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# A Pseudo-Spectral FFT Technique for Non-Periodic Problems

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A technique is developed for the use of pseudo-spectral Fast Fourier Transform methods for non-periodic time-dependent problems in fluid dynamics. Called "reduction to periodicity," it involves the evaluation of a polynomial function which approximates the departure from smooth periodicity of the dependent variable distribution at each time level. The FFT is then applied to the residual distribution. The accuracy is demonstrated in several one-dimensional problems. Stability and iterative convergence are demonstrated in one-dimensional problems with first order, second order, and fourth order time differencing, and in two-dimensional problems with first-order time differencing.

## 1. INTRODUCTION

Spectral and pseudo-spectral methods for fluid dynamics dynamics problems have been pioneered by Orszag [1–3]. The article by Orszag and Israeli [4] provides other references and an introduction to the subject; see also the monograph by Kreiss and Oliger [5] and the forthcoming monograph by Gottlieb and Orszag [6]. For periodic problems, the spatial derivatives are evaluated from the Discrete Fourier Transform using the well-known FFT (Fast Fourier Transform) algorithms. The pseudo-spectral methods (or collocation methods) are more general, simpler, and faster than the spectral methods for the variable coefficient problems of interest here. In the pseudo-spectral approach, the partial differential equations are not actually transformed as in the spectral methods; rather, the FFT is merely used to evaluate spatial derivatives in place of conventional finite difference or finite element algebraic expressions.

The use of the FFT over $M$ nodepoints corresponds to using $M$-th order trigonometric interpolation to evaluate the derivatives. This procedure is of "infinite order" [2, 4] in the sense that it may be shown to converge (ultimately) faster than any finite-order finite difference expression when all derivatives are continuous. Spectral and pseudo-spectral methods are also especially well-suited to hydrodynamic stability problems because they minimize phase-error problems, the only contribution to phase error coming from the time differencing. However, this high accuracy only occurs with periodic (and similar) boundary conditions. For viscous problems with no-slip walls, the boundary conditions are not so simple. Orszag uses Chebyshev polynomials (instead of the trigonometric polynomials of the FFT) and fast transform techniques similar to the FFT as the basis of the orthogonal expansion for these



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problems. Different problems in different coordinate systems require that new orthogonal expansions be found. "In practice, it is not a trivial matter to decide on the right expansions and the proper method for their implementation. Further, if the proper expansions are not made and the proper techniques not used to evaluate them, very inefficient and possibly inaccurate simulations may result" [4, p. 291]. (For a summary of some problems for which Fourier and Chebyshev transform methods apply, see [2, p. 108; 4, pp. 291–293].)

In order to use only the simpler, readily available FFT and still use pseudo-spectral methods for non-periodic problems, some computational artifice must be used. For the computation of a pulse propagation in Burgers equation, with the pulse extending over $0 \leqslant x \leqslant X_1$, Gazdag [7] added an artificial data set over $-X_0 \leqslant x \leqslant 0$. This data set over $X_0$ was chosen so as to give continuous functions and derivatives when the total function is extended periodically with period $X = X_0 + X_1$. Then the FFT is applied over $X$, but the results for spatial derivatives are computed only over $X_1$. