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# FINITE DIFFERENCE SCHEMES IN A MULTI-POINT STENCIL AND FINITE DIFFERENCE SCHEMES WITH THE EXACT SPECTRUM FOR PERIODIC BOUNDARY CONDITIONS

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**Abstract:** In this paper the finite difference scheme (FDS) for local approximation of periodic function's derivatives in a $2n+1$ point stencil is studied, obtaining higher order accuracy approximation. This method in the uniform grid with $N$ mesh points is used to approximate the differential operator of the second and the first order derivatives in the space, using the multi-point stencil. The matrix representation $A$ of this FDS is investigated also for other order derivatives. It is shown that the eigenvalues of FDS matrix representation $A$ can be obtained as a sum whose terms do not depend on $n$. This allows easily solving the FDS by the spectral decomposition of $A$.

The described methods are applicable for various mathematical physics problems involving periodic boundary conditions (PBC). The solutions of some problems of parabolic type partial differential equations (PDE) with PBCs are obtained, using the method of lines (MOL) to approach the PDEs in the time and the discretization in space applying the FDS of a different order of the approximation and finite difference scheme with exact spectrum (FDSES).

These methods are compared with the global approximations or pseudospectral methods, which are based on using differentiation matrices (DMs) for derivatives on a uniform grid with trigonometric interpolation.

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In this paper we show that the approximation FDS in the limit case when $n$ tends to infinity is equivalent to FDSES; moreover, FDSES is equivalent to a spectral differentiation matrix based on trigonometric (Fourier) interpolant.

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**Key Words:** approximations, eigenvalues, multi-point stencil, differentiation matrices, trigonometric interpolant

## 1. Introduction

Finite difference methods are important for approximating differential operators and solving various ordinary and partial differential equations numerically. Probably the most casual are the second order accurate FDS for approximation of the first and second order derivatives in a uniform 3-point stencil. We consider approximation of the differential operator $\partial^m/\partial x^m$ in a uniform $2n+1$, $n \geq 1$ point stencil, where $m \leq 2n$. The algebraic convergence rate is $O(N^{-2n})$.

The most attention will be devoted to the case when the function whose derivatives are to be approximated is periodic. On one hand, models of many real world processes have periodic solutions; on the other hand, because of function periodicity, the matrix representation of FDS are circulant matrices. This allows easily solving the respective FDS using the fast Fourier transform [2].

Our main result concerns the possibility to express the discrete eigenvalues of the finite difference matrix in a way which allows easily changing the approximation order and simplifies solving FDS.

We also consider global approximation methods, namely the differentiation matrices (DM), that are widely used for solving differential equations of boundary value type [3], [17], [14], [16], and FDSES. In this paper we show that both methods in the considered case are in fact equivalent. Some classical facts about the DMs are recalled below.

### 1.1. Previous Work

In the first publication about FDSES [10] the finite differences with the second order of approximation in the uniform grid are used for the approximation of the second order derivative in the space segment $x \in [0, L]$ with the homogeneous boundary conditions of first kind.

### 1.2. Differentiation Matrices

DMs are obtained when applying the pseudospectral method, where the unknown solution is expanded as a global interpolant trigonometric or polynomial interpolant. Spectral DMs for problems with PBCs are based on Fourier interpolant. In contrast, some other methods (such as finite differences) use local interpolants (such as piecewise polynomials) for expansion of the unknown solution. As pointed out in [16], the accuracy of the global method is superior compared to the accuracy of the local methods.

The pseudospectral method for solving differential equations is based on interpolants of the form [16], [17]:

$$f(x) \approx P_{N-1} = \sum_{j=1}^{N} \Phi_j(x) f(x_j).$$

Here $\{x_j\}_{j=1}^N$ is a set of grid points and $\{\Phi_j(x)\}_{j=1}^N$ is a set of interpolation functions satisfying $\Phi_j(x_k) = \delta_{jk}$ (the Kronecker delta), $f(x_k) = P_{N-1}(x_k)$, $k = \overline{1, N}$. Generally the interpolants are weighted with a weight function $\alpha(x) > 0$; we shall not consider this case in the paper. For Chebyshev and Hermite interpolation the interpolating functions $\Phi_j(x)$ are polynomials of degree $N-1$. For non-polynomial cases the interpolants are trigonometric.

The derivative operator is obtained by evaluating the $m$-th order derivatives of the interpolants at the grid points $\{x_k\}$. The operator can be represented as a matrix $D^{(m)}$ whose entries are $D_{kj}^{(m)} = \frac{\mathrm{d}^m}{\mathrm{d}\, x^m}[\Phi_j(x)]_{x=x_k}$. For boundary value problems with the PBCs the DMs $D^{(m)}$ are circulant and therefore can be given by the first row.

### 1.3. Forming FDSES from FDS

The finite difference matrix $A$ is represented in the form $A = WDW^*$; columns of $W$ are the eigenvectors of $A$, $W^*$ is the complex conjugate of $W$, $D$ is the diagonal matrix of the discrete eigenvalues. For the FDSES the elements of diagonal matrix $D$ are replaced in a specific way with the first $N$ continuous eigenvalues from the differential operator. In the case of PBCs we can show that this method is equivalent to the pseudospectral method with DMs based on trigonometric interpolant. The FDSES method in greater detail is discussed in the Section 2.1.

### 1.4. Applications

In this work new numerical algorithms are developed for solving 1D and 2D problems of the second order ordinary (ODE) and partial differential equations (PDE) with PBC. The nonlinear heat transfer equations can be written in the following form [13], [6]:

$$u_t = k(x)\, g_1(u)_{xx} + p(x)\, g_2(u)_x + q(x)\, g_3(u) + f(u), \tag{1}$$

where $u_t = \frac{\partial u}{\partial t}$, $u_x = \frac{\partial u}{\partial x}$, $u_{xx} = \frac{\partial^2 u}{\partial x^2}$; here $k(x) \geq 0$, $p(x)$ and $q(x)$ are real functions, $g_1(u)$, $g_1'(u) > 0$, $g_2(u)$ and $g_3(u)$ are trigonometric or exponential functions, $x \in (0, L)$, $t > 0$ are the space and time variables, $L$ is the period, $u = u(x,t)$ is the unknown function (for ODE we have boundary value problem with $u = u(x)$). Similarly, also a system of PDEs can be considered, where $k, p, q$ are matrices, $u$ is column-vector. For the linear heat transfer equations take $g_j(u) = u$, $j = 1, 2, 3$, $f(u) = f(x)$.

The heat transfer problem is solved numerically using the method of lines and two finite difference methods for the approximation of the spatial derivatives: local approximation with finite differences in uniform grid (FDS, FDSES) and global approximation with differentiation matrices.

Equations in the space are discretized using uniform grid $x_j = jh, j = \overline{0, N}$. The approximate functions $u(x_j, t)$ are denoted with $u_j(t)$. In the 2D problem the second argument $t$ is not discretized and method of lines (MOL) is used to solve such problems with given initial conditions at $t = 0$. For local approximation the discrete equations of the system of nonlinear ODEs are in the following form:

$$\dot{U} = KA_{2,n}g_1(U) + PA_{1,n}g_2(U) + Qg_3(U) + f(U), \tag{2}$$

where

- $K$, $P$ and $Q$ are diagonal matrices with diagonal entries $k(x_j)$, $p(x_j)$ and $q(x_j)$, $j = 1, 2, \ldots, N$, respectively;
- $A_{1,n}$ and $A_{2,n}$ are $N \times N$ circulant matrices
- $U = U(t)$, $g_r(U)$, $r = 1, 2, 3$, $f(U)$ and $\dot{U}$ are the column-vectors of length $N$ with elements $u_j(t)$, $g_r(u_j(t))$, $f(u_j(t))$, $\frac{\mathrm{d}\, u_j}{\mathrm{d}\, t}(t)$, $j = \overline{1, N}$, respectively.

