h/2}$, we should bound $||A||$. Denote each block as

$$B_\omega = \begin{pmatrix} \alpha_1 (\omega) & \alpha_2 (\omega) \\ \beta_1 (\omega) & \beta_2 (\omega) \end{pmatrix}$$

By definition,

$$||B_\omega|| = \sup_{||y||=1} \left\| \begin{pmatrix} \alpha_1 (\omega) & \alpha_2 (\omega) \\ \beta_1 (\omega) & \beta_2 (\omega) \end{pmatrix} \cdot \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \right\|$$

(14)

Using the geometric definition of the euclidean product, we obtain (14) equivalents to

$$\sup_{||y||=1} \left\| \begin{pmatrix} ||\alpha|| \cdot ||y|| \cdot \cos(\theta_1) \\ ||\beta|| \cdot ||y|| \cdot \cos(\theta_2) \end{pmatrix} \right\| = \sup_{||y||=1} \left\| \begin{pmatrix} ||\alpha|| \cdot \cos(\theta_1) \\ ||\beta|| \cdot \cos(\theta_2) \end{pmatrix} \right\|$$

$$\leq \left\| \begin{pmatrix} ||\alpha|| \\ ||\beta|| \end{pmatrix} \right\| = \sqrt{2}$$

where $\alpha = (\alpha_1, \alpha_2), \beta = (\beta_1, \beta_2), y = (y_1, y_2), \theta_1$ is the angle between $\alpha$ and $y$, while $\theta_2$ is the angle between $\beta$ and $y$. We also use the normalization condition

$$|\alpha_1(\omega)|^2 + |\beta_1(\omega)|^2 = 1, \ |\alpha_2(\omega)|^2 + |\beta_2(\omega)|^2 = 1$$

As for the matrix $A$, $\forall \mathbf{x} = (x_1, ..., x_{2N+2}) \in \mathbb{C}^{2N+2}$ we have

$$||Ax|| = \left\| \begin{pmatrix} B \cdot \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \\ \vdots \\ B \cdot \begin{pmatrix} x_{2N+1} \\ x_{2N+2} \end{pmatrix} \end{pmatrix} \right\|$$

$$\leq \sqrt{B \cdot \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}} + \ldots + \sqrt{B \cdot \begin{pmatrix} x_{2N+1} \\ x_{2N+2} \end{pmatrix} \cdot \begin{pmatrix} x_{2N+1} \\ x_{2N+2} \end{pmatrix}} = \sqrt{2}||\mathbf{x}||$$

i.e., $||A|| \leq \sqrt{2}$. 
Therefore, since $\sqrt{\frac{h}{2}} F^{-1}$ preserve norms, we obtain

$$||\Psi||_{h/2} = \| F^{-1} A \|_{h/2} = \left\| \sqrt{\frac{h}{2}} F^{-1} A \right\| \leq \sqrt{2}$$

Now we should evaluate

$$\Psi^{-1} = A^{-1} F$$

where $A^{-1}$ is a $2 \times 2$ block diagonal matrix and $F = \frac{h}{2} (F^{-1})^*$. Each block has the form

$$\frac{1}{\alpha_1(\omega)\beta_2(\omega) - \alpha_2(\omega)\beta_1(\omega)} \begin{pmatrix} \beta_2(\omega) & -\alpha_2(\omega) \\ -\beta_1(\omega) & \alpha_1(\omega) \end{pmatrix}.$$

The determinant $\alpha_1\beta_2 - \alpha_2\beta_1$ can be written as

$$\alpha_1\beta_2 - \alpha_2\beta_1 = \frac{|r_2|}{\sqrt{1 + |r_1|^2}} \frac{1}{\sqrt{1 + |r_2|^2}} \left( 1 - \frac{r_1}{r_2} \right).$$

It can be shown that that it is larger than 0.9 and less or equal to 1 for $c < 3/8$ and $-\pi \leq \omega h \leq \pi$. As an illustration please see the following figure:

![Fig. 2. The Determinent of the coefficients block](image)

Similarly to the boundedness of a block of $A$, a block of $A^{-1}$ is also bounded by $\sqrt{2}$ in the $h/2$ norm. Since $\sqrt{\frac{h}{2}} (F^{-1})^*$ preserve norms, we obtain

$$||\Psi^{-1}|| = ||A^{-1} F|| = \left\| A^{-1} \frac{h}{2} (F^{-1})^* \right\| = \left\| \sqrt{\frac{h}{2}} A^{-1} \right\| \leq \frac{10\sqrt{2}}{9} \sqrt{\frac{h}{2}} \quad (15)$$
Proving the stability is done by looking expansion of numerical solution in the \( \psi_k(\omega) \) basis:

\[
v(t) = \sum_{\omega} \hat{v}_1(t, \omega)\psi_1(\omega) + \hat{v}_2(t, \omega)\psi_2(\omega)
\]  

(16)

Substitute (16) into the scheme (7) yields:

\[
\sum_{\omega} \hat{v}_1(t, \omega)\psi_1(\omega) + \hat{v}_2(t, \omega)\psi_2(\omega) = \sum_{\omega} \hat{Q}_1(\omega)\hat{v}_1(t, \omega)\psi_1(\omega) + \hat{Q}_2(\omega)\hat{v}_2(t, \omega)\psi_2(\omega)
\]

(17)

Using the definition of \( \Psi \) from (13), equation (17) can be written in matrix form as:

\[
\begin{pmatrix}
\hat{v}_1(-\frac{N}{2}, t) \\
\hat{v}_2(-\frac{N}{2}, t) \\
\vdots \\
\hat{v}_1(\frac{N}{2}, t) \\
\hat{v}_2(\frac{N}{2}, t)
\end{pmatrix}
t = \begin{pmatrix}
\hat{Q}_1(-\frac{N}{2}) \\
\hat{Q}_2(-\frac{N}{2}) \\
\hat{\psi}_1(\frac{N}{2}) \\
\hat{Q}_1(\frac{N}{2}) \\
\hat{Q}_2(\frac{N}{2})
\end{pmatrix}
\begin{pmatrix}
\hat{v}_1(-\frac{N}{2}, t) \\
\hat{v}_2(-\frac{N}{2}, t) \\
\vdots \\
\hat{v}_1(\frac{N}{2}, t) \\
\hat{v}_2(\frac{N}{2}, t)
\end{pmatrix}
\]

(18)

Since \( \Psi^{-1} \) exists, the system (18) can be solved as a first order linear ODE. The solution is:

\[
\hat{v} = \begin{pmatrix}
e^{\hat{Q}_1(-\frac{N}{2})t}\hat{v}_1(0, -\frac{N}{2}) \\
e^{\hat{Q}_2(-\frac{N}{2})t}\hat{v}_2(0, -\frac{N}{2}) \\
\vdots \\
e^{\hat{Q}_1(\frac{N}{2})t}\hat{v}_1(0, \frac{N}{2}) \\
e^{\hat{Q}_2(\frac{N}{2})t}\hat{v}_2(0, \frac{N}{2})
\end{pmatrix}
\]

where

\[
\hat{v} = \Psi\hat{\psi}
\]

Hence we obtain,
\[ \| \mathbf{v} \|_{h/2}(t) = \| \Psi \hat{\mathbf{v}} \|_{h/2}(t) \leq \| \Psi \|_{h/2} \cdot \| \hat{\mathbf{v}} \| (t) \]

\[ \leq \| \Psi \|_{h/2} \cdot e^{\max \text{Re}(\hat{Q}_j) t} \cdot \| \hat{\mathbf{v}}(0) \| \]

\[ \leq \| \Psi \|_{h/2} \cdot \| \Psi^{-1} \| \cdot e^{\max \text{Re}(\hat{Q}_j) t} \cdot \| \mathbf{v}(0) \| \]

\[ \leq \frac{20}{9} \cdot e^{\max \text{Re}(\hat{Q}_j) t} \cdot \| \mathbf{v}(0) \|_{h/2} \]

where in the last inequality we used the bound \( \| \Psi \|_{h/2} \cdot \| \Psi^{-1} \| \leq \frac{20}{9} \sqrt{\frac{T}{2}} \) and inserted \( \sqrt{\frac{T}{2}} \) into the norm of \( \mathbf{v}(0) \). Therefore we obtain

\[ \| \mathbf{v} \|_{h/2}(t) \leq \frac{20}{9} e^{\max \text{Re}(\hat{Q}_j) t} \cdot \| \mathbf{v}(0) \|_{h/2} \]

i.e., the scheme is stable.

