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THE METHOD OF LINES AND EXPONENTIAL FITTING

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SUMMARY

When the method of lines is used for solving time-dependent partial differential equations, finite differences are commonly employed to obtain the semidiscrete equations. Usually, if the solution is expected to be smooth, symmetric difference formulae are chosen for approximating the spatial derivatives. These difference formulae are almost invariably based on Lagrange type differentiation formulae. However, if it is known in advance that periodic components of given frequency are dominating in the solution, more accurate difference formulae, based on exponentials with imaginary exponent, are available. This paper derives such formulae and presents numerical results which clearly indicate that the accuracy can be improved considerably by exploiting additional knowledge on the frequencies of the solution.

1. INTRODUCTION

A widely used approach to solving time-dependent *partial* differential equations is the method of lines. This method replaces the spatial derivatives by discrete approximations and enables us to apply well-developed time integrators for solving the resulting systems of *ordinary* differential equations. When finite differences are used to obtain the semidiscrete equations, almost invariably Lagrange-type formulae, based on polynomial interpolation of the solution, are employed to derive the difference approximations. However, in many problems arising in fluid dynamics it is known in advance that the solution is dominated by one or more periodic components of known frequency. In such cases it turns out to be better to use difference formulae based on trigonometric interpolation, that is we require that the difference formulae have a reduced truncation error for certain exponential functions with imaginary argument (see section 2). We will call such formulae *exponentially fitted* difference formulae.

In Reference 1 exponentially fitted difference approximations to first-order spatial derivatives were derived and were shown to be more accurate than conventional difference formulae in oscillatory problems. These results are summarized in section 3.1. In section 3.2, similar formulae are derived for second-order derivatives and a comparison is made with conventional difference formulae. In section 3.3, we discuss the automatic estimation of dominant frequencies in grid functions. By means of a few numerical examples we show the performance of such a frequency estimator.

Section 4 provides formulae for approximating boundary conditions to be imposed on periodic solutions.

Finally, in Section 5, we show by a number of numerical experiments that using exponentially fitted difference formulae in the space discretization of partial differential equations leads to a considerable improvement of the accuracy.

The adaption of *spatial discretizations* to known frequencies of the exact solution has received

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little attention in the literature. This is in contrast to the development of *time integrators* for solving periodic initial-value problems where a lot of work already has been done. We mention the papers of Gautschi[2] Brusa and Nigro,[3] Gladwell and Thomas[4] and van der Houwen and Sommeijer,[5] where further references to oscillatory time integrators can be found.

2. THE TRUNCATION ERROR IN THE METHOD OF LINES

We discuss the discretization of partial differential equations of the general form

$$\frac{\partial^\nu w}{\partial t^\nu} = F(w) := G\left(t, \mathbf{x}, w, \frac{\partial w}{\partial x_1}, \frac{\partial w}{\partial x_2}, \frac{\partial^2 w}{\partial x_1^2}, \frac{\partial^2 w}{\partial x_2^2}\right), \quad \mathbf{x} = (x_1, x_2)^{\mathrm{T}} \in \Omega, \quad \nu = 1, 2 \tag{1}$$

where F is the differential operator defined by the function G, and where it is known in advance that the solution is composed of components that are periodic in the space variable $\mathbf{x}$. Applying the method of lines we replace the differential operators by difference operators:

$$\frac{\partial}{\partial x_j} \sim D_j, \quad \frac{\partial^2}{\partial x_j^2} \sim D_{2+j}, \quad j = 1, 2 \tag{2}$$

and instead of (1), we consider the equation

$$\begin{aligned} &\frac{\partial^\nu W}{\partial t^\nu} = F_\Delta(W) := G(t, \mathbf{x}, W, D_1 W, D_2 W, D_3 W, D_4 W) \\ &\mathbf{x} \in \Omega_\Delta := \{\mathbf{x} \mid \mathbf{x} = (j\Delta x_1, l\Delta x_2)^{\mathrm{T}};\ j, l = 0, \pm 1, \pm 2 \end{aligned} \tag{3}$$

where W is a function of t and $\mathbf{x}$.