Unlike other boundary condition types, PBC allows to freely increase approximation order by increasing the stencil of grid points. In the case of $2n + 1$ point stencil we have to use additional conditions of periodicity $u_r = u_{N+r}$, $r = \overline{-n, n}$. This way algorithms with higher order precision (different order FDS) can be obtained.

The second advantage of PBC lies in the fact a circulant matrix is uniquely determined by its first row. For such matrices it is easy to do arithmetic operations in shorter computation time; it is also possible to get the inverse matrix (when it exists) analytically.

Another advantage is the simple solution of the pseudospectral problem. Orthonormal eigenvectors $w_k, w_k^*$ with the elements $w_{k,j} = \sqrt{N^{-1}} \exp(2\pi ijk/N)$, $w_{k,j}^* = \sqrt{N^{-1}} \exp(-2\pi ijk/N)$ do not depend on the elements of circulant matrix; here $k, j = \overline{1, N}$ and $i = \sqrt{-1}$ stands for the imaginary unit.

By solving the discrete spectral problem, we can express the matrix $A_{m,n}$ in the form $A_{m,n} = WD_{m,n}W^*$, where the columns of matrix $W$ are eigenvectors of $A_{m,n}$, $W^*$ is the conjugate transpose of $W$ and $D_{m,n}$ is a diagonal matrix with the eigenvalues $\mu_{m,k}$ of matrix $A_{m,n}$ on the diagonal (FDS), $m = 1; 2$, $k = \overline{1, N}$. Eigenvalues are obtained analytically for every multi-point stencil.

In order to compare the solution obtained by the new numerical methods with the exact solution, in the linear case the differential and discrete problems are also solved analytically using the Fourier method. We consider also some examples when the exact solution of ODE with variable coefficients or linear PDE can be found and compared to our numerical solution. Generally, when the exact solution is not known (see also the example of a nonlinear PDE) standard solvers can be used to obtain numerical solutions for comparisons.

## 2. Approximating Derivatives in the Uniform Grid

We consider the global approximation of first and second order derivatives in the uniform grid $t_k = kh$, $Nh = 2\pi$, $h = \frac{2\pi}{N}$, $k = \overline{1, N}$, using trigonometrical interpolation and local approximation of these derivatives using $2n + 1$-points stencil in this grid.

### 2.1. Global Approximations with FDSES

Traditionally, for the heat transport equation the finite difference matrix $A$ can be represented as $A = WDW$, where $W$ is the symmetrical matrix of the discrete orthonormed eigenvectors and the matrix $D$ is a diagonal matrix having the discrete eigenvalues $d_k = -\frac{4}{h^2} \sin^2(\frac{k\pi h}{2L})$, $k = \overline{1, N-1}$ on its diagonal. To obtain FDSES, the diagonal entries of $D$ are replaced with the first $N - 1$ eigenvalues from the differential operator $d_k = -(\frac{k\pi}{L})^2$, $k = \overline{1, N-1}$ (see also [7], [8], [1]).

Generally, given the finite difference matrix $A_{m,n} = WD_{m,n}W^*$ described

previously, FDSES is formed when we set the diagonal matrix $D_{m,n}$ entries $d_k$ to be the first $N$ continuous eigenvalues $\lambda_{m,k}, m = 1; 2$ instead of the discrete eigenvalues $\mu_{m,k}$: ($N$ is even)

1) $d_k = \lambda_{2,k},\ d_{k+N/2} = \lambda_{2,N/2-k},\ k = \overline{1, N/2},\ d_N = 0$ (see Fig. 1)
2) $d_k = \lambda_{1,k},\ d_{k+N/2} = -\lambda_{1,N/2-k},\ k = \overline{1, N/2-1},\ d_{N/2} = d_N = 0$ (see Fig. 2).

For odd $N$ one obtains

1) $d_k = \lambda_{2,k},\ d_{k+(N-1)/2} = \lambda_{2,(N-1)/2-k+1},\ k = \overline{1, (N-1)/2},\ d_N = 0,$
2) $d_k = \lambda_{1,k},\ d_{k+(N-1)/2} = -\lambda_{1,(N-1)/2-k+1},\ k = \overline{1, (N-1)/2},\ d_N = 0.$

In Figures 1,2 taking $N = 80, L = 1$ for FDS we show the discrete eigenvalues for $-u''$ and the imaginary parts of the discrete eigenvalues for $u'$ for different values of $n = 1; 2; 3; 4; 30$ and corresponding first $N = 80$ modified continuous eigenvalues for FDSES.

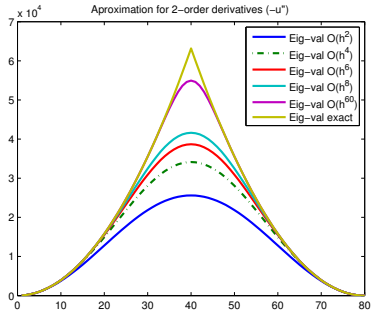



Figure 1: Eigenvalues for $-u''$ when $N = 80, L = 1, n = 1; 2; 3; 4; 30$

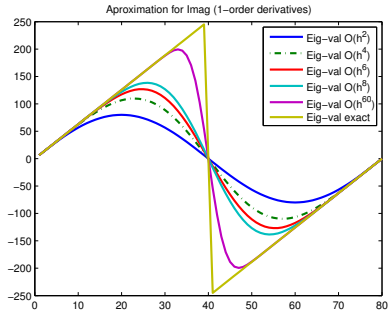



Figure 2: Imaginary part of eigenvalues for $u'$ when $N = 80, L = 1, n = 1; 2; 3; 4; 30$

For approximation of higher order derivatives, we can obtain the matrix representation for FDSES by replacing the discrete eigenvalues $\mu_{m,j},\ j = \overline{1, N}$ with the first $N$ continuous eigenvalues $\lambda_{m,j},\ j = \overline{1, N}$ of the derivatives $u^{(m)}(x)$ in the following form:

$$\lambda_{m,j} = \begin{cases} (-1)^{m/2} \left(\frac{2\pi j}{L}\right)^m, & m \text{ is even}, \\ i(-1)^{(m-1)/2} \left(\frac{2\pi j}{L}\right)^m, & m \text{ is odd}. \end{cases}$$

A downside of the FDSES method is that the matrix representation is not sparse; this is where appears the advantage of the PBC, since the matrix is

circulant and we can effectively use its spectral decomposition (with the eigenvalues described above).

### 2.2. Global Approximations with DMs

For global approximations the circulant differentiation matrices (DMs) are $D^{(1)} = \left(d^{(1)}_{k,j}\right)_{k,j=1,\dots N}$ and $D^{(2)} = \left(d^{(2)}_{k,j}\right)_{k,j=1,\dots N}$ obtained for a periodic function $f(t)$ by trigonometrical interpolation in the segment $t \in [0, 2\pi]$ [3], [17], [15], [16] :

$T_N(x) = \sum_{j=1}^{N} \Phi_j(t) f(t_j),\ \Phi_j(t_k) = \delta_{j,k},\ d^{(1)}_{k,j} = \frac{\mathrm{d}\,\Phi_j(t_k)}{\mathrm{d}\,t},\ d^{(2)}_{k,j} = \frac{\mathrm{d}^2\,\Phi_j(t_k)}{\mathrm{d}^2\,t}.$

1) $N$ **is even**,

$\Phi_j(t) = \frac{1}{N}\sin(\frac{1}{N}(t-t_j))\cot(\frac{1}{2}(t-t_j))$,

$d^{(1)}_{k,j} = 0.5(-1)^{k-j}\cot(\frac{\pi}{N}(k-j)), (k \neq j), d^{(1)}_{k,k} = 0,$ (3)

$d^{(2)}_{k,j} = -0.5(-1)^{k-j}\csc^2(\frac{\pi}{N}(k-j)), (k \neq j), d^{(2)}_{k,k} = -\frac{N^2+2}{12};$ (4)

(in this case $D^{(m)} = (D^{(1)})^m$ only holds for odd $m$),

2) $N$ **is odd**,

$\Phi_j(t) = \frac{1}{N}\sin(\frac{1}{N}(t-t_j)\csc(\frac{1}{2}(t-t_j)$,

$d^{(1)}_{k,j} = 0.5(-1)^{k-j}\csc(\frac{\pi}{N}(k-j)), (k \neq j), d^{(1)}_{k,k} = 0,$ (5)

$d^{(2)}_{k,j} = -0.5(-1)^{k-j}\csc(\frac{\pi}{N}(k-j))\cot(\frac{\pi}{N}(k-j)), (k \neq j), d^{(2)}_{k,k} = \frac{1-N^2}{12};$ (6)

(in this case $D^{(2)} = (D^{(1)})^2$ and $D^{(m)} = (D^{(1)})^m$ holds for every $m > 1$) [16].

For segment $[0, L]$ ($x = \frac{tL}{2\pi}$) the DMs are $A_1 = D^{(1)}\frac{2\pi}{L}$, $A_2 = D^{(2)}\frac{4\pi^2}{L^2}$.

### 2.3. Comparison of DMs and FDSES Methods

We will show that the FDSES method and DMs are equivalent methods. Notice that both methods have circulant matrix representation, hence it's sufficient to show that in both cases the matrices have the same eigenvalues to conclude the matrices are equal.

Recall that the eigenvalues of a circulant matrix $A = [a_1, a_2,\ \dots,\ a_{N-1}, a_N]$ can be obtained from the following expression:

$$\lambda_k = \sum_{j=1}^{N} a_j \exp\left(2\pi i k(j-1)/N\right), k = \overline{1, N}.$$

Suppose that $N$ **even**. The entries of DM $D^{(1)}$ are given by $d^{(1)}_{1,j}$ from (3). Then eigenvalues of $D^{(1)}$ are $\lambda_k = i\rho_k$, where $\rho_k = \sum_{j=1}^{M}(-1)^{j+1}\cot(\frac{\pi j}{2M})\sin(\frac{\pi jk}{M})$,

$M = N/2$, $k = \overline{1, N}$. We have

$$\rho_{k+1} - \rho_k = 2\sum_{j=1}^{M}(-1)^{j+1}\cos\frac{\pi j(2k+1)}{2M}\cos\frac{\pi j}{2M} =$$

$$= \sum_{j=1}^{M}(-1)^{j+1}\left(\cos\frac{\pi jk}{M} + \cos\frac{\pi j(k+1)}{M}\right) =$$

$$= \Re\sum_{j=1}^{M}(-1)^{j+1}\left(\left(\exp(\frac{\pi ik}{M})\right)^j + \left(\exp(\frac{\pi i(k+1)}{M})\right)^j\right) =$$

$$= \Re\left(\exp(\frac{\pi ik}{M})\frac{1-e^{i\pi k}}{1+e^{i\pi k/M}} + \exp(\frac{\pi i(k+1)}{M})\frac{1-e^{i\pi(k+1)}}{1+e^{i\pi(k+1)/M}}\right) =$$

$$= \Re\left(\frac{(1+e^{i\pi k/M})(1-(-1)^k)}{2(1+\cos(\pi k/M))} + \frac{(1+e^{i\pi(k+1)/M})(1+(-1)^k)}{2(1+\cos(\pi(k+1)/M))}\right) =$$

$$= \frac{(1+\cos(\pi k/M))(1-(-1)^k)}{2(1+\cos(\pi k/M))} + \frac{(1+\cos(\pi(k+1)/M))(1+(-1)^k)}{2(1+\cos(\pi(k+1)/M))} = 1.$$

From $\rho_0 = \rho_M = \rho_{2M} = 0$, $\rho_{M+m} = -\rho_{M-m}$, $m = \overline{1, M}$ it follows that $\lambda_k = ik$, $k = \overline{1, M-1}$, $\lambda_M = 0$, $\lambda_{k+M} = -i(M-k)$, $k = \overline{1, M-1}$, $\lambda_N = 0$. We multiply $\lambda_k$ with $\frac{2\pi}{L}$ (to consider the segment $[0; L]$ instead of $[0; 2\pi]$) and see that the obtained eigenvalues coincide with those ones of the diagonal matrix $D_{1,n}$ from FDSES.

Suppose that $N$ **odd**. The elements of $D^{(1)}$ are given by $d^{(1)}_{1,j}$ from (5); the eigenvalues of $D^{(1)}$ are $\lambda_k = i\rho_k$, where
$\rho_k = \sum_{j=1}^{M}(-1)^{j+1}\csc(\frac{\pi j}{2M+1})\sin(\frac{2\pi jk}{2M+1})$, $M = (N-1)/2, k = \overline{1, N}$. We have

$$\rho_{k+1} - \rho_k = 2\sum_{j=1}^{M}(-1)^{j+1}\cos(\frac{\pi j(2k+1)}{2M+1}) =$$

$$= 2\Re\sum_{j=1}^{M}(-1)^{j+1}\left(\exp(\frac{\pi i(2k+1)}{2M+1})\right)^j =$$

$$= 2\Re\left(\exp(\frac{\pi i(2k+1)}{2M+1})\,\frac{1-e^{i\pi M(2k+1)/(2M+1)}}{1+e^{i\pi(2k+1)/(2M+1)}}\right) =$$

$$= \Re\left(\frac{\left(1+e^{i\pi(2k+1)/(2M+1)}\right)\left(1-e^{i\pi M(2k+1)/(2M+1)}\right)}{1+\cos(\pi(2k+1)/(2M+1))}\right) = 1,$$

because $\exp(\frac{\pi i(M+1)(2k+1))}{2M+1}) = -\exp(\frac{-\pi iM(2k+1)}{2M+1})$.

From $\rho_0 = \rho_N = \rho_{2M+1} = 0$, $\rho_{M+m} = -\rho_{M-m+1}$, $m = \overline{1, M}$, it follows that $\lambda_k = ik, k = \overline{1, M}$, $\lambda_{k+M} = -i(M - k + 1)$, $k = \overline{1, M}$, $\lambda_N = 0$. By multiplying $\lambda_k$ with $\frac{2\pi}{L}$ we obtain the eigenvalues of FDSES.

### 2.4. Local Approximations with FDS in Multi-Points Stencil

We start with describing methods for higher order accuracy approximation of a smooth from the space $C^{2n+2}[0; L]$ function in an interval $[0; L]$. Consider the uniform grid $x_j = jh$, $j = \overline{0, N}$, where $Nh = L$. Let $n$ be natural number, satisfying $2n + 1 \leq N$. To obtain FDS and FDSES we use the spectral decomposition of the matrix $A_{m,n}$. Since $A_{m,n}$ is a circulant matrix, it is uniquely determined [2] by its first row:

$$A_{m,n} = h^{-m} \left[ D_0^{m,n} \ \dots \ D_n^{m,n} \ 0 \ \dots \ 0 \ D_{-n}^{m,n} \ \dots \ D_{-1}^{m,n} \right].$$

The coefficients $D_k^{m,n}$ can be obtained from the following Taylor expression for $m$-th order derivative:

$$u^{(m)}(x_j) = h^{-m} \sum_{k=-n}^{n} D_k^{m,n} u(x_{j+k}) + O(h^{2n+s-m}), \quad j = \overline{n, N-n},$$

where $s = 1$ for odd $m$, $s = 2$ for even $m$. The coefficients $D_k^{m,n}$ satisfy the following properties:

1) for all $k \in \overline{1, n}$ we have $D_{-k}^{m,n} = (-1)^m \cdot D_k^{m,n}$;

2) $D_0^{m,n} = -\sum_{k=1}^{n} (1 + (-1)^m) D_k^{m,n} = \begin{cases} -2 \sum_{k=1}^{n} D_k^{m,n}, & m \text{ is even}, \\ 0, & m \text{ is odd}. \end{cases}$

The coefficients $D_k^{m,n}$ can also be given explicitly [3]:

$$D_k^{1,n} = (-1)^{k+1} \cdot \frac{(n!)^2}{k\,(n-k)!\,(n+k)!}, \ k = \overline{1, n}, \quad D_0^{1,n} = 0.$$

and

$$D_k^{2,n} = \tfrac{2}{k}\, D_k^{1,n}, \ k = \overline{1, n}, \quad D_0^{2,n} = -2 \textstyle\sum_{k=1}^{n} D_k^{2,n}.$$

In general one can find that

$$D_k^{m,n} = (-1)^{n+m+k} \cdot e_{2n-m}^{(k)} \cdot \frac{m!}{(n-k)!\,(n+k)!},$$

where $e_{2n-m}^{(k)} = e_{2n-m}(-n, \dots, -1, 1, \dots, k-1, k+1, \dots, n)$ and $e_j$ are the elementary symmetric polynomials, defined as

$$e_j(t_1, t_2, \dots, t_K) = \sum_{1 \leq i_1 < i_2 < \dots < i_j \leq K} t_{i_1} \cdot t_{i_2} \cdot \dots \cdot t_{i_j}.$$

Let $\mu_{m,j} = h^{-m} \nu_j$ be the $j$-th eigenvalue of the matrix $A_{m,n}$ representation for FDS, but $w_j, w_j^*$ – the corresponding eigenvectors.

The matrix $W = (w_1, \ldots, w_N)$ is a symmetric unitary matrix and the matrix $A_{m,n}$ can be factored as $A_{m,n} = W\, D_{m,n}\, W^*$, where $D_{m,n}$ are diagonal matrices whose diagonal entries $\mu_{m,j}$ are eigenvalues of the matrix $A_{m,n}$.

From the properties of circulant matrices it follows that

$$\nu_j = D_0^{k,n} + \sum_{m=1}^{n} \left( D_m^{k,n}\, e^{2\pi i\, jm/N} + D_{-m}^{k,n}\, e^{-2\pi i\, jm/N} \right),$$

or

$$\nu_j = \begin{cases} -4 \sum\limits_{k=1}^{n} D_k^{m,n} \sin^2(k\alpha_j), & m \text{ is even}, \\ 2i \sum\limits_{k=1}^{n} D_k^{m,n} \sin(2k\alpha_j), & m \text{ is odd}, \end{cases} \qquad \text{where } \alpha_j = \frac{\pi\, j}{N}.$$

We note that in [3] also the case when $n \to \infty$ is considered; it is shown that in this case the FDS methods become the pseudospectral method.

The limits calculated in [3] are

$$D_k^{1,\infty} = \frac{(-1)^{k+1}}{k},\ k \neq 0; \qquad D_0^{1,\infty} = 0$$

$$D_k^{2,\infty} = 2\frac{(-1)^{k+1}}{k^2},\ k \geq 1; \qquad D_0^{2,\infty} = -4 \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^2} = -\frac{\pi^2}{3}.$$

One can notice that (for $N = 2M + 1$ being odd and choosing $L = 2\pi$) the eigenvalues tend to $\mu_{1,j} = 2ih^{-1} \sum_{k=1}^{\infty} D_k^{1,\infty} \sin \frac{2k\pi j}{N} = \frac{iN}{\pi}\rho_j$, where $\rho_j = \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k} \sin \frac{2k\pi j}{N} = \frac{\pi j}{N}$. From $\rho_{M+p} = -\rho_{M+1-p}$, $p = \overline{1, M}$ it follows that $\mu_{1,j} = ij$, $j = \overline{1, M}$ and $\mu_{1,j} = -ij$, $j = \overline{M+1, N}$.

By multiplying $\mu_{1,j}$ with $\frac{2\pi}{L}$ (to transform the segment $[0; 2\pi]$ to $[0; L]$) we conclude that the discrete eigenvalues tend to the eigenvalues of FDSES or DMs as $n \to \infty$.

A downside of using the multi-point stencil is that the matrix is not 3-diagonal; for large $n$ it is not even sparse, just as in the case of FDSES method. Again, since the matrix $A_{m,n}$ is circulant, it is important to use the spectral decomposition. At this point it's crucial to have an appropriated expression for the eigenvalues of $A_{m,n}$.

### 2.5. Coefficients for the Discrete Eigenvalues

We can see that the discrete eigenvalues $\mu_{m,j}$ depend on $n$. Now we show the following statement:

**Theorem 1.** *There exist coefficients $P_{k,m}$, depending only on $m$ and $k$*

*(but not on $n$) , which satisfy the following relation:*

$$\nu_j = \begin{cases} \sin\alpha_j \sum\limits_{k=1}^{n} P_{k,m} \sin^{2k-1}\alpha_j, & m \text{ is even,} \\ -i\cos\alpha_j \sum\limits_{k=1}^{n} k\, P_{k,m} \sin^{2k-1}\alpha_j, & m \text{ is odd.} \end{cases}$$

*Proof.* At first we consider the case when $m$ is **even**. Then

$$\nu_j = -4 \sum_{k=1}^{n} D_k^{m,n} \sin^2(k\alpha_j).$$

We denote $s = \sin^2\alpha_j$. Then $\sin^2(k\alpha_j)$ can be expressed as $\sin^2(k\alpha_j) = S_k(s)$, where $S_k$ is the $k$-th degree spread polynomial, which itself can be expressed as [12]

$$S_k(s) = s \sum_{l=0}^{k-1} \tfrac{k}{k-l} \binom{2k-1-l}{l} (-4s)^{k-1-l}.$$

The spread polynomials were introduced by N.J. Wildberger in [18].

Changing the summation index to $r = k - l$, we get

$$S_k(s) = \sum_{r=1}^{k} \tfrac{k}{r} \tfrac{(k+r-1)!}{(k-r)!\,(2r-1)!} (-4)^{r-1} s^r.$$

Therefore, $\nu_j = \sum\limits_{r=1}^{n} \left( \tfrac{(-4)^r}{r\,(2r-1)!} \sum\limits_{k=r}^{n} D_k^{m,n} \tfrac{k\,(k+r-1)!}{(k-r)!} \right) s^r.$

We have to show that the number

$$P_{m,r} = \tfrac{(-4)^r}{r\,(2r-1)!} \sum_{k=r}^{n} D_k^{m,n} \tfrac{k\,(k+r-1)!}{(k-r)!}$$

does not depend on $n$.

When $m$ is **odd**, we get $\nu_j = 2i \sum_{k=1}^{n} D_k^{m,n} \sin(2k\alpha_j)$. We will use the relation $\sin(2k\alpha_j) = U_{k-1}(\cos 2\alpha_j) \cdot \sin 2\alpha_j$, where $U_k$ are Chebyshev polynomial of the second kind. From the explicit representation of $U_k$ [11]:

$$U_k(x) = \sum_{l=0}^{k} (-2)^l \tfrac{(k+l+1)!}{(k-l)!(2l+1)!} (1-x)^l,$$

it follows that

$$U_{k-1}(\cos 2\alpha_j) = \sum_{l=0}^{k-1} (-4)^l \tfrac{(k+l)!}{(k-l-1)!(2l+1)!} \sin^{2l}\alpha_j.$$

Let $r = l + 1$, then we get

$$\sin(2k\alpha_j) = 2\cos\alpha_j \sin\alpha_j \sum_{r=1}^{k} (-4)^{r-1} \tfrac{(k+r-1)!}{(k-r)!(2r-1)!} s^{r-1}.$$

Therefore,

$$\nu_j = -i\,\cos\alpha_j\,\sin\alpha_j\,\sum_{r=1}^{n} r\,\left(\tfrac{1}{r}\cdot\tfrac{(-4)^r}{(2r-1)!}\,\sum_{k=r}^{n} D_k^{m,n}\,\tfrac{(k+r-1)!}{(k-r)!}\right)\,s^{r-1}.$$

We have to show that the number

$$P_{m,r} = \tfrac{(-4)^r}{r\,(2r-1)!}\,\sum_{k=r}^{n} D_k^{m,n}\,\tfrac{(k+r-1)!}{(k-r)!}$$

does not depend on $n$.

Therefore, we will show that the expressions

$$\eta_0 = \sum_{k=r}^{n} D_k^{m,n}\,\tfrac{k\,(k+r-1)!}{(k-r)!}, \quad \eta_1 = \sum_{k=r}^{n} D_k^{m,n}\,\tfrac{(k+r-1)!}{(k-r)!}$$

do not depend on $n$.

Observe that $\frac{(k+r-1)!}{(k-r)!} = k\cdot\prod_{l=1}^{r-1}(k^2-l^2) = k\cdot\sum_{l=0}^{r-1} c_l\cdot k^{2l}$, where the coefficients $c_0\ldots,c_{r-1}\in\mathbb{R}$ depend on $r$. Hence $\eta_1 = \sum_{l=0}^{r-1} c_l\,\sum_{k=1}^{n} D_k^{m,n}\,k^{2l+1}$. Similarly we obtain the sum $\eta_0 = \sum_{l=0}^{r-1} c_l\,\sum_{k=1}^{n} D_k^{m,n}\,k^{2l+2}$.

For each $l\in\overline{0,2n}$ the identity $\sum_{k=-n}^{n} k^l\cdot R_k(t)\equiv t^l$ holds, where

$$R_k(t) = \prod_{\substack{j=-n\\ j\neq k}}^{n}\frac{(t-j)}{(k-j)},\ t=\frac{x-x_j}{h}, \quad k=\overline{-n,n}$$

are Lagrange characteristic polynomials, defined by the relation $R_k(r)=\delta_{r,k}$, $r=\overline{-n,n}$, $k=\overline{-n,n}$. By differentiating that $m$ times, we get

$$\sum_{k=-n}^{n} k^l\cdot R_k^{(m)}(t)\equiv\begin{cases}0, & m>l,\\ m!, & m=l,\\ \frac{m!}{(l-m)!}\cdot t^{l-m}, & m<l.\end{cases}$$

Putting $t=0$ and taking into account that $R_k^{(m)}(0)=D_k^{m,n}$ gives us

$$\textstyle\sum_{k=-n}^{n} k^l\cdot D_k^{m,n} = m!\cdot\delta_{m,l}.$$

From $D_{-k}^{m,n} = (-1)^m\cdot D_k^{m,n}$ holds, thus for $l>0$ we get, that for each $l\in\overline{1,2n}$, satisfying $m\equiv l\pmod 2$, the equality $\sum_{k=1}^{n} k^l\cdot D_k^{m,n} = \frac{m!}{2}\,\delta_{m,l}$ holds and the right hand side does not depend on $n$.

Let $m' = \left\lfloor\frac{m-1}{2}\right\rfloor$, than we can write a simple expression of $P_{m,r}$ both for

even and odd values of $m$:

$$P_{m,r} = \begin{cases} \frac{(-4)^r}{r\,(2r-1)!} \cdot \frac{m!}{2}\, c_{m'} = (-4)^r\, \frac{m!}{(2r)!}\, c_{m'}, & m' \le r-1; \\ 0, & m' > r-1. \end{cases}$$

Observe that $c_l$ are coefficients of a polynomial with roots $1^2, \ldots, (r-1)^2$. According to the Vieta's theorem,

$$c_l = (-1)^{r-1-l} e_{r-1-m'}\left(1, 4, 9, \ldots, (r-1)^2\right).$$

Then

$$P_{m,r} = (-1)^{1+m'} \cdot 4^r\, \frac{m!}{(2r)!} \cdot e_{r-1-m'}\left(1, 4, 9, \ldots, (r-1)^2\right), \quad r \ge m'+1$$

and $P_{m,r} = 0$, $r \le m'$.

We conclude that

$$\nu_j = \begin{cases} \sum_{r=1}^{n} P_{m,r}\, (\sin^2 \alpha_j)^r, & m \text{ is even}, \\ -i\, \cos\alpha_j\, \sin\alpha_j\, \sum_{r=1}^{n} P_{m,r} \cdot r\, (\sin^2 \alpha_j)^{r-1}, & m \text{ is odd}. \end{cases}$$

This completes the proof. □

For instance, when $m' = 0$, (which corresponds to the cases $m = 1$ and $m = 2$), we can find that $e_{r-1}\left(1, 4, 9, \ldots, (r-1)^2\right) = ((r-1)!)^2$, hence

$$\nu_j = \begin{cases} i\, \cos\alpha_j \sum\limits_{k=1}^{n} \dfrac{4^k \cdot k}{(2k)!}\, ((k-1)!)^2\, \sin^{2k-1}\alpha_j, & m = 1; \\ -2 \sum\limits_{k=1}^{n} \dfrac{4^k}{(2k)!}\, ((k-1)!)^2\, \sin^{2k}\alpha_j, & m = 2. \end{cases}$$

### 2.6. The Spectral Representation for First and Second Derivatives

Periodic function's first and second order derivatives can be approximated in $2n+1$ stencil by finite differences with accuracy $O(h^{2n})$, using the following circulant matrices:

$$A_{1,n} = \tfrac{1}{h}[0 \quad D_1^{1,n} \ \ldots\ D_n^{1,n}\ 0\ \ldots\ 0\ -D_n^{1,n}\ \ldots\ -D_1^{1,n}],$$
$$A_{2,n} = \tfrac{1}{h^2}[D_0^{2,n} \ \ldots\ D_n^{2,n}\ 0\ \ldots\ 0\ D_n^{2,n}\ \ldots\ D_1^{2,n}],$$

respectively, where

$$D_k^{1,n} = (-1)^{k+1} \tfrac{(n!)^2}{k\,(n-k)!\,(n+k)!};$$
$$D_k^{2,n} = \tfrac{2}{k}\, D_k^{1,n},\ k = \overline{1,n}, D_0^{2,n} = -2\sum\nolimits_k^1 n D_k^{2,n}.$$

We have the following spectral representations:

$$A_{1,n} = W\, D_{1,n}\, W^*; \quad A_{2,n} = W\, D_{2,n}\, W^*.$$

Here $D_{1,n}, D_{2,n}$ are diagonal matrices with entries

$$\mu_{1,j} = \frac{i}{h}\cos(\alpha_j)\sum_{k=1}^{n} Q_{k,1}\sin^{2k-1}(\alpha_j), \quad \mu_{2,j} = -\frac{2}{h^2}\sum_{k=1}^{n} Q_{k,2}\sin^{2k}(\alpha_j),$$

respectively, on the diagonal; $Q_{k,1} = \frac{4^k \cdot k}{(2k)!}((k-1)!)^2, Q_{k,2} = \frac{Q_{k,1}}{k}$. For FDSES we can replace the discrete eigenvalues with the first $N$ continuous eigenvalues in the previously described way (see Figures 1, 2).

## 3. Some Examples of Applications

The described methods of derivative approximation, like other finite difference approximation, can be applied to estimate function's derivatives, solve ordinary and partial difference equations, etc.

### 3.1. Numerical Differentiation

Probably the simplest application of the described FDS is estimating the derivatives of a periodic function. We consider approximation of the first and second order derivatives of periodical functions in the interval $[0; L]$ for different numbers of grid points $N$ and $n$. In each case the error (the absolute value of difference between the approximation and the true derivative) for every grid point was computed; the maximal error was noted.

We notice that the advantage of using FDSES, DMs and FDS with multipoint stencil over the traditional $n = 1$ appears when $N$ should exceed $2w_0$ for approximating derivatives of functions $\sin(\frac{2\pi w_0}{L}x)$ or $\cos(\frac{2\pi w_0}{L}x)$ in the interval $[0; L]$. The spectral methods in this case are exact.

