Evaluation of Chebyshev pseudospectral methods for third order differential equations

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When the standard Chebyshev collocation method is used to solve a third order differential equation with one Neumann boundary condition and two Dirichlet boundary conditions, the resulting differentiation matrix has spurious positive eigenvalues and extreme eigenvalue already reaching O(N^5) for $N = 64$. Stable time-steps are therefore very small in this case. A matrix operator with better stability properties is obtained by using the modified Chebyshev collocation method, introduced by Kosloff and Tal Ezer [3]. By a correct choice of mapping and implementation of the Neumann boundary condition, the matrix operator has extreme eigenvalue less than O(N^4). The pseudospectral and modified pseudospectral methods are implemented for the solution of one-dimensional third-order partial differential equations and the accuracy of the solutions compared with those by finite difference techniques. The comparison verifies the stability analysis and the modified method allows larger time-steps. Moreover, to obtain the accuracy of the pseudospectral method the finite difference methods are substantially more expensive. Also, for the small N tested, $N \leqslant 16$, the modified pseudospectral method cannot compete with the standard approach.

Keywords: pseudospectral Chebyshev, third order equations, finite differences, transformed methods, accuracy

AMS subject classification: 65L05

1. Introduction

Spectral methods for solving partial differential equations have become increasingly popular because of their ability to achieve high accuracy using relatively few grid points, see Canuto et al. [1] and Fornberg [2]. Merryfield and Shizgal [4], however, pointed out one potential difficulty in integrating a differential equation such as:

$$\begin{aligned} &u_t + au_x + bu_{xxx} = 0, \quad -1 \leqslant x \leqslant 1,\ t \geqslant 0, \\ &u(\pm 1, t) = 0, \qquad u_x(-1, t) = 0, \end{aligned} \tag{1.1}$$

which contains a third-order spatial derivative. Specifically, the differential operator generates spurious positive eigenvalues when the standard Chebyshev collocation method is used. On the other hand, Mulholland [5] demonstrated that if the Neumann boundary condition is implemented wisely, the spurious positive eigenvalues can be eliminated and the eigenvalues of the resulting differentiation matrix are all negative. But in both cases, the extreme eigenvalues are still very large, and the differentiation matrices are highly non-normal. One may expect that there is a gap between Lax-stability and eigenvalue stability and that stable time-steps for explicit solvers in time are very small. The numerical experiments presented will show that the non-normality of the operator is not a problem and that the time-steps are determined by the extreme eigenvalues.

In this paper, we also use a parameter dependent transformation to stretch the Chebyshev grid, as introduced by Kosloff and Tal Ezer [3]. For an appropriate choice of mapping the resulting matrix operator has eigenvalues with negative real part and extreme eigenvalue no greater than O(N^4), up to $N = 64$. Furthermore, the modified differentiation matrix is near normal, and there is no big difference between Lax-stability and eigenvalue stability. The time-step for stability is larger than O(N^{-4}) and is always larger than that for the standard method.

In section 2, we study the spectrum of the modified differentiation matrix and show that its extreme eigenvalue is less than O(N^4). In section 3, we assess the non-normality of the standard and modified differentiation matrices. Via a study of the pseudospectra of these matrices we conclude that the standard differentiation matrix is highly non-normal whereas the modified matrix is near normal. Thus, a version of the Kreiss theorem as proved by Reddy and Trefethen [6] can be applied to ensure that eigenvalue stability implies Lax-stability. Numerical results comparing the two pseudospectral methods with finite differences are presented in section 4. Conclusions of the study are summarized in section 5.

2. The modified third order differentiation matrix

When we use the Chebyshev collocation method to discretize the spatial operator occurring in a partial differential equation, and advance in time with an explicit scheme, time-steps have to be taken restrictively small to guarantee stability. Heuristically this is explained as follows; the Chebyshev grid points

$$y_i = \cos\frac{i\pi}{N}, \quad i = 0, \ldots, N, \tag{2.1}$$

are bunched near the boundaries with minimal spacing O(N^{-2}) and the extreme eigenvalue is proportional to the reciprocal of the minimal spacing. Thus, for the third order Chebyshev differentiation matrix, we could expect the extreme eigenvalue to be as large as O(N^6), and accordingly, stable time-steps to be very small.

Kosloff and Tal Ezer [3] introduced a transformation of the domain for which the minimal spacing between grid points is $O(N^{-1})$ and collocation is with respect to a set of non-polynomial basis functions. Specifically, consider the following transformation:

$$x = g(y, \alpha) = \frac{\arcsin(\alpha y)}{\arcsin(\alpha)}, \quad x, y \in [-1, 1],$$

where y is the Chebyshev grid in (2.1), α is given by

$$\alpha = \cos \frac{j\pi}{N}, \tag{2.2}$$

and j is an integer parameter. This transformation has been successfully applied by Kosloff and Tal Ezer [3] and Renaut and Fröhlich [7] for first order and second order differential equations, respectively. Here we study the extension of its use for third order problems.

Consider the analytic eigenvalue problem

$$\begin{aligned} &u_{xxx} = \lambda u, \quad x \in [-1, 1], \\ &u(\pm 1) = 0, \qquad u_x(-1) = 0, \end{aligned} \tag{2.3}$$

where the first and third order derivatives are obtained via multiplication of u with matrices D_1 and D_3, respectively,

$$D_1 = AD \quad \text{and} \quad D_3 = BD^3 + CD^2 + ED. \tag{2.4}$$

Here D is the standard Chebyshev first order differentiation matrix, which can be written in closed form, see [1,8], and A, B, C, E are all diagonal matrices with entries given by

$$A_{ii} = \frac{1}{g'(y_i, \alpha)}, \qquad B_{ii} = \frac{1}{g'(y_i, \alpha)^3} = A_{ii}^3,$$

$$C_{ii} = -\frac{3g''(y_i, \alpha)}{g'(y_i, \alpha)^4} = -3A_{ii}\beta^2 y_i,$$

$$E_{ii} = -\frac{g'''(y_i, \alpha)}{g'(y_i, \alpha)^4} + \frac{3g''(y_i, \alpha)^2}{g'(y_i, \alpha)^5} = -A_{ii}\beta^2, \quad \beta = \arcsin(\alpha).$$

Whereas the incorporation of the Dirichlet boundary conditions $u(\pm 1) = 0$ is straightforward, the first and last rows and columns are removed from D_3, if the Neumann boundary condition, $u_x(-1) = 0$, is incorporated and used to solve for u_{N-1} the resulting operator has eigenvalues with positive real part, Merryfield [4]. Mulholland [5] recognised, however, that $u_x(-1) = 0$,

$$\sum_{j=1}^{N-1} D_1(N, j) u_j = 0,$$

can be used to solve for any u_r, $r = 1, \ldots, N-1$, to give

$$u_r = -\frac{1}{D_1(N,r)} \sum_{j=1, j\neq r}^{N-1} D_1(N,j) u_j. \tag{2.5}$$

Using (2.5) to eliminate u_r, we obtain a $(N-2)\times(N-2)$ differentiation matrix

$$\left(F^r\right)_{ij} = D_3\left(\bar{i},\bar{j}\right) - \frac{D_1(N,\bar{j})}{D_1(N,r)} D_3\left(\bar{i},r\right), \quad 1 \leqslant i,j \leqslant N-2,$$

where $\bar{i},\bar{j} = 1,\ldots,N-1$, and $\bar{i},\bar{j} \neq r$. The matrix F^r determines the properties of the method.

It can be proved that the eigenvalues of (2.3) satisfy (cf. [4,5])

$$\mathrm{e}^{3\lambda^{1/3}} = 2\sin\left(\sqrt{3}\lambda^{1/3} + \pi/6\right),$$

for which the approximate solutions are

$$\lambda_k \approx -\left[(k+1/6)\pi/\sqrt{(3)}\right]^3, \quad k = 1,2,\ldots. \tag{2.6}$$

Mulholland [5] found, for the pseudospectral operator, that the positive eigenvalues move toward the left with the eliminated variable moving toward the right, and a satisfactory set of eigenvalues occurs when the point eliminated is the furthest from the point where the Neumann boundary condition is imposed. This means that the eigenvalues of the standard matrix are extremely sensitive to the way that the Neumann boundary condition is incorporated.