The truncation error of the semidiscrete equation (3) corresponding to a given test function $w = w(t, \mathbf{x})$ is given by

$$L(w) := \frac{\partial^\nu w}{\partial t^\nu} - F_\Delta(w) = F(w) - F_\Delta(w), \quad \mathbf{x} \in \Omega_\Delta \tag{4}$$

Suppose that the solution of (1) is given by

$$w_0 := \sum_{r=1}^{R} w_0^{(r)}(t) \exp(i\mathbf{f}^{(r)} \cdot \mathbf{x}) \tag{5}$$

where the frequency vectors

$$\mathbf{f}^{(r)} := (f_1^{(r)}, f_2^{(r)})^{\mathrm{T}}, \quad r = 1, \ldots, R$$

are either known or are known to lie in a given real domain. Furthermore, let the exponential functions in (5) be eigenfunctions of the difference operators in (2) with eigenvalues defined by

$$D_j \exp(i\mathbf{f}^{(r)} \cdot \mathbf{x}) = \delta_j^{(r)} \exp(i\mathbf{f}^{(r)} \cdot \mathbf{x}), \quad j = 1, \ldots, 4 \tag{6}$$

Then from (4) and the definition of the operators F and F_Δ it follows that the magnitude of the truncation error corresponding to (5) can be reduced by minimizing the magnitude of the functions

$$\frac{\partial w_0}{\partial x_j} - D_j w_0 = \sum_{r=1}^{R} [if_j^{(r)} - \delta_j^{(r)}] w_0^{(r)}(t) \exp(i\mathbf{f}^{(r)} \cdot \mathbf{x}), \tag{7a}$$

$$j = 1, 2$$

$$\frac{\partial^2 w_0}{\partial x_j^2} - D_{2+j} w_0 = \sum_{r=1}^{R} [(if_j^{(r)})^2 - \delta_{j+2}^{(r)}] w_0^{(r)}(t) \exp(i\mathbf{f}^{(r)} \cdot \mathbf{x}) \tag{7b}$$

We observe that by *symmetric* difference operators, we obtain in (6) purely imaginary eigenvalues for $j = 1, 2$ and real eigenvalues for $j = 3, 4$. Thus, it is then feasible to minimize the magnitude of the functions (7) by minimizing the extreme values of the real-valued functions

$$if_j^{(r)} - \delta_j^{(r)}, \quad (f_j^{(r)})^2 + \delta_{j+2}^{(r)}, \quad j = 1, 2; \quad r = 1, \ldots, R \tag{8}$$

by a judicious choice of the discretization weights in the difference operators. Since we do not want too many grid points involved in the discretization molecules, the minimization of (8) is only effective if R is small, that is the exact solution is dominated by only a few Fourier components.

3. EXPONENTIALLY FITTED DIFFERENCE FORMULAE

In this section we present discretization molecules for numerical differentation of periodic functions of the form (5).

3.1. First-order derivatives

Without derivation we give a symmetric, fourth-order, four-point line discretization:[1]

$$\begin{aligned} D_1 &= \frac{1}{\Delta x_1}[\xi_1(E_1^{+1} - E_1^{-1}) + \xi_2(E_1^2 - E_1^{-2})] \\ \xi_2 &:= \frac{\dfrac{z_+}{\sin(z_+)} - \dfrac{z_-}{\sin(z_-)}}{4[\cos(z_+) - \cos(z_-)]}, \quad \xi_1 := \frac{z_+}{2\sin(z_+)} - 2\xi_2\cos(z_+) \end{aligned} \tag{9}$$

where E_1 defines the forward shift operator over one mesh width; here

$$z_+ = f_1^{(1)}\Delta x_1, \quad z_- = f_1^{(2)}\Delta x_1 \tag{10a}$$

if we want to eliminate just two frequencies from the truncation error, and

$$z_{\pm} = \Delta x_1[\tfrac{1}{2}(\bar{f}_1^2 + \underline{f}_1^2) \pm \tfrac{1}{4}\sqrt{2}(\bar{f}_1^2 - \underline{f}_1^2)]^{1/2} \tag{10b}$$

if we want to minimize the truncation error for all frequencies in the interval

$$\underline{f}_1 \leqslant f_1^{(r)} \leqslant \bar{f}_1.$$

A similar definition holds for the difference operator D_2.

The formula (9) will be called an *exponentially fitted difference formula*.

3.2. Second-order derivatives

Consider the approximation

$$\frac{\partial^2}{\partial x_1^2} \sim D_3 := \frac{1}{(\Delta x_1)^2}\sum_{l=0}^{k}\sum_{j=0}^{k}\xi_j^{(l)}(E_1^{+j} + E_1^{-j})(E_2^{+l} + E_2^{-l}) \tag{11}$$

where E_i denotes the shift operator along the x_i-axis. It is elementary to show that this approximation is second-order accurate if

$$\begin{aligned} &\sum_{j,l=0}^{k}\xi_j^{(l)} = O[(\Delta x_1)^{p+2}], \quad \sum_{j,l=0}^{k} j^2\xi_j^{(l)} = \tfrac{1}{2} + O[(\Delta x_1)^p] \\ &\sum_{j,l=0}^{k} l^2\xi_j^{(l)} = O[(\Delta x_1)^p] \end{aligned} \tag{12a}$$

holds for $p=2$, and fourth-order accurate if (12a) holds for $p=4$ and if, in addition,

$$\sum_{j,l=0}^{k} j^4\xi_j^{(l)} = O[(\Delta x_1)^2], \quad \sum_{j,l=0}^{k} l^4\xi_j^{(l)} O[(\Delta x_1)^2], \quad \sum_{j,l}^{k} j^2 l^2 \xi_j^{(l)} = O[(\Delta x_1)^2] \tag{12b}$$

We remark that usually the order terms in the order equations (12a) and (12b) are set to zero, so that polynomials of sufficiently low degree are exactly differentiated. The corresponding difference formulae will be called *conventional* formulae. The introduction of the order terms does not decrease the (algebraic) order of the difference formulae and enables us to differentiate certain exponential functions with reduced errors, as will be shown below.

Let us apply the symmetric difference operator (11) to an exponential function. This leads to the eigenvalue (cf. (6))

$$\begin{aligned} \delta_3^{(r)} &= \frac{4}{(\Delta x_1)^2} \sum_{j,l=0}^{k} \xi_j^{(l)} \cos(j\mu_1^{(r)}) \cos(l\mu_2^{(r)}) \\ \mu_j^{(r)} &:= f_j^{(r)} \Delta x_j; \quad j = 1, 2 \end{aligned} \tag{13}$$

Defining the function

$$a_1(\mu) := \mu_1^2 + 4 \sum_{j,l=0}^{k} \xi_j^{(l)} \cos(j\mu_1) \cos(l\mu_2) \tag{14}$$

it follows from (8) and (14) that we should minimize

$$|(f_1^{(r)})^2 + \delta_3^{(r)}| = \frac{1}{\Delta^2 x_1} |a_1(\mu^{(r)})|, \quad r = 1, \ldots, R \tag{15}$$

In particular, we consider the minimization of (15) for five-point line discretizations, i.e.

$$D_3 = \frac{2}{(\Delta x_1)^2} [2\xi_0 + \xi_1(E_1^{+1} + E_1^{-1}) + \xi_2(E_1^{+2} + E_1^{-2})] \tag{16}$$

where we have omitted the super index in the discretization weights. The corresponding function (14) assumes the form

$$\begin{aligned} a_1(\mu) &= \mu_1^2 + 4[\xi_0 + \xi_1 \cos(\mu_1) + \xi_2 \cos(2\mu_1)] \\ &= \mu_1^2 + 4(\xi_0 - \xi_2) + 4\xi_1 \cos(\mu_1) + 8\xi_2 \cos^2(\mu_1) =: \bar{a}_1(\mu_1) \end{aligned} \tag{17}$$

In order to minimize the extreme values of (15) we require

$$\bar{a}_1(z_r) = 0, \quad r = 1, 2, 3 \tag{18}$$

where the three zeros of $\bar{a}_1$ are located at suitable points in the frequency interval. For instance, if $R=3$ and the three frequencies in (15) are known, then we set

$$z_r = f_1^{(r)} \Delta x_1, \quad r = 1, 2, 3 \tag{19}$$

Alternatively, when it is only known that

$$\underline{f}_1 \leqslant f_1^{(r)} \leqslant \bar{f}_1, \quad r = 1, \ldots, R \tag{20}$$

