SPECTRAL APPROXIMATION OF THIRD-ORDER PROBLEMS

by

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Abstract

We consider the pseudospectral approximation of third-order problems. The spectral operator is constructed. An eigenvalue analysis with the calculation of the characteristic polynomial is presented. The eigenvalues of the spectral operator are numerically determined. An efficient preconditioner based on finite differences is constructed. Numerical results are presented.

AMS(MOS) classification: 65N35

Keywords: pseudospectral, collocation, third-order problems, eigenvalues, preconditioning.

Tables: 3

Figures: 8

1 Introduction

It is well known that pseudospectral (collocation) schemes (see [1]) can be successfully applied to second- or fourth-order problems. For smooth solutions the high (exponential) spectral accuracy can be achieved. Here we are interested in pseudospectral schemes for third-order problems. These problems occur for ion-acoustic waves in a plasma [13] and the shallow water waves [14]. They are also relevant for the Korteweg–de Vries equations [3].

First, in [10] generalized quadrature rules and interior collocation sets are provided to construct convergent pseudospectral schemes. These results are used for a model third-order evolutionary equation. No one of these sets performs better than any other, suggesting that it is sufficient to choose the most convenient set. Hence we use the standard Chebyshev Gauss-Lobatto nodes. These nodes make *Fast Fourier Transforms (FFTs)* available which are important for the efficient implementation of spectral multigrid schemes (see Heinrichs [8], [9]). In [11] both pseudospectral and spectral tau methods are compared with respect to third-order problems. The tau method was preferred because it has no spurious eigenvalues (with positive real parts). Here we give a pseudospectral scheme which also avoids spurious eigenvalues. Another approach was already proposed by Mulholland [12] where the Neumann boundary condition was incorporated in various ways. The Neumann condition was imposed weakly or by eliminating various solution points.

We present a pseudospectral scheme which was successfully used for fourth-order problems by Funaro and Heinrichs [5]. The boundary conditions are completely incorporated in the spectral approximation. An eigenvalue analysis determines the characteristic polynomial. Efficient preconditioning with finite differences is investigated. The preconditioning perfectly agrees with the results for first, second and fourth order problems (see [4], [7] and [5]). Numerical results are presented which demonstrate the efficiency of our treatment.

2 The third-order model problem

We consider the third-order evolutionary equation

$$\begin{aligned} u_t &= u_{xxx} \; in \; (x,t) \in (-1,1) \times (0,T], && (1) \\ u(\pm 1, t) &= 0 \; for \; t \in (0,T], && (2) \\ u_x(-1,t) &= 0 \; for \; t \in (0,T], && (3) \\ u(x,0) &= u_0(x) \; for \; x \in [-1,1]. && (4) \end{aligned}$$

where u_0 denotes a given function at $t = 0$. The space derivatives are now approximated by the pseudospectral scheme and the time derivative by some multi-step time scheme. For a fixed time step, the method will be stable only if the eigenvalues of the spectral differentation matrix lie in the stability region of the multi-step method. Therefore it is important that the properties of the eigenvalues are investigated. Also for an implicit time integration method the knowledge of the spectral eigenvalues is essential in order to construct efficient preconditioners and in obtaining estimates for the optimal relaxation parameters in an iterative process (see [8], [9]).

For these reasons it makes sense to study the corresponding eigenvalue problem

$$\begin{aligned} u_{xxx} &= \lambda u \; for \; x \in (-1,1), && (5) \\ u(\pm 1) &= 0, && (6) \\ u_x(-1) &= 0. && (7) \end{aligned}$$

Here u is considered as a function for fixed t and hence only dependent on x. The boundary conditions are chosen such that the eigenvalues λ are real and negative. This can easily be shown by setting up the energy norm $||\cdot||$ and proving that $\lambda ||u||^2 \leq 0$. The exakt eigenvalues of (5)–(7) are defined by the zeroes of the function f:

$$f(\lambda) \;=\; e^{3\lambda^{\frac{1}{3}}} - 2\sin\left(\sqrt{3}\lambda^{\frac{1}{3}} + \frac{\pi}{6}\right)$$

which are approximately given by

$$\lambda_k \;\cong\; -[(k+1/6)\pi/\sqrt{3}]^3 \; for \; k = 1, 2, \ldots .$$

3 Pseudospectral discretization

For the spectral approximation we use a Chebyshev collocation scheme. It is defined on the Chebyshev Gauss-Lobatto nodes given by

$$x_i = \cos \frac{i\pi}{N-1}, \; i = 0, \ldots, N-1.$$

Hence Fast Fourier Transforms (FFTs) are available for the efficient evaluation of spectral derivatives. For the approximation we employ a Chebyshev approximation $u_N \in \mathbb{P}_N$ where

$$\mathbb{P}_N = \{p : p \; polynomial \; of \; degree \; \leq N\}.$$

Now the pseudospectral scheme for (5)–(7) is defined as follows:

Find $u_N \in \mathbb{P}_N$ such that

$$\begin{aligned} u_N^{'''}(x_i) &= \lambda u_N(x_i), \; i = 1, \ldots, N-2, \\ u_N(\pm 1) &= u_N'(-1) = 0. \end{aligned}$$

Hence we have $N-2$ inner collocation and 3 boundary conditions. These are $N+1$ conditions which uniquely determine the spectral approximation u_N.

Now we give a prescription for generating the collocation matrices. Let us denote by $D = (d_{i,j})_{i,j=0,\ldots,N-1}$ (see Canuto et al. [1]) the $N \times N$ matrix corresponding to the first derivative. It is explicitely given by

$$d_{i,j} = \begin{cases} \frac{c_i}{c_j} \frac{(-1)^{i+j}}{x_i - x_j}, & i \neq j \\ -\frac{x_j}{2(1-x_j^2)}, & 1 \leq i = j \leq N-2 \\ \frac{2N^2+1}{6}, & i = j = 0 \\ -\frac{2N^2+1}{6}, & i = j = N-1. \end{cases}$$

and

$$c_i = \begin{cases} 2, & i \in \{0, N-1\} \\ 1, & i = 1, \ldots, N-2. \end{cases}$$

In particular, denoting by $l_j \in \mathbb{P}_{N-1},\ j = 0, \ldots, N-1$ the Lagrange polynomials relative to the above collocation nodes $x_i,\ i = 0, \ldots, N-1$. Now the interpolant u_N can be written as:

$$u_N = \sum_{j=1}^{N-2} u(x_j) \frac{1+x}{1+x_j} l_j(x).$$

Since $l_j(\pm 1) = 0, j = 1, \ldots, N-2$ the Dirichlet boundary conditions are automatically satisfied. The factor $1+x$ in front of l_j yields the Neumann condition in $x = -1$. Hence u_N implicitely contains the boundary conditions. Now the third derivative is given by

$$u_N^{'''}(x_i) = \sum_{j=1}^{N-2} \frac{u(x_j)}{1+x_j} [3 l_j^{''}(x_i) + (1+x_i) l_j^{'''}(x_i)],\ i = 1, \ldots, N-2.$$

The quantities $l_j^{''}(x_i), l_j^{'''}(x_i), i, j = 1, \ldots, N-2$ can be determined by computing the second and third powers of the spectral derivative matrix D.

Now the spectral operators are well defined. For these spectral discretizations we expect the high spectral accuracy. For smooth (analytical) solutions exponential convergence can be observed. We tested the accuracy for an example where the exact solution is given by

$$u(x) = 1 + \cos(\pi x). \tag{8}$$

Clearly, u satisfies the boundary conditions. We calculated the discrete L^2-error $E2$ of the third derivative which is given by $E2 = ||u^{'''} - u_N^{'''}||$. From the numerical results in table I we observe the exponential decay of the error. The rounding error accuracy is already reached for $N = 32$.

N	$E2$
8	$9.18 \cdot 10^{-4}$
16	$1.75 \cdot 10^{-11}$
32	$2.79 \cdot 10^{-13}$
64	$1.90 \cdot 10^{-12}$

Table I. Results for example (8)

4 Eigenvalue analysis and computation

Here we are interested in the eigenspectrum of the third derivative operator. For the standard spectral schemes (see [1]) it is well known that the largest eigenvalues of the first (second) derivative scale as $O(N^2)$ ($O(N^4)$). For the third derivative a behaviour as $O(N^6)$ can be expected. This will be confirmed by numerical results.

First, we present a technique for calculating the characteristic polynomial. This method was introduced by Gottlieb et al. [6] for second order problems. It was possible to show that the spectral eigenvalues are real and negative. The proof used the fact that the characteristic polynomial is related to two other polynomials forming a positive pair. This was shown by the Hurwitz property for some other polynomial. In [5] we tried a similar approach for fourth-order problems. Unfortunately, this technique could not be applied to higher-order problems. Also for third-order problems we were not able to proof that the eigenvalues are real and negative. And from the numerical calculations (see figures 1 - 4) it comes out that they are not real. The eigenvalues are complex with negative real parts. However, we were able to derive the corresponding characteristic polynomial.

We set

$$f_i = x^i T'_{N-1}, \ i = 0, 1, 2.$$

Then the eigenvalue problem takes the form

$$u''' = \lambda u + \sum_{i=0}^{2} A_i f_i, \quad u \in \mathbb{P}_N,$$

where $A_i \in \mathbb{R}, \ i = 0, 1, 2$ can be derived from the boundary conditions. Now let us consider $u_i \equiv u_i(x, \lambda) \in \mathbb{P}_N$ satisfying

$$u_i(x, \lambda) = - \sum_{k=0}^{\infty} \lambda^{-k-1} (D^{3k} f_i)(x), \ i = 0, 1, 2,$$

where D denotes the first derivative. Then we note that

$$u(x, \lambda) = \sum_{i=0}^{2} A_i u_i(x, \lambda).$$

From the boundary conditions we derive

$$\begin{aligned}
u(1,\lambda) &= A_0u_0(1,\lambda)+A_1u_1(1,\lambda)+A_2u_2(1,\lambda)=0,\\
u(-1,\lambda) &= A_0u_0(-1,\lambda)+A_1u_1(-1,\lambda)+A_2u_2(-1,\lambda)=0,\\
u'(-1,\lambda) &= A_0u_0'(-1,\lambda)+A_1u_1'(-1,\lambda)+A_2u_2'(-1,\lambda)=0.
\end{aligned}$$

The above system has nontrivial solutions $A_i, i=0,1,2$ if and only if

$$\begin{vmatrix} u_0(1,\lambda) & u_1(1,\lambda) & u_2(1,\lambda)\\ u_0(-1,\lambda) & u_1(-1,\lambda) & u_2(-1,\lambda)\\ u_0'(-1,\lambda) & u_1'(-1,\lambda) & u_2'(-1,\lambda)\end{vmatrix}=0.$$

The zeroes of the above characteristic equations yield the $N-2$ eigenvalues. For an explicit calculation it is necessary to derive the derivatives of Chebyshev polynomials in boundary points:

$$a_k = D^kT'_{N-1}(\pm 1) = (\pm 1)^{N+k}\Pi_{l=0}^{k}\frac{(N-1)^2-l^2}{2l+1}.$$

For $N=4$ we explicitely calculated the characteristic polynomial which is given by

$$4a_0^3+24a_0a_2^2\lambda^{-1}+72a_1a_2^2\lambda^{-2}=0$$

and the two eigenvalues

$$\lambda_1=-32,\quad \lambda_2=-10.6\overline{6}.$$

The eigenvalues for $N=4$ are confirmed by our numerical computations.

For increasing N we numerically calculated the eigenvalues of the spectral third derivative. In table II we present the absolute value of the minimal and maximal eigenvalues λ_{min} and λ_{max} for the spectral operators. The quantity

$$cond=\frac{\lambda_{max}}{\lambda_{min}}$$

yields a reasonable approximation of the condition number.

N	λ_{min}	λ_{max}	λ_{max}/N^6	$cond$
8	9.4822	$2.347{\cdot}10^3$	0.0089	$2.472 \cdot 10^2$
16	9.4824	$2.105{\cdot}10^5$	0.0126	$2.220 \cdot 10^4$
32	9.4824	$1.612{\cdot}10^7$	0.0150	$1.700 \cdot 10^6$
64	9.4824	$1.131{\cdot}10^9$	0.0165	$1.193 \cdot 10^8$
128	9.4824	$7.583{\cdot}10^{10}$	0.0172	$7.997 \cdot 10^9$

Table II. Results for the spectral third derivative.

From the results it becomes clear that the maximal eigenvalues are increasing as $O(N^6)$. The minimal eigenvalue approaches the smallest eigenvalue of the third derivative operator. This behaviour also becomes clear from our plots of the eigenvalues for $N = 8, 16, 32, 64$ in the figures 1 - 4. It can be observed that the eigenvalues are complex with negative real parts. Hence stability of the spectral discretization is guaranted.

5 Finite difference preconditioning

A good choice for preconditionig are bilinear finite elements as proposed by Deville and Mund [2]. We have more experience with finite differences. For $i = 2, \ldots, N-3$ the third derivative at the point x_i is approximated by upwind finite differences as follows:

$$u'''(x_i) \cong \alpha_i u(x_{i-1}) + \beta_i u(x_i) + \gamma_i u(x_{i+1}) + \delta_i u(x_{i+2}),$$

where

$$\begin{aligned}
\alpha_i &= \frac{6}{(x_{i-1} - x_{i+2})(x_{i-1} - x_{i+1})(x_{i-1} - x_i)} \\
\beta_i &= \frac{6}{(x_i - x_{i+2})(x_i - x_{i+1})(x_i - x_{i-1})} \\
\gamma_i &= \frac{6}{(x_{i+1} - x_{i+2})(x_{i+1} - x_i)(x_{i+1} - x_{i-1})} \\
\delta_i &= \frac{6}{(x_{i+2} - x_{i+1})(x_{i+2} - x_i)(x_{i+2} - x_{i-1})}
\end{aligned}$$

We still need schemes at the endpoints x_1, x_{N-2}. Here we use Taylor expansion around these points. Around x_1 we obtain

$$u(x) \cong u(x_1) + (x - x_1)u'(x_1) + \frac{1}{2}(x - x_1)^2 u''(x_1) + \frac{1}{6}(x - x_1)^3 u'''(x_1).$$

By using the boundary condition $u(x_0) = 0$ we obtain $u'''(x_1)$ in terms of the values $u(x_1), u(x_2), u(x_3)$ by solving the linear system

$$\begin{pmatrix} (x_0 - x_1) & \frac{1}{2}(x_0 - x_1)^2 & \frac{1}{6}(x_0 - x_1)^3 \\ (x_2 - x_1) & \frac{1}{2}(x_2 - x_1)^2 & \frac{1}{6}(x_2 - x_1)^3 \\ (x_3 - x_1) & \frac{1}{2}(x_3 - x_1)^2 & \frac{1}{6}(x_3 - x_1)^3 \end{pmatrix} \begin{pmatrix} u'(x_1) \\ u''(x_1) \\ u'''(x_1) \end{pmatrix} = \begin{pmatrix} -u(x_1) \\ u(x_2) - u(x_1) \\ u(x_3) - u(x_1) \end{pmatrix}$$

By solving the linear system one obtains

$$u'''(x_1) \cong \alpha_1 u(x_1) + \beta_1 u(x_2) + \gamma_1 u(x_3),$$

where

$$\alpha_1 = \frac{6}{(x_1 - x_3)(x_1 - x_2)(x_1 - x_0)}$$

$$\begin{aligned}\beta_1 &= \frac{6}{(x_2-x_3)(x_2-x_1)(x_2-x_0)}\\ \gamma_1 &= \frac{6}{(x_3-x_2)(x_3-x_1)(x_3-x_0)}.\end{aligned}$$

A similar treatment can be applied to x_{N-2}. We once more use Taylor expansion where now the boundary conditions $u(x_{N-1}) = u'(x_{N-1}) = 0$ are implemented. Here also the derivative of the Taylor polynomial is used. We have

$$u'(x) \cong u'(x_{N-2}) + (x-x_{N-2})u''(x_{N-2}) + \frac{1}{2}(x-x_{N-2})^2 u'''(x_{N-2}).$$

This leads to the linear system

$$\begin{pmatrix} 1 & (x_{N-1}-x_{N-2}) & \frac{1}{2}(x_{N-1}-x_{N-2})^2 \\ (x_{N-1}-x_{N-2}) & \frac{1}{2}(x_{N-1}-x_{N-2})^2 & \frac{1}{6}(x_{N-1}-x_{N-2})^3 \\ (x_{N-3}-x_{N-2}) & \frac{1}{2}(x_{N-3}-x_{N-2})^2 & \frac{1}{6}(x_{N-3}-x_{N-2})^3 \end{pmatrix} \begin{pmatrix} u'(x_{N-2}) \\ u''(x_{N-2}) \\ u'''(x_{N-2}) \end{pmatrix} = \begin{pmatrix} 0 \\ -u(x_{N-2}) \\ u(x_{N-3})-u(x_{N-2}) \end{pmatrix}.$$

By solving the linear system one obtains

$$u'''(x_{N-2}) \cong \beta_{N-2}u(x_{N-3}) + \gamma_{N-2}u(x_{N-2}),$$

where

$$\begin{aligned}\beta_{N-2} &= \frac{6}{(x_{N-3}-x_{N-1})^2(x_{N-3}-x_{N-2})}\\ \gamma_{N-2} &= \frac{6}{(x_{N-2}-x_{N-3})(x_{N-2}-x_{N-1})^2}.\end{aligned}$$

This leads to a finite difference matrix with four non-vanishing diagonals (one lower diagonal and two upper diagonals). In table III we present the minimal and maximal eigenvalues of the preconditioned spectral third derivative operator. It becomes obvious that we have the bounds

$$1 \le \lambda < \left(\frac{\pi}{2}\right)^3 \cong 3.8758.$$

This agrees perfectly with the case of preconditioned first derivatives, where

$$1 \leq \lambda < \frac{\pi}{2} \quad \text{(see [4])}$$

and second derivatives, where

$$1 \leq \lambda < \left(\frac{\pi}{2}\right)^2 \quad \text{(see [7])}$$

and fourth derivatives, where

$$1 \leq \lambda < \left(\frac{\pi}{2}\right)^4 \quad \text{(see [5])}.$$

The good behaviour of our preconditioner also becomes clear from our plots of the eigenvalues for $N = 8, 16, 32, 64$ (see figures 5 - 8). The eigenvalues are complex but bounded.

N	λ_{min}	λ_{max}
8	1.00	2.512
16	1.00	2.934
32	1.00	3.270
64	1.00	3.507
128	1.00	3.659

Table III. Eigenvalues of the preconditioned spectral operator.

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