For the modified differentiation matrix the eigenvalues can all be forced to have negative real part by an appropriate choice of the parameter j in (2.2). This is illustrated in figures 1–3 for $N = 32$ and $j = 1,2,3$. We see that the spread along the real axis of the real part of the eigenvalues increases with j. Also, F^{31} has eigenvalues all with negative real part when $j = 2$. In general the choice $j = 2$ is the most consistent in generating an operator for which all eigenvalues have negative real part. Figures 4(a)–(c) show the eigenvalues of F^{N-1} for $N = 16$, 32 and 64, and $j = 2$. As in Mulholland [5], when plotting the eigenvalues on the complex plane, the following transformation:

$$\begin{aligned} x &= \log_{10}\left(1 + \left|\Re(\mathrm{eig})\right|\right)\mathrm{sign}\left(\Re(\mathrm{eig})\right), \\ y &= \log_{10}\left(1 + \left|\Im(\mathrm{eig})\right|\right)\mathrm{sign}\left(\Im(\mathrm{eig})\right), \end{aligned} \tag{2.7}$$

is used.

Clearly, in some cases the exact eigenvalues are not all well approximated because complex eigenvalues occur. However, the extreme eigenvalue of the modified matrix is reduced to less than $\mathrm{O}(N^4)$, while the extreme eigenvalue of the standard matrix is $\mathrm{O}(N^5)$, for $N = 32$ and $N = 64$. In figures 5(a)–(d) we show the eigenvalue magnitudes as N is increased, where the solid line and the cross stand for the approximate eigenvalues as given by (2.6), and the eigenvalues of the modified matrix, respectively.

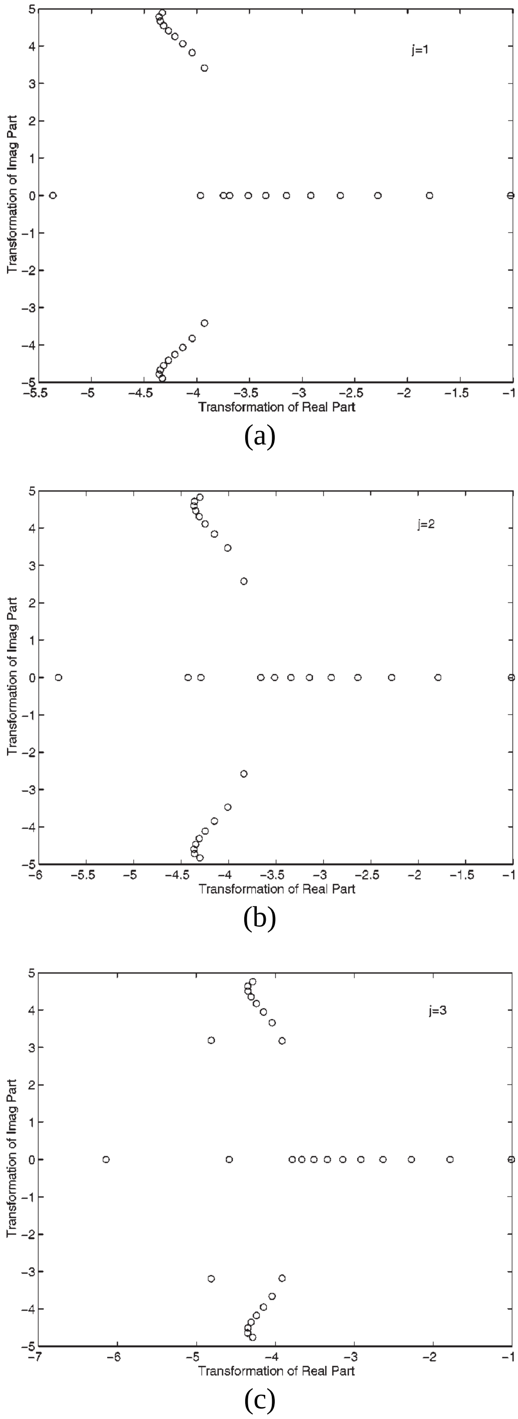
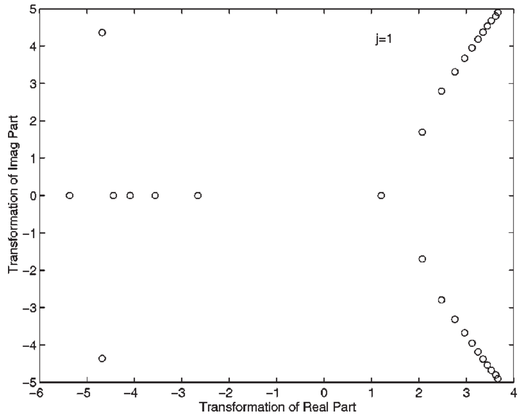
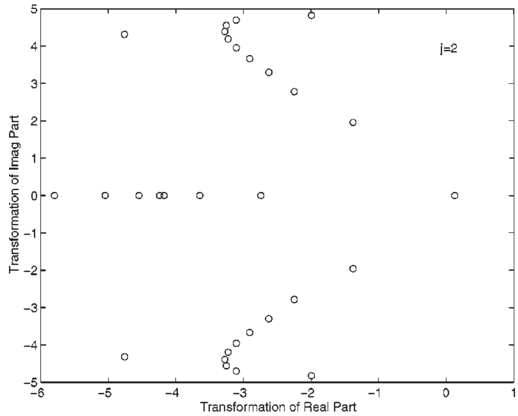


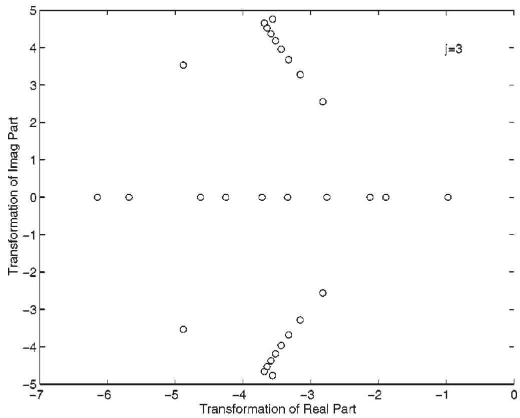
Figure 1. Spectrum of modified matrix F^1, $N = 32$. (a) $j = 1$; (b) $j = 2$; (c) $j = 3$.



(a)

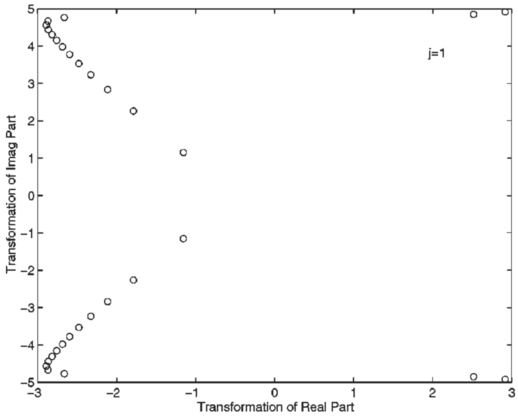


(b)

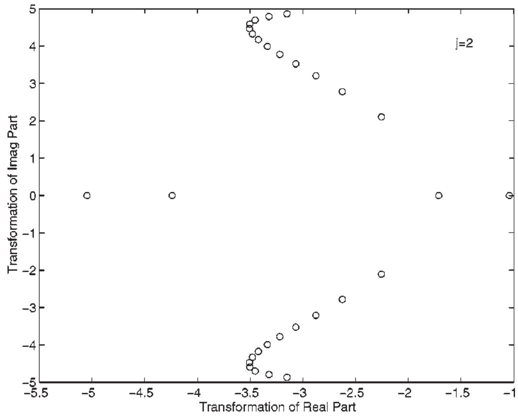


(c)

Figure 2. Spectrum of modified matrix F^{24}, $N = 32$. (a) $j = 1$; (b) $j = 2$; (c) $j = 3$.