In the Figure 3 with $N = 80, L = 1$ we show the approximation of the first and second derivatives of $\exp(\sin(4\pi x))$, obtained with the DMs $A_1$, $A_2$ from the trigonometrical interpolant and FDSES (maximal errors: $1.65e-12$ for the first derivative, $2.39e-10$ for the second derivative).

### 3.2. Solving ODEs with Constant Coefficients

The described finite differences can be used to solve numerically ODEs in form

$$\begin{cases} u''(x) + p \cdot u'(x) + q \cdot u(x) = f(x), & x \in (0, L); \\ u(0) = u(L),\ u'(0) = u'(L), \end{cases} \tag{7}$$

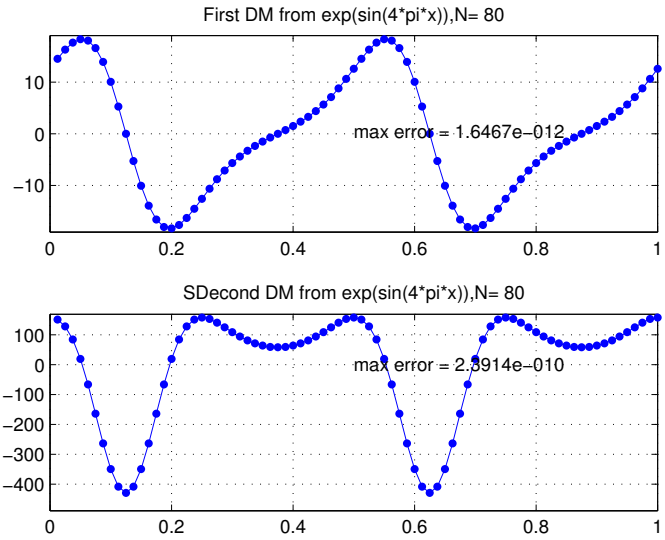



Figure 3: First and second derivatives of $\exp(\sin(4\pi x))$, obtained with the differentiation matrix $A_1$, $A_2$ of trigonometrical interpolant $N = 80$, $L = 1$. Maximal errors: $1.65e-12$ and $2.39e-10$

where $p$ and $q$ are constants (if $q = 0$, then $\int_0^1 f(x)dx = 0$ must be required).

To compare higher order FDS and spectral methods (FDSES, DM) with the exact solution, we also consider some analytical methods for solving the BVP.

### 3.2.1. The Fourier Method in the Real Form

Express $f(x) = \sum_{k=1}^{\infty}(b_{kc}\cos\frac{2\pi kx}{L} + b_{ks}\sin\frac{2\pi kx}{L}) + \frac{b_{0c}}{2}$, where

$$b_{kc} = \frac{2}{L}\int_0^L f(s)\cos\frac{2\pi ks}{L}ds, \quad b_{ks}(t) = \frac{2}{L}\int_0^L f(s,t)\sin\frac{2\pi ks}{L}ds.$$

Then the solution is

$$u(x) = \sum_{k=1}^{\infty}(a_{kc}\cos\frac{2\pi kx}{L} + a_{ks}\sin\frac{2\pi kx}{L}) + \frac{a_{0c}}{2},$$

where the unknown coefficients $a_{kc}, a_{ks}$ can be obtained from the following real system of two linear algebraic equations:

$$\begin{cases} a_{kc}(\lambda_{2,k} + q) - a_{ks}p\,\Im(\lambda_{1,k}) = b_{kc}, \\ a_{ks}(\lambda_{2,k} + q) + a_{kc}p\,\Im(\lambda_{1,k}) = b_{ks}, \\ qa_{0c} = b_{0c}. \end{cases} \tag{8}$$

Similarly, to solve the linear 1D heat transfer problem (1) with given initial conditions at $t = 0$, the method of lines is used and we have ODEs to determine the coefficients $a_k(t), a_{kc}(t), a_{ks}(t)$ depending on $t$ [5], [8].

For the **discrete problem** with $2n+1$ points stencil we have FDS or system of $N$ linear algebraic equations

$$A\,U = F,$$

where $U, F$ are column vectors of length $N$, the matrix $A = A_{2,n} + p\,A_{1,n} + q\,I$ is $N \times N$ circulant matrix and $I$ is the $N \times N$ identity matrix.

Using the spectral decomposition of $A_{2,n}$ and $A_{1,n}$ and noticing $W^*W = I$, we get

$$(D_{2,n} + p\,D_{1,n} + q\,I)\,\tilde{U} = \tilde{F},$$

where $\tilde{U} = W^*\,U$, $\tilde{F} = W^*\,F$. The matrix $D_{2,n} + p\,D_{1,n} + q\,I$ is a diagonal matrix with the elements $\mu_{2,k} + p\mu_{1,k} + q$, $k = \overline{1,N}$ on the diagonal. Hence we can easily find the vector $\tilde{U}$ and then the vector $U = W\tilde{U}$. For FDSES we can replace the eigenvalues in the diagonal-matrices in a previously described way. For DM we need replace the circulant matrices $A_{2,n}, A_{1,n}$ with circulant matrices $A_1, A_2$, to obtain the trigonometrical interpolation.

### 3.2.2. The Real Discrete Fourier Method

The elements $f_j$ of the column vector $F$ are obtained using the trigonometrical interpolation [9], [4]:

$$f_j = \sum_{k=1}^{*N_2}(b_{kc}\cos\tfrac{2\pi kj}{N} + b_{ks}\sin\tfrac{2\pi kj}{N}) + \tfrac{b_{0c}}{2},$$

where

$$b_{kc} = \tfrac{2}{N}\sum_{j=1}^{N} f_j\cos\tfrac{2\pi kj}{N},\ b_{ks} = \tfrac{2}{N}\sum_{j=1}^{N} f_j\sin\tfrac{2\pi kj}{N},\ k = \overline{1,N_2}$$

and $N_2 = \frac{N}{2}$, $\sum_{k=1}^{*N_2}\beta_k := \sum_{k=1}^{N_2-1}\beta_k + \frac{\beta_{N/2}}{2}$.

To find the solution $u_j = \sum_{k=1}^{*N_2}(a_{kc}\cos\frac{2\pi kj}{N} + a_{ks}\sin\frac{2\pi kj}{N}) + \frac{a_{0c}}{2}$ we need to determine the unknown functions $a_{kc}, a_{ks}$. We use the spectral representation of the matrices $A_{2,n}, A_{1,n}$ to obtain

$$\begin{aligned} f_j = (A_{2,n}u)_j + p\,(A_{1,n}u)_j + qu_j = \sum_{k=1}^{*N_2}\mu_{2,k}(a_{kc}\cos\tfrac{2\pi kj}{N} + a_{ks}\sin\tfrac{2\pi kj}{N}) + \\ + p\sum_{k=1}^{*N_2}\Im(\mu_{1,k})(-a_{kc}\sin\tfrac{2\pi kj}{N} + a_{ks}\cos\tfrac{2\pi kj}{N}) + \\ + q\sum_{k=1}^{*N_2}(a_{kc}\cos\frac{2\pi kj}{N} + a_{ks}\sin\frac{2\pi kj}{N}) + \frac{a_{0c}}{2} \end{aligned}$$

From the orthonormality condition it follows that

$$\frac{2}{N}\sum_{j=1}^{N}\cos\frac{2\pi kj}{N}\sin\frac{2\pi mj}{N}=\frac{2}{N}\sum_{j=1}^{N}\sin\frac{2\pi kj}{N}\sin\frac{2\pi mj}{N}=\frac{2}{N}\sum_{j=1}^{N}\cos\frac{2\pi kj}{N}\cos\frac{2\pi mj}{N}=\delta_{k,m},$$

and to determine the functions $a_{kc}, a_{ks}$ we obtain the system (8), where the eigenvalues $\lambda_{2,k}, \lambda_{1,k}$ are replaced with the discrete eigenvalues $\mu_{2,k}, \mu_{1,k}$. Thus, to find the discrete coefficients $a_{kc}, a_{ks}$ with FDSES and DM we obtain the initial system (8).