then suitable values for z_r can be obtained by identifying the zeros of $\bar{a}_1(z)$ with the zeros of a Chebyshev polynomial shifted to the interval of frequencies (20).[1] This results in

$$z_2 = \sqrt{\tfrac{1}{2}(\bar{f}_1^2 + \underline{f}_1^2)}\, \Delta x_1, \quad z_1 = \sqrt{z_2^2 - (z_2^2 - \underline{f}_1^2 \Delta^2 x_1) \cos\left(\frac{\pi}{6}\right)},$$

$$z_3 = \sqrt{z_2^2 - (z_2^2 - \bar{f}_1^2 \Delta^2 x_1)\cos\left(\frac{\pi}{6}\right)} \tag{21}$$

The conditions (18) imply that exponential functions of the form

$$\exp\left(i\frac{z_r x_1}{\Delta x_1}\right), \quad r = 1, 2, 3$$

are exactly differentiated by the difference operator (16).

For future reference, we give the solution of equation (18):

$$\begin{aligned}
\xi_2 &= \frac{1}{8}\frac{z_1^2(c_2 - c_3) + z_2^2(c_3 - c_1) + z_3^2(c_1 - c_2)}{(c_1 - c_2)(c_3 - c_1)(c_2 - c_3)} \\
\xi_1 &= -\frac{1}{4}\frac{z_1^2 - z_2^2}{c_1 - c_2} - 2\xi_2(c_1 + c_2) \\
\xi_0 &= \xi_2 - \xi_1 c_1 - 2\xi_2 c_1^2 - \tfrac{1}{4}z_1^2: \quad c_r = \cos(z_r), \quad r = 1, 2, 3
\end{aligned} \tag{22}$$

The discretization (16), (22) will be called an *exponentially fitted difference formula*.

We observe that the usual 5-point line discretization arises if $a(z)$ has all its zeros at the origin. The corresponding weights are given by

$$\xi_0 = -\tfrac{5}{8}, \quad \xi_1 = \tfrac{2}{3}, \quad \xi_2 = -\tfrac{1}{24} \tag{23}$$

This discretization satisfies (12) with $p = 4$ so that it is fourth-order accurate. It can be shown that the discretizations (16), (22), (19) and (16), (22), (21) are also fourth-order accurate.

In order to compare the truncation errors of the discretizations (16), (22) and (23), we derive expressions for the extreme values of $|\bar{a}|$ on the frequency interval (20) if the mesh size tends to zero. For (23) we easily find

$$|\bar{a}_1(\bar{f}_1 \Delta x_1)| \approx \tfrac{1}{90}(\bar{f}_1 \Delta x_1)^6 \text{ as } \Delta x_1 \to 0 \tag{24}$$

Since, in the case (22), the zeros of $\bar{a}$ vanish as the mesh size decreases, we find a similar expression to (24) only differing by the order constant; numerically we found for the case where the left end point of the frequency interval is the origin

$$|\bar{a}_1(\bar{f}_1 \Delta x_1)| \approx \frac{1}{3000}(\bar{f}_1 \Delta x_1)^6 \text{ as } \Delta x_1 \to 0 \tag{25}$$

3.3. *Automatic estimation of dominant frequencies*

In actual computation, it is convenient to estimate automatically the main frequencies of the numerical solution. Suppose that at $t = \bar{t}$ ($\bar{t}$ fixed) the numerical solution is expected to be an approximation to the function

$$u(\mathbf{x}) := \sum_{r=1}^{R} a_r \exp(i\,\mathbf{f}^{(r)} \cdot \mathbf{x}), \quad a_r \in \mathbb{C}, \quad \mathbf{f}^{(r)} \in \mathbb{R}^2 \tag{26}$$

A straightforward technique for determining the frequency vectors $\mathbf{f}^{(r)}$ is based on the minimization of the expression

$$\sum_{j=1}^{N} |u(\mathbf{x}_j) - U_j|^2 \tag{27}$$

where U_j denotes the numerical approximation to $u(\mathbf{x}_j)$ and $\{\mathbf{x}_j\}_{j=1}^{N}$ represents a set of grid points.