### 2.1.3 Estimation of the Error

In most schemes the error is of the same order as the truncation error which is typically calculated using Taylor’s expansions. In this scheme, however, the error is much smaller than the truncation error. This order reduction caused by the interaction between the operator \( Q \) and the truncation error.

In order to investigate this relation, we perform the analysis in the eigenvectors space.

It is assumed that the solution is smooth enough, i.e. \( \mathbf{u} \in C^6 \). Since the smoothness of the function equivalence to the coefficients decay in the spectral analysis, the coefficients \( \hat{u}(t, \omega) \) decay fast as \( \omega^{-6} \).

Therefore it is sufficient to look at \( \omega h << 1 \).

From (19) the equation for the error:

\[ \frac{\partial \mathbf{E}}{\partial t} = Q \mathbf{E} + \mathbf{T}_e \]  

The expansion of \( \mathbf{E} \) in the \( \{ \psi_j \} \) basis is

\[ \mathbf{E}(t) = \sum_\omega \hat{E}_1(t, \omega) \psi_1(\omega) + \hat{E}_2(t, \omega) \psi_2(\omega) \]  

where \( \mathbf{E} = \Psi \hat{\mathbf{E}}, \mathbf{T}_e = \Psi \hat{\mathbf{T}}_e \).

Therefore we can write

\[ \frac{\partial \mathbf{E}}{\partial t} = \Lambda \mathbf{E} + \mathbf{T}_e \]  

\[ \text{(21)} \]
where
\[
\Lambda = \text{diag} \left( \hat{Q}_1 \left( -\frac{N}{2} \right), \hat{Q}_2 \left( -\frac{N}{2} \right), \ldots, \hat{Q}_1 \left( \frac{N}{2} \right), \hat{Q}_2 \left( \frac{N}{2} \right) \right)
\] (22)

The solution for the error in norm from (21):
\[
\left\| \hat{E} \right\| = \left\| e^{\hat{Q}_1 \left( S \right) t} \hat{E}_1 \left( \frac{N}{2} \right) e^{\hat{Q}_2 \left( S \right) t} \hat{E}_2 \left( \frac{N}{2} \right) \right\| + e^{\Lambda t} \cdot \int_0^t e^{-\Lambda \tau} \hat{T}_e d\tau
\] (23)

For \( \omega h \ll 1 \) the eigenvalues and eigenvectors' coefficients are:
\[
\hat{Q}_1(\omega) = -\omega^2 + \frac{(1 + 4c)\omega^4}{12 - 24c} \left( \frac{h}{2} \right) + O(h^4)
\]
\[
\alpha_1 = 1 - \frac{c^2}{32(1 - 2c)^2} \left( \frac{\omega h}{2} \right)^6 + O \left( \omega^7 \right), \quad \beta_1 = -\frac{ic}{4 - 8c} \left( \frac{\omega h}{2} \right)^3 + O(h^5)
\]
\[
\hat{Q}_2(\omega) = -\frac{4 - 8c}{(h/2)^2} + (1 - 4c)\omega^2 + O(h^2)
\]
\[
\alpha_2 = \frac{ic}{2c - 1} \left( \frac{\omega h}{2} \right)^2 + O(h^3), \quad \beta_2 = 1 + O(h^2)
\]

Since the initial error, \( E_0 \), is either 0 or at most of the order of machine error, the term \( e^{\Lambda t} \hat{E}_0 \) can be neglected.

Since we do spectral analysis of the error, it is also sufficient to look at the low modes and focus on the case where \( \omega h \ll 1 \).
We shall first evaluate \( T_e \). Recall that:
\[(T_e)_j = \frac{1}{12} \left( \frac{h}{2} \right)^2 (u_j)_{xxxx} + c \left[ \left( \frac{h}{2} \right) (u_j)_{xxx} + \frac{1}{2} \left( \frac{h}{2} \right)^2 (u_j)_{xxxx} \right] + O(h^3) = O(h) \quad \text{(24)}\]

\[(T_e)_{j+1/2} = \frac{1}{12} \left( \frac{h}{2} \right)^2 (u_{j+1/2})_{xxxx} + c \left[ - \left( \frac{h}{2} \right) (u_{j+1/2})_{xxx} + \frac{1}{2} \left( \frac{h}{2} \right)^2 (u_{j+1/2})_{xxxx} \right] + O(h^3) = O(h) \quad \text{(25)}\]

Denote \( T_e = T_\ell + T_h \), where

\[T_h = c \left( \frac{h}{2} \right) \text{diag} (1, -1, 1, -1, ..., 1, -1) u_{xxx} + O(h^3)\]

\[T_\ell = \frac{6c + 1}{12} \left( \frac{h}{2} \right)^2 u_{xxxx} + O(h^4)\]

The expansion of \( u \) in the \( \{ \psi_j \} \) basis is

\[u(t) = \sum_\omega \hat{u}_1(t, \omega) \psi_1(\omega) + \hat{u}_2(t, \omega) \psi_2(\omega)\]

\( u \) can also be expanded in Fourier series as

\[u(t) = \frac{1}{\sqrt{2\pi}} \sum_\omega \hat{u}(t, \omega) e^{i\omega x} + \hat{u}(t, \nu) e^{i\nu x}\]

where

\[\hat{u}(t, \omega) = \alpha_1 \hat{u}_1(t, \omega) + \alpha_2 \hat{u}_2(t, \omega)\]

\[\hat{u}(t, \nu) = \beta_1 \hat{u}_1(t, \omega) + \beta_2 \hat{u}_2(t, \omega)\]

If we replace \( u_{xxx}, u_{xxxx} \) in (26) by the representation in (26), we obtain

\[T_h = \frac{1}{\sqrt{2\pi}} \sum_\omega (i\omega)^3 \hat{u}(t, \omega) \text{diag} (1, -1, 1, -1, ..., 1, -1) e^{i\omega x} + O(h^3)\]

\[+ (i\nu)^3 \hat{u}(t, \nu) \text{diag} (1, -1, 1, -1, ..., 1, -1) e^{i\nu x} + O(h^3)\]

\[T_\ell = \frac{6c + 1}{12} \left( \frac{h}{2} \right)^2 \frac{1}{\sqrt{2\pi}} \sum_\omega (i\omega)^4 \hat{u}(t, \omega) e^{i\omega x} + (i\nu)^4 \hat{u}(t, \nu) e^{i\nu x} + O(h^4)\]
In order to evaluate $\hat{T}_e$ we use the following representation

$$\hat{T}_e = \Psi^{-1} T_e = \Psi^{-1} T_\ell + \Psi^{-1} T_h = \hat{T}_\ell + \hat{T}_h$$

and treat the terms $\hat{T}_\ell = A^{-1} F T_\ell, \hat{T}_h = A^{-1} F T_h$ separately, where notice that $F = \frac{h}{2} (F^{-1})^*$. 

For the term $A^{-1} F T_h$, the m-position which represent the $\omega_m$ frequency in the vector $F T_h$ is

$$\frac{h}{2} \frac{1}{\sqrt{2\pi}} e^{-i\omega_m x^T} \cdot \left( \frac{h}{2} \right) \frac{1}{\sqrt{2\pi}} \sum_\omega (i\omega)^3 \hat{u}(t, \omega) \text{diag}(1, -1, 1, -1, ..., 1, -1) e^{i\omega x} + (i\nu)^3 \hat{u}(t, \nu) \text{diag}(1, -1, 1, -1, ..., 1, -1) e^{i\nu x} + O(h^3)$$

$$= c \left( \frac{h}{2} \right)^2 \frac{1}{2\pi} e^{-i\omega_m x^T} \cdot \sum_\omega (i\omega)^3 \hat{u}(t, \omega) e^{i\nu x} + (i\nu)^3 \hat{u}(t, \nu) e^{i\omega x} + O(h^3)$$

$$= c \left( \frac{h}{2} \right) (i\nu (\omega_m))^3 \hat{u}(t, \nu (\omega_m)) + O(h^3)$$

where the last equality in (26) is valid due to the orthogonality of the terms: $<e^{i\omega_m x}, e^{i\omega_n x}>_{h/2} = 0$, $<e^{i\nu_m x}, e^{i\nu_n x}>_{h/2} = 0$.

Similarly, for the n-position in the vector which represent the $\nu_n$ frequency, we obtain $c \left( \frac{h}{2} \right) (i\omega_n)^3 \hat{u}(t, \omega_n)$.

Now, in order to evaluate $A^{-1} F T_h$, we use the Taylor expansions of the coefficients blocks in the matrix $A^{-1}$. Since we consider $\omega h << 1$, we look at the terms in the middle of the vector $F T_h$, where $\omega = 0, \pm 1, \pm 2, \ldots, \omega << N, \nu = O(N)$.

When we multiply a $2 \times 2$ block of $A^{-1}$ with the proper rows of $\omega = O(1), \nu = O(N)$, we obtain

$$\begin{pmatrix} O(1) & O(h) \\ O(h^3) & O(1) \end{pmatrix} \cdot c \left( \frac{h}{2} \right) \begin{pmatrix} (i \cdot O(N))^3 \hat{u}(t, O(N)) \\ (i \cdot O(1))^3 \hat{u}(t, O(1)) \end{pmatrix}$$

(26)

Since $\omega h << 1$, and from the relation (8) we can say that $(i\nu)^3 = O(1/h^3)$. From the smoothness assumption, $\hat{u}(\nu) = O(h^6)$, which yields $(i\nu)^3 \cdot \hat{u}(\nu) = O(h^3)$, and (26) is

$$\begin{pmatrix} O(h^2) \\ O(h) \end{pmatrix}$$
For the term $A^{-1}\mathcal{F}\mathbf{T}_\ell$, the m-position which represent the $\omega_m$ frequency in the vector $\mathcal{F}\mathbf{T}_\ell$ is

\[
\frac{h}{2} \left( \frac{1}{12} \left( \frac{h}{2} \right)^2 \right) e^{-i\omega_m x} \cdot \left( \frac{6c + 1}{12} \left( \frac{h}{2} \right)^2 \sum_\omega \left( (i\omega)^4 \hat{u}(t, \omega) e^{i\omega x} + (i\nu)^4 \hat{u}(t, \nu) e^{i\nu x} \right) + O(h^4) \right)
\]

\[
= \frac{6c + 1}{12} \left( \frac{h}{2} \right)^3 \left( \frac{1}{2\pi} \sum_\omega \left( (i\omega)^4 \hat{u}(t, \omega) \sum_{0 \leq j \leq 2N+1} e^{i(h-\omega_m)j\pi/2} + (i\nu)^4 \hat{u}(t, \nu) \sum_{0 \leq j \leq 2N+1} e^{i(h-\omega_m)j\pi/2} \right) + O(h^4) \right)
\]

\[
= \frac{6c + 1}{12} \left( \frac{h}{2} \right)^2 (i\omega_m)^4 \hat{u}(t, \omega_m) + O(h^4)
\]

(27)

where again the one before last equality in (27) is valid due to the orthogonality of the terms: $<e^{i\omega_m x}, e^{i\omega_n x}>_{h/2} = 0$, $<e^{i\nu_m x}, e^{i\nu_n x}>_{h/2} = 0$. And similarly, for the n-position in the vector which represent the $\nu_n$ frequency, we obtain the same.

Again we look at the terms in the middle of the vector $\mathcal{F}\mathbf{T}_1$, where $\omega = 0, \pm 1, \pm 2, \ldots, \omega << N, \nu = O(N)$. For example, when we multiply a block of $A^{-1}$ with the proper rows of $\omega = O(1), \nu = O(N)$, we obtain

\[
\begin{pmatrix}
O(1) & O(h) \\
O(h^3) & O(1)
\end{pmatrix}
\cdot
\frac{6c + 1}{12} \left( \frac{h}{2} \right)^2
\begin{pmatrix}
(i \cdot O(1))^4 \hat{u}(t, O(1)) \\
(i \cdot O(N))^4 \hat{u}(t, O(N))
\end{pmatrix}
\]

(28)

Since $(i\nu)^4 \cdot \hat{u}(\nu) = O(h^4)$ similarly as in the case of $A^{-1}\mathcal{F}\mathbf{T}_h$, we obtain that (28) is

\[
\begin{pmatrix}
O(h^2) \\
O(h^4)
\end{pmatrix}
\]

In summary, (26) and (28) yield
As for the high frequency modes:  

\[ \hat{T}_h = A^{-1}F T_h = \begin{pmatrix} \vdots \\ \hat{T}_{h_1} \\ \hat{T}_{h_2} \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ O(h^2) \\ O(h) \\ \vdots \end{pmatrix} \]

Now, we should bound the terms of the second term on the right-hand-side of (23) can be bounded by:

\[
\left\| e^{A t} \int_0^t e^{-A \tau} \hat{T}_\omega d\tau \right\| \leq \begin{pmatrix} \max_{0 \leq \tau \leq t} \hat{T}_1 (\tau, -\frac{N}{2}) & \frac{e^{Q_1(-\frac{N}{2})^t -1}}{Q_1(-\frac{N}{2})} \\ \max_{0 \leq \tau \leq t} \hat{T}_2 (\tau, -\frac{N}{2}) & \frac{e^{Q_2(-\frac{N}{2})^t -1}}{Q_2(-\frac{N}{2})} \\ \vdots \\ \max_{0 \leq \tau \leq t} \hat{T}_1 (\tau, \frac{N}{2}) & \frac{e^{Q_1(\frac{N}{2})^t -1}}{Q_1(\frac{N}{2})} \\ \max_{0 \leq \tau \leq t} \hat{T}_2 (\tau, \frac{N}{2}) & \frac{e^{Q_2(\frac{N}{2})^t -1}}{Q_2(\frac{N}{2})} \end{pmatrix}
\]

We should evaluate them, where

\[ \hat{T}_1 = \hat{T}_{h_1} + \hat{T}_{\ell_1} \]
\[ \hat{T}_2 = \hat{T}_{h_2} + \hat{T}_{\ell_2} \]

As for the high frequency modes: \( \hat{Q}_2(\omega) \) are negative and of the order of \( O \left( \frac{1}{h^2} \right) \). Therefore \( e^{\hat{Q}_2(\omega)t} \approx 0, \frac{e^{\hat{Q}_2(\omega)t} - 1}{\hat{Q}_2(\omega)} = O(h^2) \) and \( \forall \omega : O \left( \max_{0 \leq \tau \leq t} |\hat{T}_2 (\tau, \omega)| \cdot h^2 \right) \approx O(h^3) \).

As for the low frequency modes(\( \omega \neq 0 \)):

\[ \left| \frac{e^{\hat{Q}_1(\omega)t} - 1}{\hat{Q}_1(\omega)} \right| = \left| \frac{e^{(-\omega^2 + H.O.T.)t} - 1}{-\omega^2 + H.O.T.} \right| \leq \frac{1}{\omega^2} \leq O(1) \]
For $\omega = 0$, recall that $\hat{Q}_1(0) = 0$, hence from L'Hopital's rule we have

$$\left| \lim_{s \to 0} \frac{e^{st} - 1}{s} \right| = \left| \frac{e^{st}}{1} \right| = t = O(1)$$

Therefore we obtain $O\left( \max_{0 \leq \tau \leq t} |\hat{T}_1(\tau, \omega)| \cdot 1 \right) = O(h^2)$.

Eventually, from (29) these yield

$$||E||_{h/2} \leq ||\Psi||_{h/2} \cdot ||\hat{E}|| \leq \sqrt{2e^{\Lambda t}||\hat{E}||}(0) + O(h^2) \quad (30)$$

Note that from the structure of the truncation error (24),(25) we would expect that for $c = -\frac{1}{6}$ the order of the error also will be higher than 2. However this is not the case, since in [2] it was shown that the explicit form of the error is:

$$E(t) = e^{-\omega^2 t} \left[ \left( \frac{1 + 4c}{12 - 24c} \left( \frac{\omega h}{2} \right)^2 + O(h^4) \right) e^{i\omega x} \right. \right.$$  

$$+ \left. \left( \frac{ic}{4 - 8c} \left( \frac{\omega h}{2} \right)^3 + O(h^5) \right) e^{ivx} \right] \quad (31)$$

and it can be seen from (31) that for $c = -\frac{1}{4}$ we obtain 3rd-order.

This is illustrated in the following numerical example.

### 2.1.4 Numerical Example

The scheme was run for $u(x, t) = e^{\cos(2\pi(x-t))}$ on the interval $[0, 1]$ and $N = 32, 64, 128$ with 4-order Runga-Kutta time propagator. We run the scheme with $c = 0, -1/4, 1/6, -1/6$ and in the next figure it can be seen that for $c = -1/4$ we obtain a 3rd-order convergence rate at time $t = 1$:

### 2.2 5th Order Scheme - Numerical Example

Consider the following 4th-order approximation of two-point block:

for internal points:
The scheme was run for \( u(x, t) = e^{\cos(2\pi(x-t))} \) on the interval \([0, 1]\) and \(N = 32, 64, 128\) with 4-order Runga-Kutta time propagator. We run the scheme with \(c = 0, 4/13, 1/6, -1/6\) and in the next figure it can be seen that for \(c = 4/13\) we obtain a 5th-order convergence rate at time \(t = 1\):

\[
\frac{d^2}{dx^2} u_j \approx \frac{1}{12(h/2)^2}\left[(-u_{j-1} + 16u_{j-1/2} - 30u_j + 16u_{j+1/2} - u_{j+1}) + c(-u_{j-1} + 5u_{j-1/2} - 10u_j + 10u_{j+1/2} - 5u_{j+1} + u_{j+3/2})\right]
\]

\[
\frac{d^2}{dx^2} u_{j+1/2} \approx \frac{1}{12(h/2)^2}\left[(-u_{j-1/2} + 16u_j - 30u_{j+1/2} + 16u_{j+1} - u_{j+3/2}) + c(u_{j-1} - 5u_{j-1/2} + 10u_j - 10u_{j+1/2} + 5u_{j+1} - u_{j+3/2})\right]
\]

3 Two-point Block Finite Difference Schemes for IBVP Heat Equation

In this section we present the schemes and analysis of the boundary problem. We developed schemes for Dirichlet boundary problem and for Neumann boundary problem.
Consider the differential boundary value problem of the non-homogeneous heat equation:

\[
\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + F(x, t), \quad x \in [0, \pi], \ t \geq 0
\]

\[
u(t = 0) = f(x)
\]  

(32)

with Dirichlet boundary conditions:

\[
u(0, t) = g_0(t), \ \nu(\pi, t) = g_\pi(t)
\]  

(33)

or with Neumann boundary conditions:

\[
u_x(0, t) = g_0(t), \ \nu_x(\pi, t) = g_\pi(t)
\]  

(34)

We analogize both problems. We tried to generalize the periodic case directly for the boundary case. Though numerical experiments showed this is possible, the analysis is more complicated. Therefore we suggest to work in other discretization, which first we present for the periodic problem.
For both boundary problem, we would like to define a new grid without the boundaries:
\[ x_{j+1/4} = jh + h/4, h = \frac{\pi}{N}, x_{j+3/4} = x_j + 3h/4, j = 0, \ldots, N - 1, \]
altogether there are 2N points.
This grid is derived from the grid of the periodic problem on \([0, 2\pi]\) which has 4N points:
\[ x_{j+1/4} = jh + h/4, h = \frac{\pi}{N}, x_{j+3/4} = x_j + 3h/4, j = 0, \ldots, 2N - 1, x_{2N} = 2\pi. \]
Note that also \(x_N = \pi\). For simplicity, we again assume that \(N\) is even. See Figure 5 for illustration.

![Fig. 5. The grid for scheme (35).](image)

The scheme in each block is:

\[
\frac{d^2}{dx^2} u_{j+1/4} \approx \frac{1}{(h/2)^2} \left[ \left( u_{j-1/4} - 2u_{j+1/4} + u_{j+3/4} \right) + c \left( -u_{j-1/4} + 3u_{j+1/4} - 3u_{j+3/4} + u_{j+5/4} \right) \right] \\
\frac{d^2}{dx^2} u_{j+3/4} \approx \frac{1}{(h/2)^2} \left[ \left( u_{j+1/4} - 2u_{j+1/4} + u_{j+5/4} \right) + c \left( u_{j-1/4} - 3u_{j+1/4} + 3u_{j+3/4} - u_{j+5/4} \right) \right] 
\]

(35)

Now we would like to find \(\hat{Q}\).

For this grid, the analysis of the periodic problem is the done in the manner as the analysis in the previous section.

Since we have two grid points less than before, we obtain that in this notations the values for \(\omega\) are \(\omega = -N + 1, \ldots, N\). We split the spectrum according

\[
\nu = \nu(\omega) = \begin{cases} 
\omega - 2N & \omega > 0 \\
\omega + 2N & \omega \leq 0 
\end{cases}
\]

where the following relations hold:

\[
\forall \omega > 0 : e^{i\nu x_{j+1/4}} = -ie^{i\omega x_{j+1/4}}, e^{i\nu x_{j+3/4}} = ie^{i\omega x_{j+3/4}} \\
\forall \omega \leq 0 : e^{i\nu x_{j+1/4}} = ie^{i\omega x_{j+1/4}}, e^{i\nu x_{j+3/4}} = -ie^{i\omega x_{j+3/4}}
\]
We look for eigenvectors of the form of (10) and obtain a similar equation to (11). The symbols are the same as in (12) but \( r_1, r_2 \) are
\[
\tilde{r}_{1,2} = \frac{(-4 + 8c) \cos(\omega(h/2)) + \Delta}{2c(2\sin(\omega(h/2)) + \sin(2\omega(h/2)))}
\]

For \( \omega = -N + 1, \cdots, N, \omega \neq 0 \) the eigenvectors are similarly as before
\[
\tilde{\psi}_k(\omega) = e^{i\omega x} + \tilde{r}_k e^{i\nu x}, \, k = 1, 2
\]
(36)
Note that for \( \omega = N \) the eigenvectors are \( \frac{1}{\sqrt{2\pi}} \sin(Nx), \frac{1}{\sqrt{2\pi}} \cos(Nx) \) respectively.
For \( \omega = 0 \) the eigenvectors are \( \tilde{\psi}_1(0) = \frac{1}{\sqrt{2\pi}} e^{i0x} = \frac{1}{\sqrt{2\pi}} 1, \tilde{\psi}_2(0) = \frac{1}{\sqrt{2\pi}} e^{iNx} \) similarly as before.

We obtained the symbols an eigenvectors that enable us to do the analysis of the periodic problem as in the previous section.

3.2 The Eigenvectors of The IBVP

We would like to investigate the IBVP problem, and use the eigenvectors of the periodic problem in order to produce eigenvectors.
The motivation is to look for eigenvectors which have a similar form as in the analytic problem. i.e., if we reflect them from \([0, \pi]\) to \([0, 2\pi]\), we will obtain the eigenvectors of the periodic problem.
Denote the eigenvectors in general as
\[
\phi_k(\omega) = \tilde{\psi}_k(\omega) + \tilde{\gamma} \tilde{\psi}_k(-\omega), \, k = 1, 2.
\]

For Dirichlet boundaries, we look for eigenvectors of the form of \( \phi_k(\omega) = \tilde{\psi}_k(\omega) - \tilde{\psi}_k(-\omega), \, k = 1, 2 \), i.e., \( \tilde{\gamma} = -1 \). This is due to the fact that \( \{\sin(\omega x)\}_\omega \) are eigenvectors for the classic Dirichlet problem.
For Neumann boundaries, we look for eigenvectors of the form of \( \phi_k(\omega) = \tilde{\psi}_k(\omega) + \tilde{\psi}_k(-\omega), \, k = 1, 2 \), i.e., \( \tilde{\gamma} = 1 \). This is due to the fact that \( \{\cos(\omega x)\}_\omega \) are eigenvectors for the classic Neumann problem.

It can be seen as in the periodic problem that for each \( \omega \) there are two types of eigenvectors, \( \psi_1(\omega), \psi_2(\omega) \) and two types of eigenvalues \( \hat{Q}_1(\omega), \hat{Q}_2(\omega) \) respectively which hold \( \hat{Q}_{1,2}(\omega) = \hat{Q}_{1,2}(\omega) \).
For every \( \omega = -N + 1, \cdots, N - 1, \omega \neq 0 \), the following holds for \( k = 1, 2 \):
\[
\begin{align*}
\hat{Q}\tilde{\psi}_k(\omega) &= \hat{Q}_k(\omega)\tilde{\psi}_k(\omega) \\
\hat{Q}\tilde{\psi}_k(-\omega) &= \hat{Q}_k(\omega)\tilde{\psi}_k(-\omega)
\end{align*}
\]
if we subtract or sum this equations, this yields

\[ Q\phi_k(\omega) = \hat{Q}_k(\omega)\phi_k(\omega) \]

with \( \gamma = \mp 1 \) respectively.

We obtain that \( \phi_1(\omega), \phi_2(\omega) \) with \( \gamma = \mp 1 \) are also eigenvectors for the periodic problem.

Because of the form of \( \phi_1(\omega), \phi_2(\omega) \), for all \( \omega \neq 0, N \) only half of the frequencies (the non-negative ones) can be considered for each of the boundary value problems.

As mentioned, since the discretization of each of the boundary problem is taken from the proper periodic problem, it is obtained that for \( \omega = 1, ..., N - 1 \), \( \phi_1(\omega), \phi_2(\omega) \) are eigenvectors for Dirichlet with \( \gamma = -1 \) and \( \phi_1(\omega), \phi_2(\omega) \) are eigenvectors for Neumann with \( \gamma = 1 \).

For each of the cases, Dirichlet or Neumann, we need two more eigenvectors. Recall that \( \psi_1(0), \psi_2(0), \psi_1(N), \psi_2(N) \) are eigenvectors for the new periodic problem which can also be expressed as

\[
\frac{1}{\sqrt{2\pi}} \cos(0x) = \frac{1}{\sqrt{2\pi}}, \frac{1}{\sqrt{2\pi}} \sin(2Nx), \frac{1}{\sqrt{2\pi}} \sin(Nx), \frac{1}{\sqrt{2\pi}} \cos(Nx)
\]

respectively. Naturally from the classic Dirichlet and Neumann boundary problems, \( \frac{1}{\sqrt{2\pi}} \sin(2Nx), \frac{1}{\sqrt{2\pi}} \sin(Nx) \) are eigenvectors for the current Dirichlet problem and \( \frac{1}{\sqrt{2\pi}} \cos(0x), \frac{1}{\sqrt{2\pi}} \cos(Nx) \) are eigenvectors for the current Neumann problem with the corresponding eigenvalues of the periodic problem.

In summary, \( \frac{1}{\sqrt{2\pi}} \sin(2Nx), \frac{1}{\sqrt{2\pi}} \sin(Nx), \phi_1(\omega), \phi_2(\omega) \) with \( \gamma = -1 \) for \( \omega = 1, ..., N-1 \) are eigenvectors for the Dirichlet problem and \( \frac{1}{\sqrt{2\pi}} \cos(0x), \frac{1}{\sqrt{2\pi}} \cos(Nx), \phi_1(\omega), \phi_2(\omega) \) with \( \gamma = 1 \) for \( \omega = 1, ..., N-1 \) are eigenvectors for the Neumann problem.

### 3.2.1 An Example of the Eigenvalues for N=6

In order to substantiate the results presented above, we present the numeric symbols which obtained in the periodic two-point block approximation with \( N = 6 \):
The appropriate eigenvalues for both IBVP problem:

| $\omega$ | Dirichlet symbols | Neumann symbols |
|----------|-------------------|-----------------|
| 0        | -87.5415          | 0               |
| 1        | -85.5642,-0.99994 | -85.5642,-0.99994 |
| 2        | -79.8974,-3.99654 | -79.8974,-3.99654 |
| 3        | -71.288,-8.9584   | -71.288,-8.9584 |
| 4        | -60.8583,-15.7405 | -60.8583,-15.7405 |
| 5        | -50.1805,-23.7481 | -50.1805,-23.7481 |
| 6        | -29.1805          | -43.7708        |

Table 1
Dirichlet and Neumann symbols

3.3 Second and Third Order Scheme for The Reflected Dirichlet IBVP for Two-Point Block

3.3.1 Analysis

For constructing the scheme we calculate the ghost points next to the boundaries as $x_{-1/4} = -\frac{h}{4}, x_{N+1/4} = \pi + \frac{h}{4}$.

The scheme at the ghost points $u_{-1/4}, u_{N+1/4}$ is computed as follows, by using interpolation of 2 points and the boundaries:

$$u_{-1/4} = -u_{1/4} + 2g_0 + \left(\frac{h}{4}\right)^2 u_{xx}(0, t) + O(h^4) \quad (37)$$

$$u_{N+1/4} = -u_{N-1/4} + 2g_\pi + \left(\frac{h}{4}\right)^2 u_{xx}(\pi, t) + O(h^4) \quad (38)$$

where $u_{xx}(0, t), u_{xx}(\pi, t)$ can be calculated from the PDE:

$$u_{xx}(0, t) = u_t(0, t) - F(0, t)$$
$$u_{xx}(\pi, t) = u_t(\pi, t) - F(\pi, t)$$

(39)
Consider the approximation of two-point block.

for internal points, \( j = 1, \ldots, N - 2 \):

\[
\frac{d^2}{dx^2} u_{j+1/4} \approx \frac{1}{(h/2)^2} \left[ (u_{j-1/4} - 2u_{j+1/4} + u_{j+3/4}) + c(-u_{j-1/4} + 3u_{j+1/4} - 3u_{j+3/4} + u_{j+5/4}) \right]
\]

\[
\frac{d^2}{dx^2} u_{j+3/4} \approx \frac{1}{(h/2)^2} \left[ (u_{j+1/4} - 2u_{j+3/4} + u_{j+5/4}) + c(u_{j-1/4} - 3u_{j+1/4} + 3u_{j+3/4} - u_{j+5/4}) \right]
\]

on the boundaries the scheme is different due to the ghost points:

\[
\frac{d^2}{dx^2} u_{1/4} \approx 2(1 - c)g_0 + (1 - c) \left( \frac{h}{4} \right)^2 u_{xx}(0, t) + O(h^4)
\]

\[
+ \frac{1}{(h/2)^2} \left[ (-3u_{1/4} + u_{3/4}) + c(4u_{1/4} - 3u_{3/4} + u_{5/4}) \right]
\]