For the discrete linear 2D heat transfer equations (2) we have ODEs to determine the corresponding coefficients $a_k(t), a_{kc}(t), a_{ks}(t)$ depending on $t$ [5], [8].

In view of this approach, the spectral decomposition of $A_{m,n}$ and the Theorem 1 in particular becomes significant, since it allows us to increase $n$ very easily – one has to add one more addend to each eigenvalue $\mu_j$, rather than recompute them again.

**Example 1**: $p = 3, q = -1, f(x) = \cos(4\,\pi\,x) - 3\,\sin(28\,\pi\,x), \quad L = 1.$
The exact solution is $u(x) = u_1(x) + 3\,u_2(x)$ where

$$u_1(x) = \frac{-(16\pi^2+1)\,\cos(4\pi x)+12\,\pi\,\sin(4\pi x)}{(16\pi^2+1)^2+(12\pi)^2};$$
$$u_2(x) = \frac{84\pi\,\cos(28\pi x)+(784\pi^2+1)\,\sin(28\pi x)}{(784\pi^2+1)^2+(84\pi)^2}.$$

Several solutions were computed corresponding to different $n$ values, namely $n = 1$ (the standard FDS in 3-point stencil), $n = 7$, $n = 15$, $n = 49$. The FDSES and DM methods are solving this problem exactly, if $N \geq 28$.

The results are displayed in the Table 1; the "–" means the number of grid points is not large enough to choose the corresponding value of $n$.

Table 1: Maximal error of different numerical solutions

| | $N = 15$ | $N = 35$ | $N = 55$ | $N = 75$ | $N = 99$ |
|---|---|---|---|---|---|
| $n = 1$ | 0.067 | 0.00034 | 0.00012 | 6.25e-05 | 3.52e-05 |
| $n = 7$ | – | 2.24e-05 | 2.14e-07 | 4.81e-09 | 1.29e-10 |
| $n = 15$ | – | 4.57e-06 | 4.19e-10 | 1.46e-13 | 3.07e-16 |
| $n = 49$ | – | – | – | – | 2.60e-16 |

### 3.3. Solving ODEs with Variable Coefficients

When $p$ and $q$ are functions, $p = p(x)$, $q = q(x)$, the matrix $A$ of the linear system of $N$ algebraic equations is not circulant:

$$A = A_{2,n} + P \cdot A_{1,n} + Q,$$

where $P, Q$ are $N \times N$ diagonal matrices with diagonal elements $p_j = p(x_j)$ and $q_j = q(x_j)$, respectively. The matrices $A_{2,n}, A_{1,n}$ can be formed using the spectral decomposition $A_{2,n} = WD_{2,n}W^*$, $A_{1,n} = WD_{1,n}W^*$ in two ways:

1) for the multi-point stencil FDS diagonal matrices $D_{2,n}, D_{1,n}$ are chosen with elements $\mu_{2,k}, \mu_{1,k}$,
2) for the FDSES or DM diagonal matrices $D_{2,n}, D_{1,n}$ are chosen with elements $\lambda_{2,k}, \lambda_{1,k}, k = \overline{1, N}$ in the previously described way.

The vector $U$ can be found as $U = A^{-1}F$.

**Example 2**: Suppose that

$$\begin{aligned} q(x) &= -(2k_0\pi)^2 \left(\sin(2k_0\,\pi\,x) - \cos^2(2k_0\,\pi\,x)\right), \\ p(x) &= 4k_0\pi\cos(2k_0\,\pi\,x), \\ f(x) &= f_1(x)f_0(x), \end{aligned}$$

where

$$f_0(x) = \exp(-\sin(2k_0\,\pi\,x)), \qquad f_1(x) = \cos(4\,\pi\,x).$$

We can see that function $v(x) = u(x)/f_0(x)$ is the solution of ODEs with constant coefficients $v''(x) = f_1(x)$, $x \in (0, 1)$ with PBCs. This solution is in the following form:

$$v(x) = -\frac{\cos(4\pi x)}{16\pi^2} + C,$$

where $C$ is an arbitrary constant. The exact solution is

$$u(x) = -\frac{\cos(4\pi x)}{16\pi^2} f_0(x) + C f_0(x),$$

where it follows from $u(0) = 0$ that $C = \frac{1}{16\pi^2}$.

We show in Table 2 the maximal errors of solutions obtained with global methods (FDSES, DM) for $N = 20, 30, 40, 80, 100, 160$; $k_0 = 2, 5/\sqrt{3}, 8, 14$ and local approximations for different $n$.

The equation $v''(x) = f_1(x)$ can be discretized as $A_{2,n}V = F_1$. In this case FDSES and DM methods are exact, but for FDS with $N = 20, k_0 = 2$ the maximal errors of solutions are $3.1e-04$ $(n = 1)$; $2.8e-15$ $(n = 7)$ and $1.7e-18$ $(n \geq 15)$.

Table 2: The maximal errors obtained with global (FDSES=DMs) and local approximations for different $n$

| $k_0$ | $N$ | FDSES | $n=1$ | $n=2$ | $n=10$ | $n=40$ |
|---|---|---|---|---|---|---|
| 2 | 20 | 4.5e-06 | 1.1e-02 | 2.1e-03 | 3.3e-05 | 1.2e-06 |
| $5/\sqrt{3}$ | 30 | 7.0e-05 | 1.2e-02 | 3.9e-03 | 8.7e-05 | 7.4e-05 |
| 2 | 40 | 2.2e-11 | 2.5e-03 | 1.6e-04 | 1.1e-08 | 3.6e-11 |
| 8 | 80 | 2.6e-06 | 7.1e-03 | 1.3e-03 | 4.1e-05 | 2.7e-05 |
| 8 | 100 | 4.7e-08 | 7.0e-02 | 9.4e-03 | 1.0e-05 | 1.1e-07 |
| 14 | 160 | 3.0e-07 | 1.4e-02 | 3.0e-03 | 7.7e-05 | 8.9e-06 |

### 3.4. Solving Linear PDEs

For the heat transfer equation, using the method of lines (MOL) we obtain a linear system of ODEs:

$$\dot{U}(t) = KA_{2,n}\,U(t) + PA_{1,n}\,U(t) + Q\,U(t) + F(t), \qquad U(0) = U_0,$$

where

- $K$, $P$ and $Q$ are diagonal matrices with diagonal entries $k(x_j)$, $p(x_j)$ and $q(x_j)$, $j = 1, 2, \ldots, N$, respectively;
- $U(t)$, $F(t)$ and $U_0(t)$ are the column-vectors with elements $u_j(t) \approx u(x_j, t)$, $f_j(t) = f(x_j, t)$ and $u_j(0) = u_0(x_j)$, $j = \overline{1, N}$, respectively.

Using the spectral decomposition of the matrices, we obtain FDS and FDSES approximations for the linear system of ODEs. If the coefficients $k, p, q$ are constant, the solution can also be found analytically using the Fourier method.

The stability of the MOL is reduced to inequality $\Re(p_k) \leq 0$, where $p_k$, $k = \overline{1, N}$ are the eigenvalues of the right side difference operator.

**Example 3**: using Example 2 with $k(x) = 1$, $f(x,t) = -f_1(x)f_0(x)$, $L = 1$, $u_0(x) = \frac{1}{16\pi^2} f_0(x)$, $k_0 = 2$, $N = 20$ we obtain the stationary solution for $t = 0.1$ with 42 time step for FDSES (max. error $4.0e-06$), FDS ($n \geq 7$) (max. error $2.0e-05$)and with 45 time step for FDS ($n = 1$), (max. error $3.0e-03$).

In Figures 4, 5 the stationary solutions for $k_0 = 14$, $n = 1; 2$, $N = 160$, obtained with FDS and FDSES or DM are shown.