Most numerical libraries for large scale computing contain a suitable least-squares routine for solving this problem (e.g. NAG routine E04FCF). The efficiency of the least-squares algorithm for finding the frequencies $\mathbf{f}^{(r)}$ (and the coefficients a_r) that minimize (27) decreases when the number of parameters increases. Therefore, it is advantageous to replace (27) by an expression in which fewer parameters are involved. In particular, it would be nice when only the frequency parameters $\mathbf{f}^{(r)}$ are left. We illustrate the derivation of such an expression by a few examples.

Example 1. Let in (26) x be scalar and let $R = 1$, i.e.

$$u(x) = a_1 \exp(if^{(r)}x) \tag{28}$$

By applying the operator $P(E)$, where E is the forward shift operator and

$$P(z) = \sum_{j=-m}^{m} p_j z^j \tag{29}$$

we obtain the identity

$$P(E)u(x) - P(e^{if^{(1)}\Delta x})u(x) \equiv 0 \tag{30}$$

Suppose that $P(z)$ satisfies the condition

$$P(z) = P(1/z) \tag{31}$$

i.e. $p_j = p_{-j}$, and define

$$P^*(z) := p_0 + 2\sum_{j=1}^{m} p_j \cos(jz) \tag{32}$$

Then (30) assumes the form

$$P(E)u(x) - P^*(f^{(1)}\Delta x)u(x) \equiv 0 \tag{33}$$

This identity suggests the minimization of the *one-parameter expression*

$$\sum_{j=1}^{N} |[P(E) - P^*(f^{(1)}\Delta x)]\,U_j|^2 \tag{34}$$

Simple examples of a suitable function $P(z)$ are given by $P_1(z) = z + (1/z)$ and $P_2(z) = z - 2 + (1/z)$.

Example 2. Next we consider the case $R = 2$:

$$u(x) = a_1 \exp(if^{(1)}x) + a_2 \exp(if^{(2)}x) \tag{35}$$

Let us define the functions

$$v(x) := P(E)u(x), \quad w(x) := P^2(E)u(x) \tag{36}$$

Then we easily derive the identity

$$P^*(f^{(1)}\Delta x)P^*(f^{(2)}\Delta x)u(x) - [P^*(f^{(1)}\Delta x) + P^*(f^{(2)}\Delta x)]v(x) + w(x) \equiv 0 \tag{37}$$

As in the preceding example, this identity straightforwardly leads to a *two-parameter expression* to be minimized over the two frequency parameters.

In order to illustrate the performance of a frequency estimator based on (37) we have listed a few results in Table I for both functions $P_1(z)$ and $P_2(z)$. The choice of these functions is determined by efficiency considerations. The functions $u(x)$ correspond to the functions $w(0, x)$ used in our numerical experiments reported in Section 5. The results obtained show that the inaccuracy of the

Table I. Estimation of dominant frequencies

Problem	$2\pi/\Delta x$	$P_1(z)$ $f^{(1)}$	$P_1(z)$ $f^{(2)}$	$P_2(z)$ $f^{(1)}$	$P_2(z)$ $f^{(2)}$
1. $u(x) = \sin(\sin(x))$	8	0	1·10	0	1·45
	16	1·00	2·99	1·00	2·99
3. $u(x) = \tan(\sin(x))$	16	1·00	3·32	1·01	3·32
4. $u(x) = \sin(4x) + \sin(5x) + \sin(6x)$	16	4·05	5·90	4·05	5·90
5. $\sin(x) + \sin(1{\cdot}2x)$	8	1·00	1·20	1·00	1·20

estimated frequencies is at most 10 per cent for $P_1(z)$ and 40 per cent for $P_2(z)$. The latter error occurs for problem 1 on the coarsest grid. The other results appeared not to be sensitive to the choice of the function $P(z)$.

4. EXPONENTIALLY FITTED EXTRAPOLATION

In order to apply the symmetric difference operator (9) and (16), (22) near the boundary points we need to extrapolate, beyond the boundary, the numerical solution obtained at internal grid points. When *conventional* difference operators are used, then we may employ polynomial extrapolation; for example, the sixth-order formula

$$w(\mathbf{x}) \approx [6(E_1 + E_1^5) - 15(E_1^2 + E_1^4) + 20E_1^3 - E_1^6]w(\mathbf{x}) \tag{38}$$

However, when using *exponentially fitted* discretizations, then polynomial extrapolation is inaccurate, unless still higher order formulae are applied. A more attractive alternative is the use of exponentially fitted extrapolation formulae.