\[
\frac{d^2}{dx^2} u_{3/4} \approx -2cg_0 + c \left( \frac{h}{4} \right)^2 u_{xx}(0, t) + O(h^4)
\]

\[
+ \frac{1}{(h/2)^2} \left[ (u_{1/4} - 2u_{3/4} + u_{5/4}) + c(-4u_{1/4} + 3u_{3/4} - u_{5/4}) \right]
\]

\[
\frac{d^2}{dx^2} u_{N-3/4} \approx -2cg_\pi + c \left( \frac{h}{4} \right)^2 u_{xx}(\pi, t) + O(h^4) + \frac{1}{(h/2)^2} \left[ (u_{N-5/4} - 2u_{N-3/4} + u_{N-1/4}) + c(-u_{N-5/4} + 3u_{N-3/4} - 4u_{N-1/4}) \right]
\]

\[
\frac{d^2}{dx^2} u_{N-1/4} \approx 2(1 - c)g_\pi + (1 - c) \left( \frac{h}{4} \right)^2 u_{xx}(\pi, t) + O(h^4) + \frac{1}{(h/2)^2} \left[ (u_{N-3/4} - 3u_{N-1/4}) + c(u_{N-5/4} - 3u_{N-3/4} + 4u_{N-1/4}) \right]
\]

The truncation errors are:

for \( j = 1, \ldots, N - 2 \) :
The truncation errors are different on the boundaries due to the ghost points:

\[(T_e)_{j+\frac{1}{4}} = \frac{1}{12} \left( \frac{h}{2} \right)^2 \frac{\partial^4 u_{j+\frac{1}{4}}}{\partial x^4} + \]
\[c \left[ \left( \frac{h}{2} \right) \frac{\partial^3 u_{j+\frac{1}{4}}}{\partial x^3} + \frac{1}{2} \left( \frac{h}{2} \right)^2 \frac{\partial^4 u_{j+\frac{1}{4}}}{\partial x^4} + \frac{1}{4} \left( \frac{h}{2} \right)^3 \frac{\partial^5 u_{j+\frac{1}{4}}}{\partial x^5} \right] + O(h^4) = O(h)\]

\[(T_e)_{j+\frac{3}{4}} = \frac{1}{12} \left( \frac{h}{2} \right)^2 \frac{\partial^4 u_{j+\frac{3}{4}}}{\partial x^4} + \]
\[c \left[ -\left( \frac{h}{2} \right) \frac{\partial^3 u_{j+\frac{3}{4}}}{\partial x^3} + \frac{1}{2} \left( \frac{h}{2} \right)^2 \frac{\partial^4 u_{j+\frac{3}{4}}}{\partial x^4} - \frac{1}{4} \left( \frac{h}{2} \right)^3 \frac{\partial^5 u_{j+\frac{3}{4}}}{\partial x^5} \right] + O(h^4) = O(h)\]

It can be seen that the difference between the internal truncation errors and the truncation errors on the boundaries is of order of \(O(h^2)\).

Now the scheme can be written as:
\[ \frac{\partial \mathbf{v}}{\partial t} = Q_D \mathbf{v} + B_D + F , \quad t \geq 0 \tag{40} \]

\[ \mathbf{v}(t = 0) = \mathbf{f} . \]

where \( Q_D \) is the discretization matrix and \( B_D \) is the boundary vector:

\[
B_D = \begin{pmatrix}
2(1 - c)g_0 + (1 - c) \left( \frac{h}{\pi} \right)^2 u_{xx}(0, t) + O(h^4) \\
-2cg_0 + c \left( \frac{h}{\pi} \right)^2 u_{xx}(0, t) + O(h^4) \\
\vdots \\
0 \\
-2cg_\pi + c \left( \frac{h}{\pi} \right)^2 u_{xx}(\pi, t) + O(h^4) \\
2(1 - c)g_\pi + (1 - c) \left( \frac{h}{\pi} \right)^2 u_{xx}(\pi, t) + O(h^4)
\end{pmatrix} \tag{41}
\]

Note that the stability is preserved here since \( \phi_k(\omega), k = 1, 2 \) are linear combinations of \( \psi_k(\omega), k = 1, 2 \) and for them we proved stability in section 2.

### 3.3.2 Estimation of The Error

The analysis here is similar to the one presented in section 2. The only difference here is the truncation error.

It is assumed again that the solution is smooth enough, i.e. \( \mathbf{u} \in C^5 \) and according to this assumption the coefficients \( \hat{\mathbf{u}}(t, \omega) \) decay fast as \( \omega^{-6} \). Therefore it is sufficient to look at \( \omega h << 1 \).

From (4) the equation for the error:

\[ \frac{\partial \mathbf{E}}{\partial t} = Q \mathbf{E} + \mathbf{T}_e \tag{42} \]

with homogeneous boundaries.

The expansion of \( \mathbf{E} \) in the \( \phi_j \) basis is

\[ \mathbf{E}(t) = \sum_\omega \hat{E}_1(t, \omega) \phi_1(\omega) + \hat{E}_2(t, \omega) \phi_2(\omega) \tag{43} \]

where \( \mathbf{E} = \Phi \hat{\mathbf{E}}. \)
As in the previous section we obtain the solution for the error from the discretized equation:

\[
\|\hat{E}\| = \left\| \begin{pmatrix}
  e^{\hat{Q}_1 (-\frac{N}{2}) t} \hat{E}_1 (0, -\frac{N}{2}) \\
  e^{\hat{Q}_2 (-\frac{N}{2}) t} \hat{E}_2 (0, -\frac{N}{2}) \\
  \vdots \\
  e^{\hat{Q}_1 (\frac{N}{2}) t} \hat{E}_1 (0, \frac{N}{2}) \\
  e^{\hat{Q}_2 (\frac{N}{2}) t} \hat{E}_2 (0, \frac{N}{2}) \\
\end{pmatrix}
\right\| + e^{\Lambda t} \cdot \int_0^t e^{-\Lambda \tau} \left( T_e \right) d\tau
\]

\[
\leq \| e^{\Lambda t} \hat{E}_0 \| + \left\| e^{\Lambda t} \cdot \int_0^t e^{-\Lambda \tau} \left( T_e \right) d\tau \right\| \tag{44}
\]

where \( \Lambda \) is the eigenvalues matrix as before. Since the initial error, \( E_0 \), is either 0 or, at most of the order of machine error, the term \( e^{\Lambda t} \hat{E}_0 \) can be neglected as before. Denote

\[
\Phi = \begin{pmatrix}
  \vdots & \vdots & \vdots & \vdots \\
  \phi_1 (0) & \phi_2 (0) & \cdots & \phi_1 (N) & \phi_2 (N) \\
  \vdots & \vdots & \vdots & \vdots 
\end{pmatrix}
\]

Now denote \( T_e = T_I + T_B \), where \( T_I \) is the truncation error of the periodic problem in the previous section and \( T_B \) is the difference between the truncation error of the boundary problem and periodic problem:
(T_B)_{1/4} = -\frac{1}{192} \left( \frac{h}{2} \right)^2 \frac{\partial^4 u_{1/4}}{\partial x^4} + \frac{1}{384} \left( \frac{h}{2} \right)^3 \frac{\partial^5 u_{1/4}}{\partial x^5} \\
+ c \left[ \frac{1}{192} \left( \frac{h}{2} \right)^2 \frac{\partial^4 u_{1/4}}{\partial x^4} - \frac{1}{384} \left( \frac{h}{2} \right)^3 \frac{\partial^5 u_{1/4}}{\partial x^5} \right] + O(h^4) = O(h^2)

(T_B)_{3/4} = -\frac{1}{192} \left( \frac{h}{2} \right)^2 \frac{\partial^4 u_{3/4}}{\partial x^4} + \frac{1}{384} \left( \frac{h}{2} \right)^3 \frac{\partial^5 u_{3/4}}{\partial x^5} \\
+ c \left[ \frac{1}{192} \left( \frac{h}{2} \right)^2 \frac{\partial^4 u_{3/4}}{\partial x^4} + \frac{1}{384} \left( \frac{h}{2} \right)^3 \frac{\partial^5 u_{3/4}}{\partial x^5} \right] + O(h^4) = O(h^2)

(T_B)_{N-1/4} = -\frac{1}{192} \left( \frac{h}{2} \right)^2 \frac{\partial^4 u_{N-1/4}}{\partial x^4} + \frac{1}{384} \left( \frac{h}{2} \right)^3 \frac{\partial^5 u_{N-1/4}}{\partial x^5} \\
+ c \left[ \frac{1}{192} \left( \frac{h}{2} \right)^2 \frac{\partial^4 u_{N-1/4}}{\partial x^4} - \frac{1}{384} \left( \frac{h}{2} \right)^3 \frac{\partial^5 u_{N-1/4}}{\partial x^5} \right] + O(h^4) = O(h^2)

(T_B)_{N-3/4} = -\frac{1}{192} \left( \frac{h}{2} \right)^2 \frac{\partial^4 u_{N-3/4}}{\partial x^4} + \frac{1}{384} \left( \frac{h}{2} \right)^3 \frac{\partial^5 u_{N-3/4}}{\partial x^5} \\
+ c \left[ \frac{1}{192} \left( \frac{h}{2} \right)^2 \frac{\partial^4 u_{3/4}}{\partial x^4} + \frac{1}{384} \left( \frac{h}{2} \right)^3 \frac{\partial^5 u_{N-3/4}}{\partial x^5} \right] + O(h^4) = O(h^2)

Any different position of the vector $T_B$ is zero.

Similar to the analysis was given in the previous section, $T_I = T_{Ie} + T_{Ih}$, where

$T_{Ih} = \frac{c}{12} \left( \frac{h}{2} \right) \text{ diag } (1, -1, 1, -1, \ldots, 1, -1) u_{xxx}$

$T_{Ie} = \frac{6c + 1}{12} \left( \frac{h}{2} \right)^2 u_{xxxx} + O(h^3)$

$T_B = \frac{c - 1}{192} \left( \frac{h}{2} \right)^2 u_{xxxx} + O(h^3)$

And we would like to evaluate $\hat{T}_{Ih}, \hat{T}_{Ie}$. Since we treat non-homogeneous boundary problem, here, instead of the terms $(iv)^3 \hat{u}(t, \nu) = O(h^3)$ we have $u_{xxx}, u_{xxxx}$ which decay at least as $\frac{1}{N} = O(h)$.

Therefore, as in section 2, we can obtain that $T_{Ih} = O(h^2), \hat{T}_{Ie} = O(h^3)$. Also, $\hat{T}_B = O(h^3)$.

The second term on the right-hand-side of (44) can be bounded by:
Runga-Kutta time propagator. We run the scheme with $c$

Eventually these yield

The scheme was run where we considered Dirichlet boundary conditions for

For the high frequency modes: $\hat{Q}_2(\omega)$, we obtain:

For terms with the low frequency mode: $\hat{Q}_1(\omega)$ are of the order of $O(1)$, therefore

The matrices $\Phi, \Phi^{-1}$ are at most an order change of columns of the matrices $\Psi, \Psi^{-1}$, thus their norms $\|\Phi\|_{h/2} \leq 2\|\Psi\|_{h/2} = 2\sqrt{2}$, $\|\Phi^{-1}\|_{h/2} \leq 2\|\Psi\|_{h/2} = \frac{20\sqrt{2}}{9}$ are bounded.

Eventually these yield

3.4 Numerical Example

The scheme was run where we considered Dirichlet boundary conditions for $u(x, t) = e^{i\omega(x-t)}$ on the interval $[0, 1]$, and $N$ = 32, 64, 128 with 4-order Runga-Kutta time propagator. We run the scheme with $c = 0, -1/4, 1/6, -1/6$
and in the next figure it can be seen that for $c = -1/4$ we obtain a 3th-order convergence rate at time $t = 1$:

![Convergence plot](image)

Fig. 6. Convergence plot of 3rd order scheme for non-homogeneous Dirichlet (37), $\log_{10} \|E\|$ vs. $\log_{10} (\frac{h}{2})$ for $c = 0, -1/4, 1/6, -1/6$. 

32
3.5 Second and third Order Scheme for the Reflected Neumann Problem for Two-Point Block

Consider the case of the previous section only with Neumann boundaries \( \text{(34)} \). The problem has the same eigenvalues and eigenvectors for the approximation of two-point block so the analysis here is the same. The difference here is in the ghost points \( u_{-1/4}, u_{N+1/4} \) which are computed as follows, by using interpolation of 2 points and the boundaries:

\[
\begin{align*}
    u_{-1/4} &= u_{1/4} - \left( \frac{h}{2} \right) u(0, t)_x - \frac{1}{3} \left( \frac{h}{4} \right)^3 u(0, t)_{xxx} + O(h^5) \\
    u_{N+1/4} &= u_{N-1/4} + \left( \frac{h}{2} \right) u(\pi, t)_x + \frac{1}{3} \left( \frac{h}{4} \right)^3 u(\pi, t)_{xxx} + O(h^5)
\end{align*}
\]

where \( u(0, t)_{xxx}, u(\pi, t)_{xxx} \) are known from the PDE:

\[
\begin{align*}
    u_{xxx}(0, t) &= u_{xx}(0, t) - F_x(0, t) \\
    u_{xxx}(\pi, t) &= u_{xx}(\pi, t) - F_x(\pi, t)
\end{align*}
\]

3.5.1 Numerical Example

The scheme was run under the same conditions as the previous example, with the exception that now Neumann boundary conditions have been considered. We run the scheme with \( c = 0, -1/4, 1/6, -1/6 \) and in the next figure it can be seen that for \( c = -1/4 \) we obtain a 3rd-order convergence rate at time \( t = 1 \):
3.6 5th Order Scheme - Numerical Example

Consider the following 4th-order approximation of two-point block:

for internal points, $j = 1, ..., N - 2$:

$$\frac{d^2}{dx^2} u_{j+1/4} \approx \frac{1}{12(h/2)^2} \left[ (-u_{j-3/4} + 16u_{j-1/4} - 30u_{j+1/4} + 16u_{j+3/4} - u_{j+5/4}) \\
+ c(-u_{j-3/4} + 5u_{j-1/4} - 10u_{j+1/4} + 10u_{j+3/4} - 5u_{j+5/4} + u_{j+7/4}) \right]$$

$$\frac{d^2}{dx^2} u_{j+3/4} \approx \frac{1}{12(h/2)^2} \left[ (-u_{j-1/4} + 16u_{j+1/4} - 30u_{j+3/4} + 16u_{j+5/4} - u_{j+7/4}) \\
+ c(u_{j-3/4} - 5u_{j-1/4} + 10u_{j+1/4} - 10u_{j+3/4} + 5u_{j+5/4} - u_{j+7/4}) \right]$$

It can be seen from the scheme that two ghost points are needed for every boundary, and the approximations at $x = 3/4, N - 3/4$ are also affected by the ghost points.

The ghost points for Dirichlet Boundary problem are computed as follows, by using interpolation of 2 points and the boundaries:
\[ u_{-1/4} = -u_{1/4} + 2g_0 + \left( \frac{h}{4} \right)^2 u_{xx}(0, t) + \frac{1}{12} \left( \frac{h}{4} \right)^4 u_{xxxx}(0, t) + O(h^6) \]
\[ u_{-3/4} = -u_{3/4} + 2g_0 - 9 \left( \frac{h}{4} \right)^2 u_{xx}(0, t) - \frac{81}{12} \left( \frac{h}{4} \right)^4 u_{xxxx}(0, t) + O(h^6) \]
\[ u_{N+1/4} = -u_{N-1/4} + 2g_{\pi} + \left( \frac{h}{4} \right)^2 u_{xx}(\pi, t) + \frac{1}{12} \left( \frac{h}{4} \right)^4 u_{xxxx}(\pi, t) + O(h^6) \]
\[ u_{N+3/4} = -u_{N-3/4} + 2g_{\pi} - 9 \left( \frac{h}{4} \right)^2 u_{xx}(\pi, t) - \frac{81}{12} \left( \frac{h}{4} \right)^4 u_{xxxx}(\pi, t) + O(h^6) \]

where \( u_{xx}(0, t), u_{xx}(\pi, t) \) are known from the PDE as before and also \( u_{xxxx}(0, t), u_{xxxx}(\pi, t) \):

\[ u_{xxxx}(0, t) = u_{txx}(0, t) - F_{xx}(0, t) \]
\[ u_{xxxx}(\pi, t) = u_{txx}(\pi, t) - F_{xx}(\pi, t) \]

Hence the scheme is different on the boundaries due to the ghost points:

\[ \frac{d^2}{dx^2} u_{1/4} \approx (30 + 8c) g_{D_0} + (7 - 4c) \left( \frac{h}{4} \right)^2 u_{xx}(0, t) + \frac{(-65 - 76c)}{12} \left( \frac{h}{4} \right)^4 u_{xxxx}(0, t) \]
\[ + \frac{1}{12(h/2)^2} \left[ (-46u_{1/4} + 17u_{3/4} - u_{5/4}) \right] + c(-15u_{1/4} + 11u_{3/4} - 5u_{5/4} + u_{7/4}) \]

\[ \frac{d^2}{dx^2} u_{3/4} \approx (-2 - 8c) g_{D_0} + (-1 + 4c) \left( \frac{h}{4} \right)^2 u_{xx}(0, t) + \frac{(-1 + 76c)}{12} \left( \frac{h}{4} \right)^4 u_{xxxx}(0, t) \]
\[ + \frac{1}{12(h/2)^2} \left[ (17u_{1/4} - 30u_{3/4} + 16u_{5/4} - u_{7/4}) \right] + c(15u_{1/4} - 11u_{3/4} + 5u_{5/4} - u_{7/4}) \]

\[ \frac{d^2}{dx^2} u_{N-1/4} \approx (30 + 8c) g_{D_n} + (7 - 4c) \left( \frac{h}{4} \right)^2 u_{xx}(\pi, t) + \frac{(-65 - 76c)}{12} \left( \frac{h}{4} \right)^4 u_{xxxx}(\pi, t) \]
\[ + \frac{1}{12(h/2)^2} \left[ (-46u_{N-1/4} + 17u_{N-3/4} - u_{N-5/4}) \right] + c(-15u_{N-1/4} + 11u_{N-3/4} - 5u_{N-5/4} + u_{N-7/4}) \]

\[ \frac{d^2}{dx^2} u_{N-3/4} \approx (-2 - 8c) g_{D_n} + (-1 + 4c) \left( \frac{h}{4} \right)^2 u_{xx}(\pi, t) + \frac{(-1 + 76c)}{12} \left( \frac{h}{4} \right)^4 u_{xxxx}(\pi, t) \]
\[ + \frac{1}{12(h/2)^2} \left[ (17u_{N-1/4} - 30u_{N-3/4} + 16u_{N-5/4} - u_{N-7/4}) \right] + c(15u_{N-1/4} - 11u_{N-3/4} + 5u_{N-5/4} - u_{N-7/4}) \]
The ghost points for Neumann Boundary problem are computed as follows, by using interpolation of 2 points and the boundaries:

\[
\begin{align*}
u_{-1/4} &= u_{1/4} - \left( \frac{h}{2} \right) g_{0x} - \frac{1}{3} \left( \frac{h}{4} \right)^3 g_{0xxx} - \frac{1}{60} \left( \frac{h}{4} \right)^5 g_{0xxxxx} + O(h^7) \\
u_{-3/4} &= u_{3/4} - 3 \left( \frac{h}{2} \right) g_{0x} - 9 \left( \frac{h}{4} \right)^3 g_{0xxx} - \frac{243}{60} \left( \frac{h}{4} \right)^5 g_{0xxxxx} + O(h^7) \\
u_{N+1/4} &= u_{N-1/4} + \left( \frac{h}{2} \right) g_{\pi x} + \frac{1}{3} \left( \frac{h}{4} \right)^3 g_{\pi xxx} + \frac{1}{60} \left( \frac{h}{4} \right)^5 g_{\pi xxxxx} + O(h^7) \\
u_{N+3/4} &= u_{N-3/4} + 3 \left( \frac{h}{2} \right) g_{\pi x} + 9 \left( \frac{h}{4} \right)^3 g_{\pi xxx} + \frac{243}{60} \left( \frac{h}{5} \right)^5 g_{\pi xxxxx} + O(h^7)
\end{align*}
\]

where \(g_{0xxx}, g_{\pi xxx}\) are known from the PDE as before and also \(g_{0xxxxx}, g_{\pi xxxxx}\):

\[
\begin{align*}
g_{N0xxxxx} &= u_{xxxxx}(0, t) = u_{txx}(0, t) - F_{xxx}(0, t) \\
g_{N\pi xxxxx} &= u_{xxxxx}(\pi, t) = u_{txxx}(\pi, t) - F_{xxx}(\pi, t)
\end{align*}
\]

3.7 Numerical Example

The scheme was run under the same conditions as the previous example of 3rd-order Dirichlet. We run the scheme with \(c = 0, 4/13, 1/6, -1/6\) and in the next figure it can be seen that for \(c = -1/4\) we obtain a 5th-order convergence rate at time \(t = 1\):
4 Summary

In this paper, we present proofs of stability and convergence for the periodic heat equation. Also and mainly in this paper, we derived a methodology for constructing high-order finite-difference semi-discrete schemes for initial boundary value problems. A new approach to handle the approximations on the boundaries is offered.

We have set the groundwork for using the schemes, which were developed for second derivative in space for a periodic problem in [2], in initial boundary value problems. Specifically, we illustrated the schemes on the homogeneous and non-homogeneous heat equation as was done in the periodic problem.

We presented a 3rd-order accurate approximations with Dirichlet or Neumann boundaries conditions for $\frac{\partial^2}{\partial x^2}$. The scheme uses terms with lower order than the standard terms of 2nd-order scheme. They make the truncation error oscillatory and eventually raise the order of the actual error.

We demonstrated how to impose Dirichlet or Neumann boundary conditions and developed a 5th-order accurate approximation for $\frac{\partial^2}{\partial x^2}$, using the same method. The method can be generalized systematically even for higher order accurate approximations.
Generalizations of the method for high order accurate schemes for periodic and IBVP’s are left for future work.

References

[1] S. Abarbanel, A. Ditkowski, B. Gustafsson, On error bounds of finite difference approximations to partial differential equations—temporal behavior and rate of convergence, Journal of Scientific Computing 15 (1) (2000) 79–116.

[2] A. Ditkowski, High order finite difference schemes for the heat equation whose convergence rates are higher than their truncation errors, in: Spectral and High Order Methods for Partial Differential Equations ICOSAHOM 2014, Springer, 2015, pp. 167–178.

[3] B. Gustafsson, The convergence rate for difference approximations to mixed initial boundary value problems, Mathematics of Computation 29 (130) (1975) 396–406.

[4] B. Gustafsson, The convergence rate for difference approximations to general mixed initial-boundary value problems, SIAM Journal on Numerical Analysis 18 (2) (1981) 179–190.

[5] B. Gustafsson, H.-O. Kreiss, J. Oliger, Time-dependent problems and difference methods, John Wiley & Sons, 1995.

[6] M. Zhang, C.-W. Shu, An analysis of three different formulations of the discontinuous galerkin method for diffusion equations, Mathematical Models and Methods in Applied Sciences 13 (03) (2003) 395–413.