The function $v(x,t) = u(x,t)/f_0(x)$ is the solution of the heat transfer equation

$$\frac{\partial v(x,t)}{\partial t} = \frac{\partial^2 v(x,t))}{\partial x^2} - f_1(x)$$

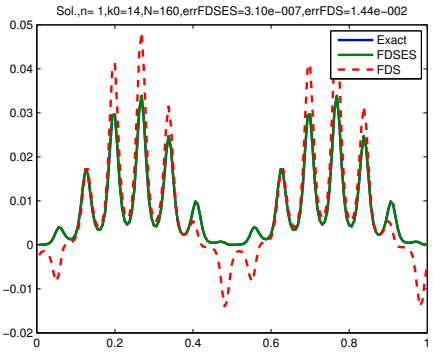



Figure 4: Solutions: exact, FDS ($n = 1$), FDSES with $k_0 = 14, N = 160$.

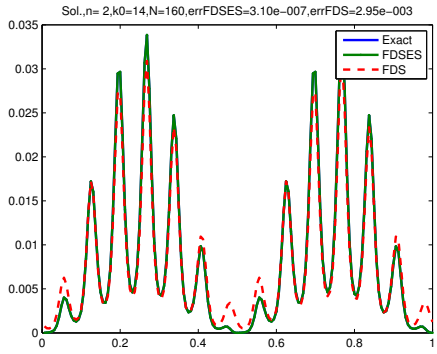



Figure 5: Solutions: exact, FDS ($n = 2$), FDSES with $k_0 = 14, N = 160$.

with PBCs. The exact solution for $v(x,0) = \frac{1}{16\pi^2}$ is

$$v(x,t) = f_1(x) \cdot \frac{\exp(-16\pi^2 t) - 1}{16\pi^2} + \frac{1}{16\pi^2} \underset{t\to\infty}{\longrightarrow} \frac{1 - f_1(x)}{16\pi^2}.$$

### 3.5. Solving Nonlinear PDEs

We shall consider the initial-boundary value problem for solving the nonlinear heat transfer equation (1) with $k = 1, p = q = 0$ where $g_1(u) = u^{\sigma+1}$, $f(u) = au^{\beta}$ are power functions with $a > 0$, $\beta \geq 1$, $\sigma \geq 0$, $u(x,t) \geq 0$, $u_0(x) \geq 0$.

In [13] for $a = 1$ it is proved for the first kind boundary conditions that

1) for $\beta < \sigma + 1$ there exists a global bounded solution for all $t$,
2) for $\beta \geq \sigma + 1$ there exists a global bounded solution for sufficient small $||u_0||$, but for larger $||u_0||$ there exists a finite value of time $T_*$ for which $u(x,t) \to \infty$ if $t \to T_*$.

The initial value problem for ODEs is in the form

$$\dot{\mathbf{U}} + \mathbf{AG} = \mathbf{F}, \quad \mathbf{U(0)} = \mathbf{U_0},$$

where $G, F$ are column vectors with elements $g_k = g(u(x_k,t))$, $f_k = af(u(x_k,t))$, $k = \overline{1,N}$.

Numerical experiments were carried out with the `MATLAB` solver `ode23s`, choosing $L = 1$ and $u_0(x) = x(1-x) \geq 0$ and setting $a = 5$, $\sigma = \beta = 3$, $(\beta < \sigma + 1)$, $t = 10$, $N = 6, 10, 20$ with first kind boundary conditions [6]. In the Table 3 the maximal errors of our numerical experiments are shown for the

Table 3: The maximal errors using FDS and FDSES

| $N$ | FDS | FDSES |
|---|---|---|
| 6 | 0.0125 | 0.0011 |
| 10 | 0.0046 | 0.0003 |
| 20 | 0.0013 | 0.0001 |

FDS and FDSES methods.

**Example 4**: in the Figures 6, 7, 8 and 9 four type solutions are shown with $u_0(x) = \sin^{100}(\pi x)$, $N = 50, \sigma = 3$ for periodical boundary conditions:

1) $\beta = 5$, $a = 100$, $T_1 = 5.481100$, $T_2 = 5.481131$, the solution "blows up" locally with $T_* = 5.481204$;
2) $\beta = 4$, $a = 100$, $T_1 = 0.20200$, $T_2 = 0.2026$ , the solution "blows up" globally with $T_* = 0.2020262$;
3) $\beta = 5$, $a = 1$, $T_1 = 0.05$, $T_2 = 25$, the solution tends to zero if $t \to \infty$;
4) $\beta = 4$, $a = 0.01$, $T_1 = 0.05$, $T_2 = 2500$, the solution tends to the stationary limit.

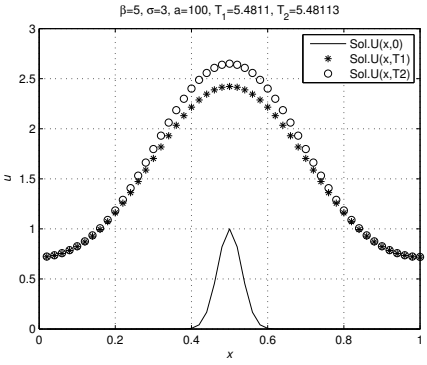



Figure 6: $U \to \infty$ for $x = 0.5$

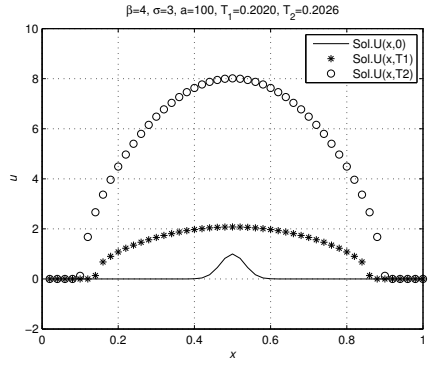



Figure 7: $U \to \infty$ for $x \in (0, 1)$

## 4. Conclusions

Our main result was the Theorem 1, which shows that the eigenvalues of the corresponding local approximation matrices can be expressed as a sum whose coefficients are irrespective of $n$. For a periodic function the described methods can provide high accuracy finite difference approximation (more accurate than

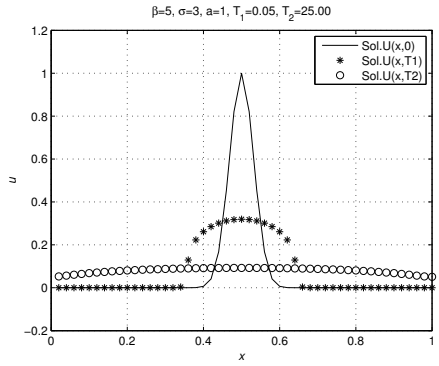



Figure 8: $U \to 0$ if $t \to \infty$

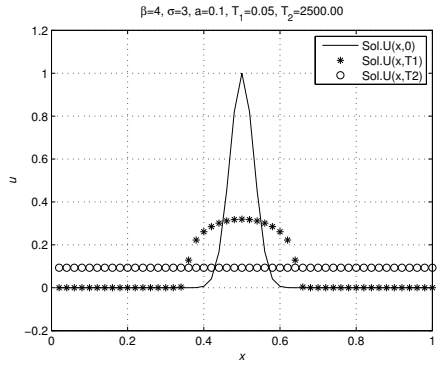



Figure 9: $U \to$ stationary if $t \to \infty$

in a 3-point stencil, as it is expected) while using the spectral decomposition also allows to avoid exact calculation of the FDS coefficients.

FDSES and DM methods were described (also note that these methods can be viewed as the limiting case of the FDS method). When solving linear ODEs and PDEs with constant coefficients, it was shown that FDSES is equivalent with the pseudospectral method.

The advantages of the FDSES or DM method when solving ODEs and PDEs with variable coefficients are demonstrated via several numerical examples in comparison with FDS for 3-points stencil.

Note that also similar FDS for approximation of higher order derivatives can be obtained, with analogue matrix representation's eigenvalue expression.

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