Let us start with the symmetric interpolation formula

$$w(\mathbf{x}) \approx A_1 w(\mathbf{x}) := \sum_{l=0}^{k} \sum_{j=1}^{k} \zeta_j^{(l)}(E_1^j + E_1^{-j})(E_2^l + E_2^{-l})w(\mathbf{x}) \tag{39}$$

and require that this approximation has a small truncation error for functions of the form (5). Then, the extrapolation weights should be such that

$$\begin{aligned} w_0 - A_1 w_0 &= \sum_{r=1}^{R} [1 - \alpha_1^{(r)}] w_0^{(r)}(t) \exp(\mathrm{i}\mathbf{f}^{(r)} \cdot \mathbf{x}) \\ \alpha_1^{(r)} &:= 4 \sum_{l=0}^{k} \sum_{j=1}^{k} \zeta_j^{(l)} \cos(j\mu_1^{(r)}) \cos(l\mu_2^{(r)}) \end{aligned} \tag{40}$$

is small in magnitude. This is achieved by minimizing the magnitude of the function

$$b_1(\mu) := 1 - \alpha_1^{(r)} = 1 - 4 \sum_{l=0}^{k} \sum_{j=1}^{k} \zeta_j^{(l)} \cos(j\mu_1) \cos(l\mu_2) \tag{41}$$

over the range of frequencies. (Notice that $b_1(\mu)$ does not have the same form as the function $a_1(\mu)$ defined by (14): this can be traced back to the fact that $a_1(\mu)$ corresponds to the truncation error of a *difference* operator, whereas $b_1(\mu)$ corresponds to the truncation error of an *extrapolation* formula.) This minimax problem is similar to that discussed in section 3.2 for the function (14) and the (approximate) solution of this problem can be obtained along the same lines.

In our numerical experiments we will apply the seven-point formula that arises for

$$k=3,\quad \zeta_j^{(l)}=0 \quad \text{for } l\neq 0. \tag{42}$$

Defining

$$b_1(\mu)=\bar{b}_1(\mu_1):=1-4[\zeta_1\cos(\mu_1)+\zeta_2\cos(2\mu_1)+\zeta_3\cos(3\mu_1)] \tag{43}$$

we arrive at the fitting conditions (cf. (18))

$$\bar{b}_1(z_r)=0,\quad r=1,2,3 \tag{44}$$

where the three zeros of $\bar{b}_1$ coincide with (19) or (21). By solving (44), we obtain the extrapolation weights and the resulting extrapolation formula is then given by

$$w(\mathbf{x})\approx\left[-\frac{\zeta_2}{\zeta_3}(E_1+E_1^5)-\frac{\zeta_1}{\zeta_3}(E_1^2+E_1^4)+\frac{1}{2\zeta_3}E_1^3-E_1^6\right]w(\mathbf{x}) \tag{45}$$

Just as the difference formula (16), (22), the extrapolation formula (45) presents an approximation to the formula that really minimizes the magnitude of the function (41). In the special case where $\zeta_j^{(l)}=0$ for $l\neq 0$, it is possible to solve the minimax problem exactly, because $b_1(\mu)$ can then be expressed as a polynomial in $\cos(\mu_1)$ and for polynomials minimax solutions are available.

5. NUMERICAL EXPERIMENTS

By means of numerical examples we will show that the exponentially fitted discretization formulae derived in the preceding sections lead to considerably larger accuracies than the conventional discretizations, for both linear and non-linear problems. The problems are specified in Table II.

The initial conditions are taken from the exact solution. In cases where the solution is periodic with respect to the given x-interval, we compare results obtained by imposing Dirichlet boundary conditions and by imposing a periodicity condition. We confine our experiments to equations of the form

$$\frac{\partial^2 w}{\partial t^2}=G\left(x,t,w,\frac{\partial^2 w}{\partial x^2}\right) \tag{46}$$

The spatial discretization was based on 5-point formulae; we present results obtained by conventional and by exponentially fitted formulae ((16) with (23) and with (22)). In the case of Dirichlet boundary conditions, we used the polynomial extrapolation formula (38) for conventional discretizations and the exponentially fitted formula (45) otherwise.

The time integration was performed by the second-order Runge–Kutta–Nyström method generated by the Butcher array:[5]

$$\begin{array}{c|cccc} 1/2 & 0 & & & \\ 1/2 & 0 & 1/30 & & \\ 1/2 & 0 & 0 & 1/12 & \\ \hline & 0 & 0 & 0 & 1/2 \\ & 0 & 0 & 1 & 1 \end{array} \tag{47}$$

This method has zero dissipation and phase-lag order $q=6$. The periodicity interval is given by $[0,(2{\cdot}75)^2]$.

The accuracy of the results is measured by the number of correct digits, i.e. by

$$cd:=-\log_{10}|\text{ maximal absolute error at the end point } t=T| \tag{48}$$

In the table of results, cd(P) and cd(D) correspond to results obtained by imposing periodic and

Table II. Numerical results

Problem	T	$2\pi/\Delta x$	$T/\Delta t$	$\{f_1^{(r)}\}$	cd(P)	cd(D)
1. $w_{tt} = w_{xx}$	1	8	16	$\{0, 0, 0\}$	1·80	1·30
$w = \sin(\sin(x+t))$				$\{1, 2, 3\}$	2·99	2·89
$0 \leqslant x \leqslant 2\pi$		16	32	$\{0, 0, 0\}$	2·92	2·17
$0 \leqslant t \leqslant T$				$\{1, 3, 5\}$	4·19	4·19
2. $w_{tt} = \dfrac{(1+w^2)w_{xx}}{1+\sin^2(\sin(x+t))}$	1	8	16	$\{0, 0, 0\}$	1·83	1·32
				$\{1, 2, 3\}$	3·00	2·90
		16	32	$\{0, 0, 0\}$	2·92	2·18
$w = \sin(\sin(x+t))$				$\{1, 3, 5\}$	4·20	4·20
$0 \leqslant x \leqslant 2\pi$	10	16	32	$\{0, 0, 0\}$	1·88	1·83
$0 \leqslant t \leqslant T$				$\{1, 3, 5\}$	4·17	4·06
3. $w_{tt} = \dfrac{(1+w^2)w_{xx}}{1+\tan^2(\sin(x+t))}$	1	16	32	$\{0, 0, 0\}$	1·95	1·46
				$\{1, 2, 3\}$	2·21	1·74
$w = \tan(\sin(x+t))$				$\{1, 3, 5\}$	2·70	2·45
$0 \leqslant x \leqslant 2\pi, 0 \leqslant t \leqslant T$				$(0, 2, 4)$	1·98	1·75
4. $w_{tt} = w_{xx}$						
$w = \sin 4(x+t) + \sin 5(x+t)$	1	16	32	$\{0, 0, 0\}$	−0·06	−0·65
$+ \sin 6(x+t)$				$[3, 7]$	0·62	−0·02
$0 \leqslant x \leqslant 2\pi, 0 \leqslant t \leqslant T$				$[4, 6]$	1·58	1·06
				$[4{\cdot}5, 5{\cdot}5]$	1·11	0·60
5. $w_{tt} = w^2\Big[w_{xx} - \dfrac{1}{w} + w$	1	8	16	$\{0, 0, 0\}$	−0·62	1·16
$+ 0{\cdot}44\sin(1{\cdot}2x + t)\Big]$				$[0{\cdot}9, 1{\cdot}3]$	−0·61	3·26
$w = \sin(x+t) + \sin(1{\cdot}2x + t)$				$[1, 1{\cdot}2]$	−0·61	3·28
$0 \leqslant x \leqslant 2\pi, 0 \leqslant t \leqslant T$				$[1{\cdot}05, 1{\cdot}1]$	−0·61	3·34
6. $w_{tt} = w_{xx} + \dfrac{6xt}{8\pi^3}(x^2 - t^2)$	1	8	16	$\{0, 0, 0\}$	0·98	1·31
				$\{1, 2, 3\}$	0·84	1·40
$w = \sin(\sin(x+t)) + \left(\dfrac{xt}{2\pi}\right)^3$		16	32	$\{0, 0, 0\}$	0·54	2·15
$0 \leqslant x \leqslant 2\pi, 0 \leqslant t \leqslant T$				$\{1, 3, 5\}$	0·52	1·84

Dirichlet boundary conditions, respectively. We observe that imposing periodic boundary conditions in cases where the initial conditions are not periodic *with respect to the given x-interval* leads to singularities in the exact solution at the boundary points (e.g. problem 5) caused by an inconsistency of the initial-boundary values.

The purpose of the experiments listed in Table II is to show that the use of exponentially fitted space discretizations, instead of conventional discretizations, will *improve the accuracy considerably in all cases where the exact solution is periodic*. This assertion is supported by the

Table III. cd(D) values for various frequency intervals $[\underline{f}_1, \bar{f}_1]$

Problem 7	$\frac{2\pi}{\Delta x}$	$\frac{1}{\Delta t}$	$\{0,0,0\}$	$[0,1]$	$[0,2]$	$[0,3]$
$w_{tt} = w_{xx}$	8	16	2·06	1·92	1·44	0·70
$w = 1/(1+x+t)$	16	32	2·78	2·71	2·48	2·06
$0 \leqslant x \leqslant 2\pi, 0 \leqslant t \leqslant 1$	32	64	3·78	3·74	3·62	3·78

Table IV. Numerical results for problem 2 with $\Delta x = 2\pi/16$, $\Delta t = 1/32$

	$\{f_1^{(r)}\} = \{0,0,0\}$		$\{f_1^{(r)}\} = \{1,3,5\}$	
t	cd(P)	cd(D)	cd(P)	cd(D)
0·2	3·75	3·25	4·47	4·47
0·4	3·33	2·65	4·26	4·26
0·6	3·02	2·30	4·17	4·17
0·8	2·91	2·16	4·16	4·16
1·0	2·92	2·18	4·20	4·20
2·0	2·54	2·03	4·27	4·29
4·0	2·25	1·90	4·14	4·25

results obtained for the problems 1–5. Even in a case where the true frequencies differ completely from the predicted frequencies, such as in the last row of problem 3, the exponentially fitted formulae are competitive with the conventional formulae. Also, notice that changing from periodic to Dirichlet boundary conditions decreases the accuracy of conventional space discretizations much more than the accuracy of the exponentially fitted discretizations.

The last problem of Table II was obtained from problem 1 by adding a *non-oscillatory term* to the exact solution. As a consequence, only the oscillatory part of the solution will be computed with increased accuracy by the exponentially fitted method, whereas the non-oscillatory part is computed with considerably reduced accuracy. The results in Table II indicate that in such cases there is no advantage in using exponentially fitted methods. Notice that imposing periodic boundary conditions leads to bad accuracies because of the inconsistency in the initial-boundary values.

Next, we integrated a problem with no space oscillations at all. In Table III, results are given for the conventional discretization (arising if the frequencies are $\{0,0,0\}$) and for three frequency intervals. At first, if the grid is rather coarse, the exponentially fitted method is considerably less accurate than the conventional method. On finer grids, however, the accuracies become more and more comparable because the exponentially fitted method converges to the conventional method.

Finally, we considered the error behaviour as a function of t. The results for problem 2 listed in Table II already indicate that the conventional method is more sensitive to long interval integration than the exponentially fitted method. Table IV presents more detailed information on the error behaviour of the various methods.

6. CONCLUDING REMARKS

Below we summarize the main properties of exponentially fitted space discretizations in comparison with conventional discretizations using the same number of grid points:

(i) The *additional costs* are negligible.
(ii) The *order of accuracy* does not change (cf. Table III).
(iii) The *accuracy* improves considerably if
    (a) only a few (approximately known) frequencies dominate the solution (cf. problems 1–4)
    (b) all dominating frequencies are located in a small interval (cf. problems 5).
(iv) The properties (i), (ii) and (iii) also hold for *non-linear* problems.
(v) If the solution contains *non-periodic components*, then there is no advantage in using exponentially fitted space discretizations (cf. problem 6).
(vi) If the solution contains no periodic components, then conventional discretization methods are to be preferred.

Furthermore, we remark that the frequency estimator described in Section 3.3 yields reliable results and can be used as a part of a computer implementation of exponentially fitted space discretizations.

Finally, we observe that a similar approach can be followed in designing space discretizations that are fitted to exponentials with real arguments (i.e. in (5) $i\mathbf{f}^{(r)}$ is real valued).

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