(a)



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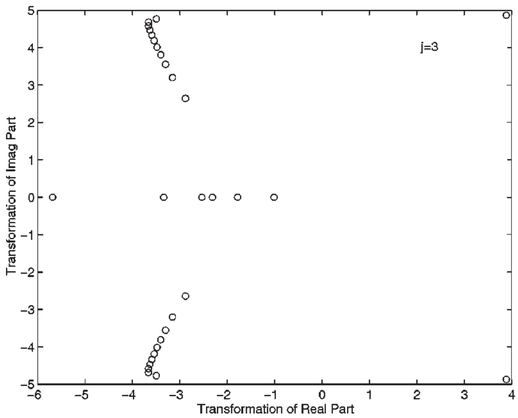


(c)

Figure 3. Spectrum of modified matrix F^{31}, $N = 32$. (a) $j = 1$; (b) $j = 2$; (c) $j = 3$.

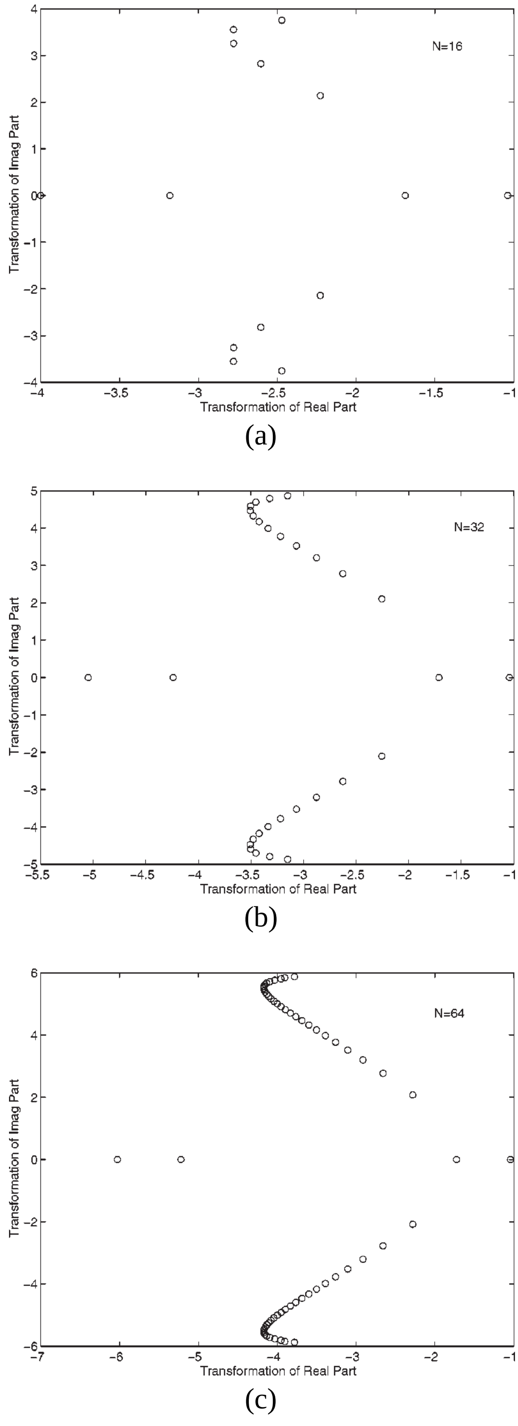


Figure 4. Spectrum of modified matrix F^{N-1}. (a) $N = 16$; (b) $N = 32$; (c) $N = 64$.

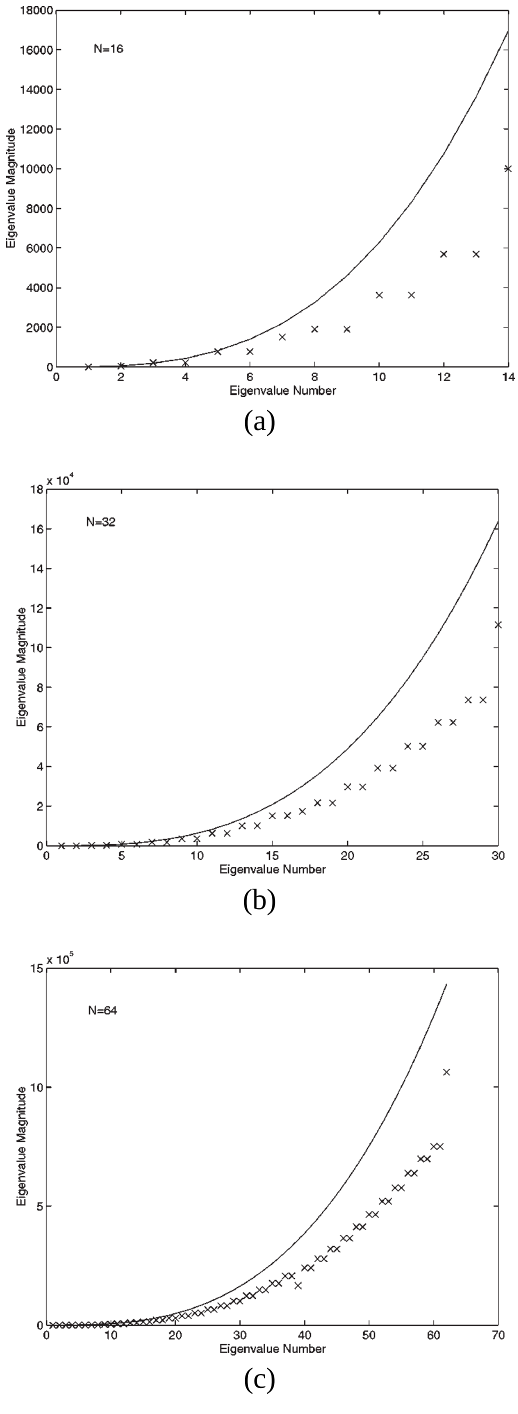
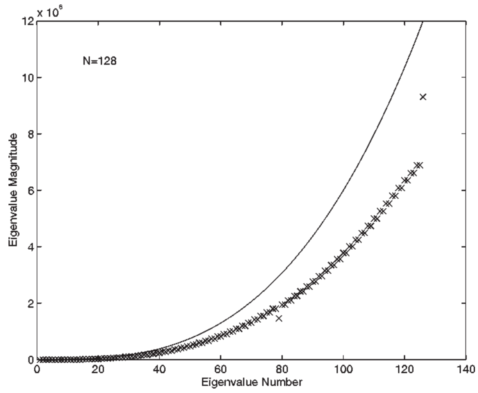


Figure 5. Magnitudes of eigenvalues (2.6) compared with eigenvalues of modified matrix. (a) $N = 16$; (b) $N = 32$; (c) $N = 64$.



(d)

Figure 5. (Continued.) (d) $N = 128$.

As noted by Mulholland [5] for the standard matrix, only approximately $N/3$ of the eigenvalues are accurately approximated. But the modulus of the largest eigenvalue now does not exceed that of the approximate eigenvalue of the largest modulus. It is therefore important to determine whether or not the stable time-step can be estimated from the eigenvalue of the largest modulus. This depends on the relative sensitivities of the eigenvalues, or, equivalently, on the degree of non-normality of the matrix.

3. Measures of non-normality

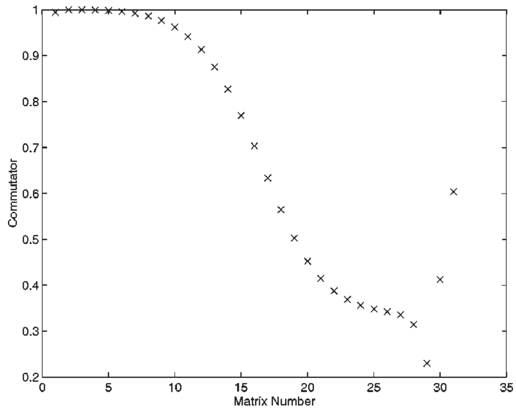
A matrix D is called normal if it satisfies $D^TD = DD^T$. A normal matrix has diagonal Schur form, which means that its eigenvectors can be taken to be orthogonal. Thus, its eigenvalues are insensitive to perturbation.

The following quantities can be used to assess the degree of non-normality of a matrix D:

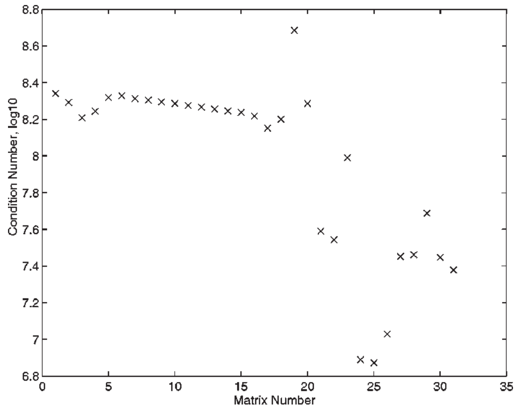
1. Commutator $C(D) := \|DD^T - D^TD\|/\|DD^T\|$. If D is normal $C(D) = 0$.
2. Condition number $\kappa(V)$: V is the matrix of normalized eigenvectors D. If D is normal $\kappa(V) = 1$.
3. Comparison of spectral radius and the 2-norm of D: identical if D is normal.
4. $\|T\|$, where T is the strictly triangular part of the Schur form of D.

The above quantities provide only partial information about non-normality. In particular a matrix may have large commutator or large condition number, while its eigenvalues are relatively insensitive to perturbations. However, together they provide some insight for a family of matrices.

For comparison we study first F^r, $r = 1, \ldots, N-1$, and N fixed. We plot the commutator, condition number $\kappa(V)$, the comparison of spectral radius and the 2-norm of the matrix, and the 2-norm of the Schur triangular matrix T in figures 6(a)–(d), respectively, for $N = 32$, and $\log_{10}$ scale in the figures 6(b)–(d). For the modified



(a)



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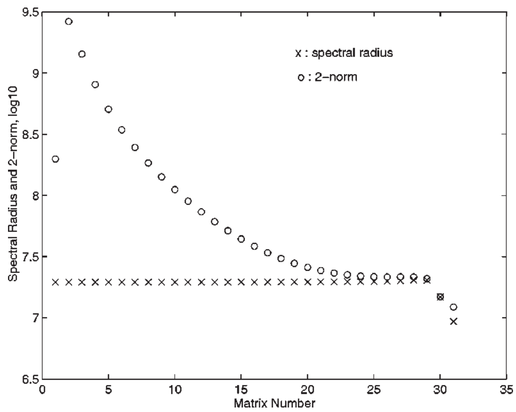
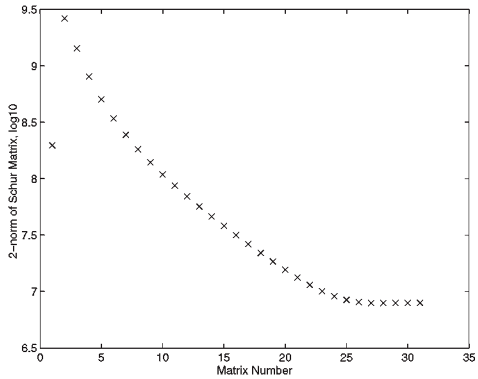


(c)

Figure 6. Measures of non-normality for standard matrix, $N = 32$. (a) Commutator; (b) condition number; (c) comparison of spectral radius and the 2-norm.



(d)

Figure 6. (Continued.) (d) 2-norm of Schur matrix.

Table 1
Measures of non-normality for standard matrix.

N	16	32	64	128
Commutator	0.6127	0.6033	0.6011	0.6005
Condition number	2.9137e+3	2.3896e+7	1.4334e+13	1.7063e+12
Spectral radius	1.4609e+5	9.3406e+6	5.9747e+8	3.8232e+10
2-norm of T	1.2822e+5	7.9293e+6	5.0309e+8	3.2128e+10

matrix parameter j in (2.2) is chosen so that all the eigenvalues of the resulting matrices have negative real part, namely $j = 2$ for F^1 and F^{31} and $j = 3$ otherwise, figures 7(a)–(d).

From these figures, we can see that:

1. For the standard differentiation matrices, although the commutators are not very big, the condition numbers and 2-norm of T are very large, on the order of 10^7, suggesting non-normality.

2. For the modified differentiation matrix, roughly with $r \geqslant 29$, all four measures are minimal. For $r = 31$, $\kappa(V) = 66.2304$. Hence these matrices have the best properties with respect to normality. On the other hand, for r small all the quantities are of the same order of magnitude as for the standard matrix.

3. We conclude that F^{N-1} is closest to normality in all cases.

Tables 1 and 2 provide a direct comparison of the standard and modified matrices F^{N-1}. Again these measurements suggest that the modified matrices are nearer to normality than the standard matrices.

For non-normal matrices eigenvalue analysis is insufficient to determine the stability of a method. But due to a version of the Kreiss-matrix theorem presented in [6], stability can be examined via a study of the pseudospectrum of the matrix.

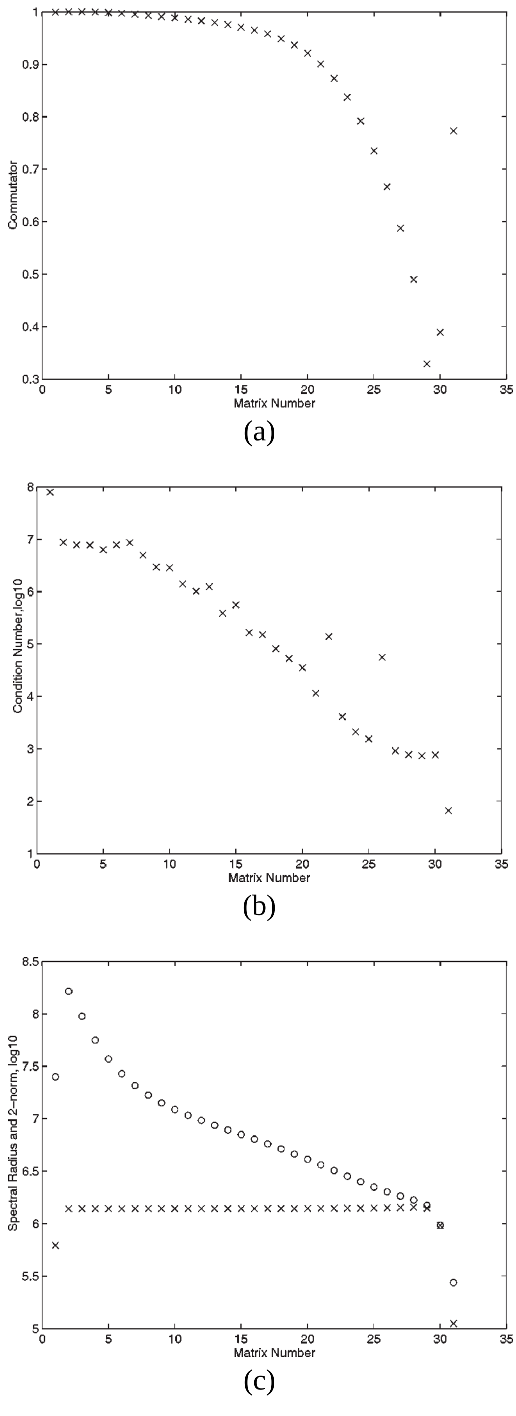
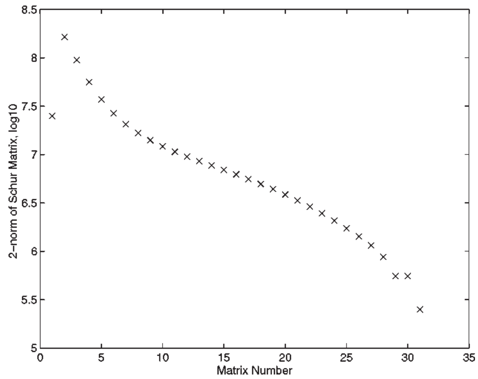


Figure 7. Measures of non-normality for modified matrix, $N = 32$. (a) Commutator; (b) condition number; (c) comparison of spectral radius and the 2-norm.



(d)

Figure 7. (Continued.) (d) 2-norm of Schur matrix.

Table 2
Measures of non-normality for modified matrix.

N	16	32	64	128
Commutator	0.7610	0.7732	0.7804	0.7901
Condition number	60.7740	66.2304	66.3685	64.8007
Spectral radius	9.9975e+3	1.1153e+5	2.6392e+6	2.3187e+7
2-norm of T	2.1881e+4	2.5031e+5	2.4188e+6	2.1346e+7

Let $\|\cdot\|$ be an appropriate norm, and let $S_{N,\Delta t}$ be the discrete solution operator on a grid of N points with time-step Δt:

$$S_{N,\Delta t} : v^n \to v^{n+1}, \qquad v^{n+1} = S^n_{N,\Delta t} v^0, \tag{3.1}$$

where v^n represents the computed solution at time step n. Lax-stability is defined by

$$\|S^n_{N,\Delta t}\| \leqslant C, \quad \text{for all } N,\ n \text{ such that } n\Delta t \leqslant \tau,$$

where τ is some time and $C = C(\tau)$ is a constant. Eigenvalue stability is defined by

$$\|S^n_{N,\Delta t}\| \leqslant C, \quad \text{for all } n \text{ and fixed } N \text{ and } \Delta t. \tag{3.2}$$

Unless the operators $\{S_{N,\Delta t}\}$ are normal, condition (3.2) is necessary but not sufficient for Lax-stability (3.1).

Definition (ε-pseudospectrum [6]). Given $A \in C^{N\times N}$ and $\varepsilon > 0$, the ε-pseudospectrum of A is the set

$$\Lambda_\varepsilon(A) := \{z \in C\colon\ z \text{ is an eigenvalue of } A + E, \text{ with } E \in C^{N\times N} \text{ and } \|E\|_2 \leqslant \varepsilon\}.$$

A number $\lambda_\varepsilon \in \Lambda_\varepsilon(A)$ is called an ε-pseudoeigenvalue of A.

Let Δ denote the open disk in the complex plane

$$\Delta := \{z \in C\colon\ |z| < 1\},$$

and given a point $z \in C$ and a set $X \subseteq C$, let $\mathrm{dist}(z, X)$ denote the usual distance between a point and a set. Then the connection between power-boundedness of matrix operators and the pseudospectrum is made clear in the version of the Kreiss-matrix theorem presented in [6].

Theorem. Let $\{A_\nu\}$ be a family of matrices or bounded linear operators of dimensions $N_\nu \leqslant \infty$. If the powers of these matrices satisfy

$$\|A_\nu^n\| \leqslant C \quad \text{for all } n \geqslant 0,$$

for some constant C, independent of ν, then their ε-pseudoeigenvalues $\{\lambda_\varepsilon\}$ satisfy

$$\mathrm{dist}(\lambda_\varepsilon, \Delta) \leqslant C\varepsilon \quad \text{for all } \varepsilon \geqslant 0. \tag{3.3}$$

Conversely, (3.3) implies

$$\|A_\nu^n\|_2 \leqslant 2\mathrm{e}\min\{N_\nu, n\}C \quad \text{for all } n > 0. \tag{3.4}$$

Thus, ignoring the factor e in front of C in (3.4), (3.3) is a necessary and sufficient condition for the powerboundness of the operators $\{S_{N,\Delta t}\}$. Equivalently, for stability the eigenvalues of $A_\nu + E$ should lie in Δ and it suffices to study the pseudospectra of the operators, which for near-normal matrices are just the union of ε-balls around the spectra.

In figures 8 and 9 pseudospectra for $N = 32$ are plotted on a $\log_{10}$–$\log_{10}$ scale using transformation (2.7) for the standard and modified matrices, respectively. In each case E is generated randomly 50 times for each perturbation, $\varepsilon = 10^{-3}$, 10^{-2}, 10^{-1} and 1. Note that the biggest entries of these matrices are of the order 10^5 and the smallest ones are of the order 10^2 (absolute value). Because of (2.7) the scattering of the pseudospectra is wider than it appears in the pictures. In these figures the circles indicate the exact eigenvalues. In figures 10 and 11 pseudospectra of F^{N-1} are plotted for $N = 16$, 24 and 64. We conclude:

1. The standard matrix is highly non-normal: the complex eigenvalues are very sensitive to perturbations.
2. The modified matrix, if it is obtained by eliminating a point near the Neumann boundary, is near normal: its eigenvalues are insensitive to perturbations.

Thus, for the modified method, the difference between Lax-stability and eigenvalue stability should be negligible, suggesting that a stable time-step will be

$$\Delta t = \mathrm{O}(N^{-4}).$$

In figures 12 and 13 the contour levels $\|(zI - A)^{-1}\|_2 = 10^{-k}$ for standard and modified matrices, respectively, are plotted. The exact eigenvalues are denoted

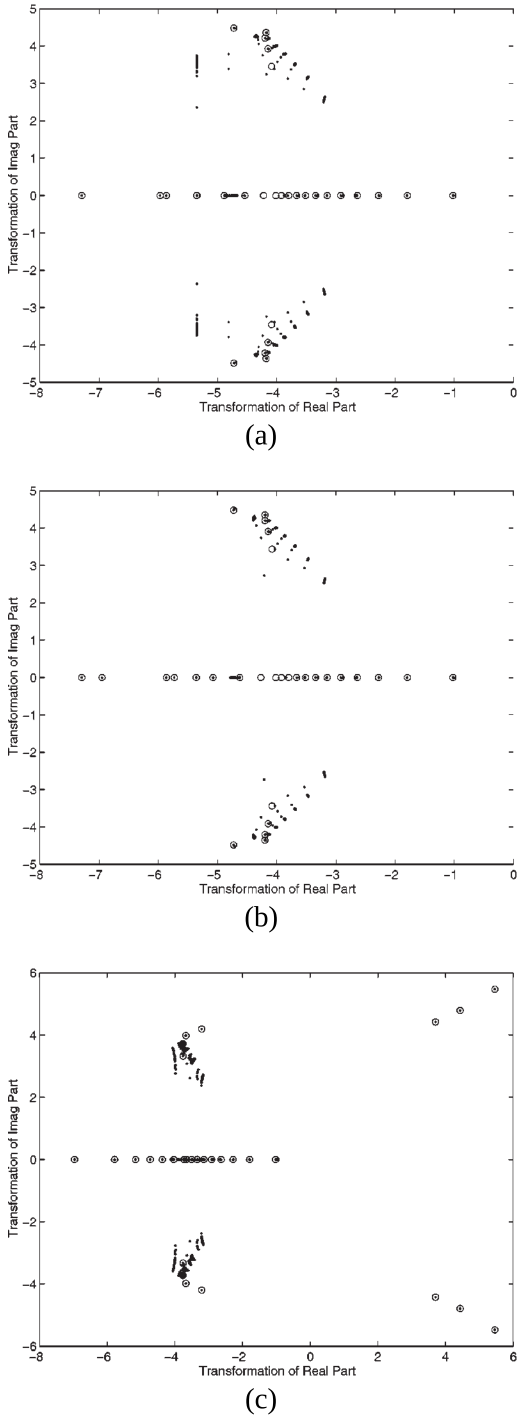
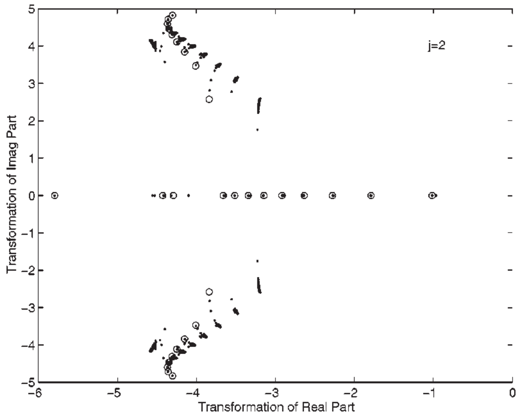
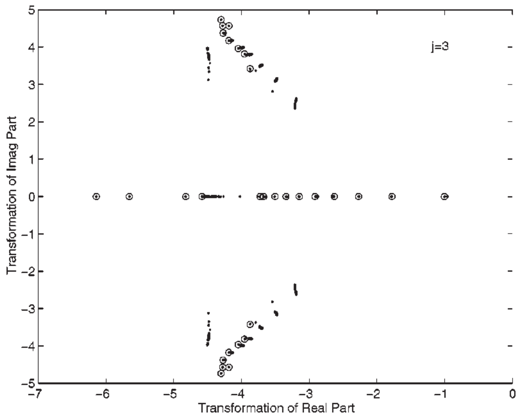


Figure 8. Pseudospectra of standard matrix F^r, $N = 32$. (a) $r = 1$; (b) $r = 8$; (c) $r = 31$.



(a)



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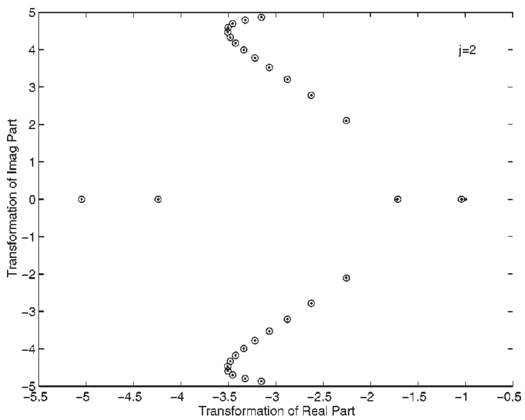
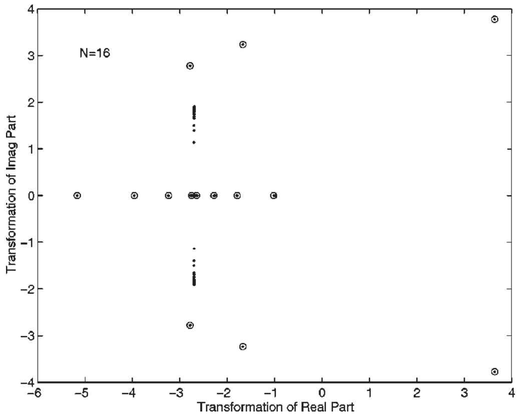
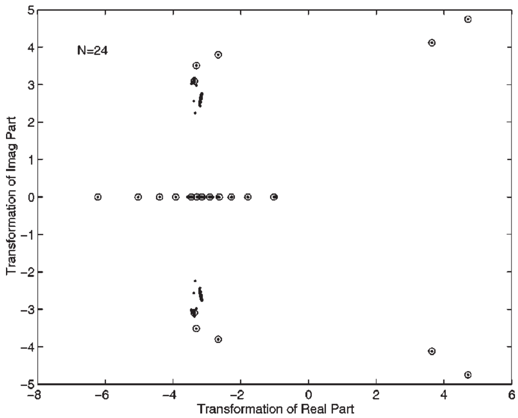


(c)

Figure 9. Pseudospectra of modified matrix F^r, $N = 32$. (a) $r = 1$; (b) $r = 8$; (c) $r = 31$.



(a)



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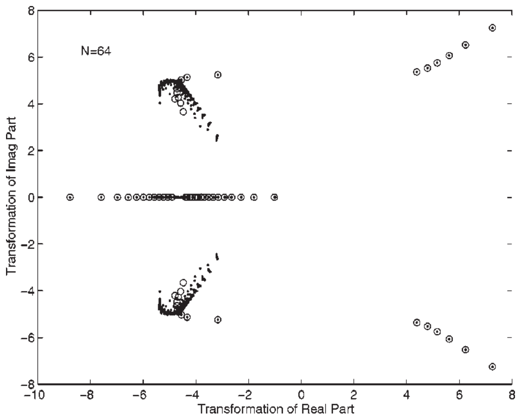
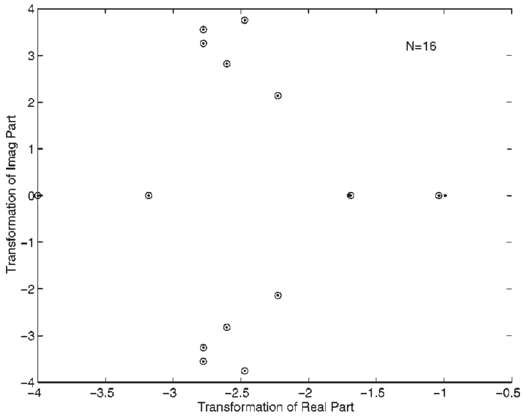
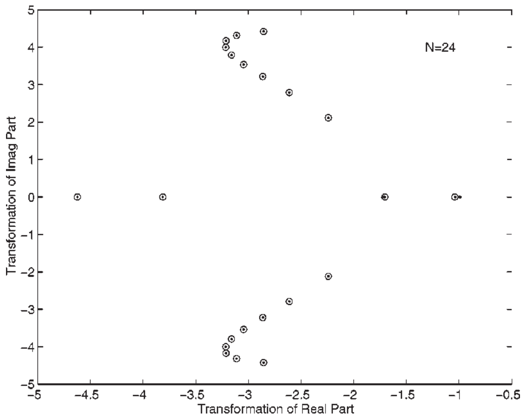


(c)

Figure 10. Pseudospectra of standard matrix. (a) $N = 16$; (b) $N = 24$; (c) $N = 64$.



(a)



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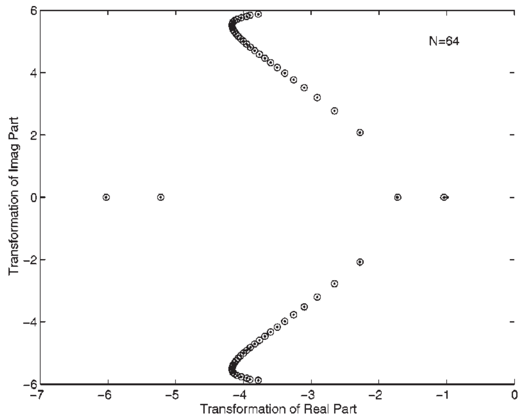
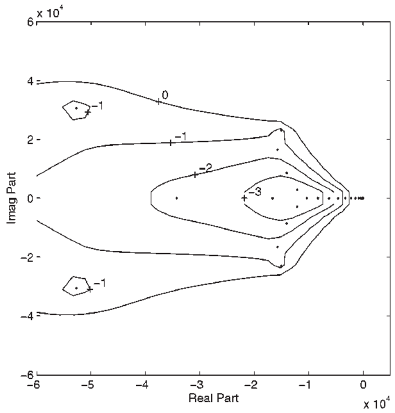
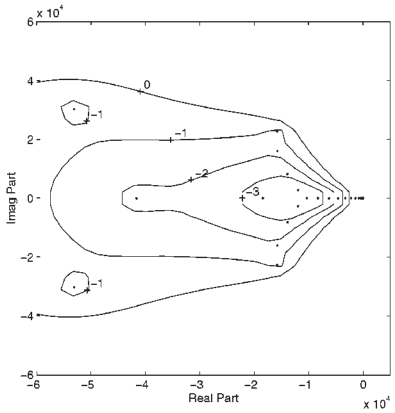


(c)

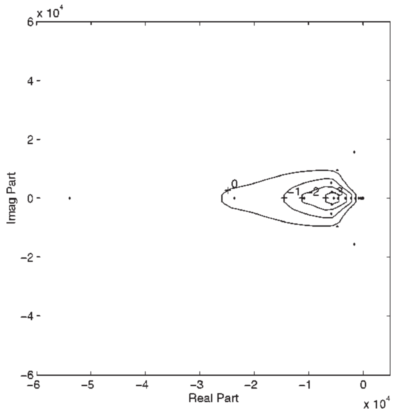
Figure 11. Pseudospectra of modified matrix. (a) $N = 16$; (b) $N = 24$; (c) $N = 64$.



(a)

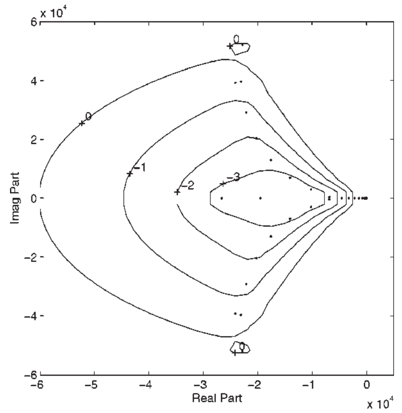


(b)

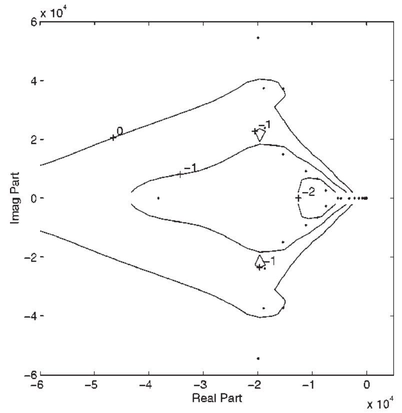


(c)

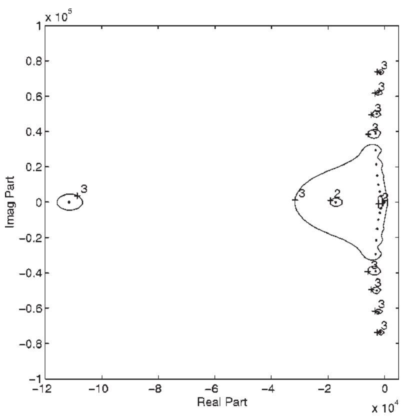
Figure 12. Contours of pseudospectrum for varying tolerance: standard matrix F^r, $N = 32$. (a) $r = 1$; (b) $r = 8$; (c) $r = 31$.



(a)



(b)



(c)

Figure 13. Contours of pseudospectrum for varying tolerance: modified matrix F^r, $N = 32$. (a) $r = 1$; (b) $r = 8$; (c) $r = 31$.

by dots. For the modified method, it is significant that even when the perturbation is as large as 10^3, the eigenvalues are rather insensitive, see figure 13. This suggests that when we apply the modified Chebyshev collocation method to a third order differential equation which contains low order terms, the resulting matrix should also be near normal.

4. Numerical comparison with finite differences

In this section, we apply the pseudospectral method, the modified pseudospectral method and a finite difference method to solve two test problems:

Example 1.

$$\begin{aligned} u_t &= -\frac{1}{\sqrt{3}}u_x + \frac{1}{8\sqrt{3}}u_{xxx}, \\ u(\pm 1, t) &= \exp\bigl(-t \pm 1\sqrt{3}\bigr)(\cos \pm 1 + \sin \pm 1), \\ u_x(-1, t) &= \exp\bigl(-t - \sqrt{3}\bigr)\bigl(\bigl(1 - \sqrt{3}\bigr)\cos 1 - \bigl(1 - \sqrt{3}\bigr)\sin 1\bigr), \end{aligned}$$

for which the solution is

$$u(x, t) = \exp\bigl(-t + \sqrt{3}x\bigr)(\cos x + \sin x).$$

Example 2.

$$\begin{aligned} u_t &= -3u_x + u_{xxx}, \\ u(-1, t) &= 0, \\ u(1, t) &= \frac{1}{3}\exp(-2t)\exp(1)\bigl(5 + \exp(-6)\bigr), \\ u_x(-1, t) &= 0, \end{aligned}$$

for which the solution is

$$u(x, t) = \frac{1}{3}\exp(-2t)\bigl((2 + 3x)\exp(x) + \exp(-3)\exp(-2x)\bigr).$$

For the pseudospectral implementations Euler's method is used to advance in time and the Neumann boundary condition is implemented as follows: in the numerical scheme, considered for the equation $u_t = f(u)$, and where n and i indicate the steps in time and space, respectively, we first solve

$$u_i^{n+1} = u_i^n + \Delta t f(u^n)_i, \quad i = 1, \ldots, N-2, \tag{4.1}$$

and then use the boundary condition at $x = -1$ to solve for u_{N-1}^{n+1}

$$u_{N-1}^{n+1} = \frac{1}{D_1(N, N-1)}\left(u_x(-1, t) - \sum_{i \neq N-1} D_1(N, i)u_i^{n+1}\right).$$

For the modified pseudospectral method the parameter j in the transformation of the grid ranges from 1 to $N/2-1$, and the method coincides with the standard method for $j = N/2$. For each N the complete range of r, $r = 1,\dots,N-1$, was tested. Note that for a given time-step the cost of the modified and the standard pseudospectral methods is the same per time-step. Also, because the boundary conditions are different in each case we may expect to see different values of Δt for which the solution is stable even when N is fixed.

For the finite difference formulation we use second order central difference approximations for the first and third order derivatives at all points away from the boundaries. The stencil for the third order derivative is obviously too wide to approximate the third order derivative at one point in from the boundary. At $x = -1$ the Neumann boundary condition is imposed with the second order central difference approximation for the first order derivative. In this way a ghost value outside the grid is obtained, so that the central difference stencil for the third order derivative can be applied at one point in from the boundary. At the $x = 1$ boundary a one-sided stencil is used to approximate the third order derivative to second order for the grid point one in from the boundary. The update in time is carried out using Adams–Bashforth order 2 (AB2). Other multistep schemes were considered for the update of the boundary equation, using one or two steps only, but when evaluated for both test problems we determined that AB2 was consistently better. Moreover, it is easy to show that Euler's method is unconditionally unstable for the interior equation and that AB2 is stable for $k/h^2 < 4/(3\sqrt(3)b)$ when $\mathrm{O}(a) \approx \mathrm{O}(b)$, as is the case in the examples considered here.

The numerical computations and their costs are summarized in tables 3 and 4. The costs of the FD scheme increase linearly with N as would be expected from the

Table 3
Largest stable time-step and error.

N		4		8			16		
Ex.	Meth.	Δt	E	Δt	E	Flops	Δt	E	Flops
1	FD	2.00(−1)	7.24(−2)	2.50(−2)	2.12(−2)	3.60(4)	3.13(−3)	5.98(−3)	5.56(5)
1	MPS	1.00(−1)	2.47(−2)	2.50(−2)	8.00(−2)	4.01(4)	3.91(−4)	4.91(−2)	8.19(6)
	(r,j)	(1, 1)			(7, 2)			(9, 2)	
1	SPS	1.00(−1)	2.46(−2)	6.25(−3)	5.10(−4)	1.60(5)	4.88(−5)	9.05(−6)	6.55(7)
	r	1			4			1–12	
2	FD	2.50(−2)	8.67(−3)	3.13(−3)	1.25(−3)	1.40(5)	1.95(−4)	2.92(−4)	4.39(6)
2	MPS	1.25(−2)	5.07(−2)	1.56(−3)	3.25(−1)	6.40(5)	4.88(−5)	8.60(−3)	6.55(7)
	(r,j)	(1, 1)			(7, 2)			(1, 1)	
2	SPS	1.25(−2)	7.99(−3)	3.91(−4)	1.53(−5)	2.56(6)	6.10(−6)	2.935(−7)	5.24(8)
	r	1			6			1–12	
N^{-3}		1.56(−2)		1.95(−3)			2.44(−4)		
N^{-4}		3.90(−2)		2.44(−4)			1.53(−5)		
N^{-5}		9.76(−4)		3.05(−5)			9.53(−7)		

Table 4
Time-step for minimal error.

N		4		8			16		
Ex.	Meth.	Δt	E	Δt	E	Flops	Δt	E	Flops
1	FD	2.00(−1)	7.24(−2)	2.50(−2)	2.12(−2)	3.60(4)	3.13(−3)	5.98(−3)	5.56(5)
1	MPS	2.50(−2)	1.97(−2)	6.25(−3)	7.67(−2)	1.60(5)	9.77(−5)	1.14(−2)	3.27(7)
	(r, j)	(1, 2)			(7, 2)			(1–12,6)	
1	SPS	2.50(−2)	1.79(−2)	1.56(−3)	1.82(−4)	6.40(5)	1.22(−5)	2.26(−6)	1.16(8)
	r	1			4			1–12	
2	FD	2.50(−2)	6.67(−3)	3.13(−3)	1.25(−3)	1.40(5)	1.95(−4)	2.92(−4)	4.39(6)
2	MPS	1.25(−2)	5.07(−2)	3.91(−4)	2.12(−5)	2.56(6)	1.22(−5)	4.72(−7)	1.16(8)
	(r, j)	(1, 1)			(1, 3)			(1, 4)	
2	SPS	1.25(−2)	7.99(−3)	9.77(−5)	3.82(−6)	1.02(7)	1.53(−6)	7.34(−8)	9.29(8)
	r	1			5			1–12	

Table 5
Range of (r, j) yielding stable solutions for example 2.

N	r	j	Δt	E
8	1	1–4	1.95(−4)	2.01(−2)–8.74(−6)
	2	2–4	1.95(−4)	1.12(−2)–8.84(−6)
	3	2–4	1.95(−4)	2.28(−2)–8.42(−6)
	4	2–4	1.95(−4)	5.30(−2)–9.35(−8)
	5	2–4	1.95(−4)	3.95(−2)–8.12(−6)
	6	2–4	3.91(−4)	3.99(−2)–9.36(−6)
	7	1–3	9.77(−5)	1.53(−1)–3.35(−4)
16	1	1–8	6.10(−6)	8.60(−3)–2.93(−7)
	2	2–8	6.10(−6)	6.29(−3)–2.93(−7)
	3	2–8	6.10(−6)	1.57(−2)–2.93(−7)
	4	2–8	6.10(−6)	6.22(−2)–2.93(−7)
	5	2–8	6.10(−6)	5.76(−2)–2.93(−7)
	6	2–8	6.10(−6)	2.08(−1)–2.93(−7)
	7	2–8	6.10(−6)	1.00(−1)–2.93(−7)
	8	2–8	6.10(−6)	3.77(−1)–2.93(−7)
	9	2–8	6.10(−6)	1.22(−1)–2.93(−7)
	10	2–8	6.10(−6)	3.76(−1)–2.93(−7)
	11	2–8	6.10(−6)	1.10(−1)–2.93(−7)
	12	2–8	6.10(−6)	2.00(−1)–2.93(−7)
	13	2–5	6.10(−6)	6.55(−2)–8.39(−7)
	14	2–3	6.10(−6)	5.31(−2)–1.61(−3)
	15	2–2	6.10(−6)	1.21(−2)

sparsity of the update matrices. On the other hand, these matrices are dense for the pseudospectral methods and the costs increase quadratically with N. For each N the largest stable time-step and the time-step, within a factor of 4 of the maximum, giving the best solution as measured with respect to the relative error measured in the max norm, $E = \|\text{exact} - \text{numerical}\|_1 / \|\text{exact}\|_1$, are given. In each case the values given

Table 6
Convergence of FD scheme with N.

	Example 1			Example 2		
N	Δt	E	flops	Δt	E	flops
4	2.00(−1)	7.24(−2)	2.4(3)	2.50(−2)	8.67(−3)	9.2(3)
8	2.50(−2)	2.12(−2)	3.6(4)	3.13(−3)	1.25(−3)	1.4(5)
16	3.13(−3)	5.98(−3)	5.6(5)	1.95(−4)	2.92(−4)	4.4(6)
32	1.95(−4)	1.55(−3)	1.7(7)	1.22(−5)	7.28(−5)	1.4(8)
64	1.22(−5)	3.90(−4)	5.6(8)	7.63(−7)	1.82(−5)	4.4(9)
128	7.63(−7)	9.76(−5)	1.8(10)	4.77(−8)	4.55(−6)	7.1(10)

are within a factor 2 of the exact value, i.e. the stable time-step is less than twice the value stated. For comparison N^{-k}, $k = 3, \ldots, 5$, are also given. In table 5 the range of (r, j) for which stable solutions can be found is given, with the stable time-step and relative error for the second example only. The time-step given is that which gives a stable solution for the complete range of j stated. Clearly, comparing with table 3, for the smaller values of j a larger time-step may be taken to still give a stable solution. On the other hand, the error is still the same, at least to two significant figures, because the modified methods have error largely independent of the time-step. Convergence, roughly $O(h^2)$, of the FD scheme is shown in table 6 over the range $N = 4, \ldots, 64$.

We observe that for stable schemes the error for the modified method, for fixed r, is fixed with respect to the first two significant figures for smaller time-steps, indicating that error is due to spatial discretization. On the other hand, for the standard method the error decreases approximately by a factor 2 as $\mathrm{d}t \to \mathrm{d}t/2$, consistent with the order one accuracy of Euler's method in time. This is seen in more extensive results obtained and not summarized here. In either case the results are largely independent of r, if the scheme is stable, see table 5. But the results do depend on j very closely, and more accuracy is achieved as $j \to N/2$, the Chebyshev scheme.

The error behavior of the finite difference method is also contaminated by the error of the spatial discretization and the temporal error is not seen. Therefore for both the FD and the MPS results the best results that are given are indeed best over even smaller time-steps. On the other hand, for the SPS case decreasing the time-step leads to improvement in the error, by a factor of 2 as $\mathrm{d}t \to \mathrm{d}t/2$. Also, the costs associated with the methods increase in the same proportion.

5. Conclusions

The modified Chebyshev method suggested by Kosloff and Tal Ezer [3] theoretically has better stability properties than the standard method. Specifically, subject to an appropriate choice of parameter:

1. The eigenvalues all have negative real part.

2. The extreme eigenvalue is in the range O(N^3) to O(N^4) for N from 4 to 64.
3. The matrix is near normal.

When the finite difference and pseudospectral methods are compared with respect to cost and accuracy we conclude that the method of choice is dependent on the accuracy required. Specifically:

1. If high accuracy is required, without concern for cost, the standard pseudospectral method is the method of choice, giving the least error for a given choice of N. To obtain accuracy equivalent to the $N = 8$ SPS method, N is required to be greater than 64 and 128 for examples 1 and 2, respectively. The associated costs are greater by a factor of at least 10^3 and 10^4, respectively.
2. The cost to achieve the best result with the MPS method is only about twice that of the best result with finite differences for the small values of N considered in this study. The result is, however, substantially improved. Therefore the modified method stands to provide a good compromise between the high spectral accuracy of the SPS method and the much lower accuracy of the FD method.
3. The stable time-steps for the pseudospectral methods are in all cases much better than the worst case predictions of N^{-6}. Stable time-steps are approximately a factor of N larger for the MPS method as compared to the SPS method. In the latter case a stable time-step is achieved between N^{-4} and N^{-5}. This will worsen as N increases, but in practice N is rarely taken large because of the dramatic increase in cost that occurs. Rather, a multidomain approach with moderate sized N would be preferred.
4. Note that the FD formulation considered was only second order in space. But even in this case the implementation was not straightforward because of the wide stencil required just to generate a second order approximation to a third order derivative. The local form of the FD formulation poses more and more problems as the order of the differential equation increases and the order of the spatial approximation to the derivatives becomes wider. Because pseudospectral methods are inherently global this is not an issue.

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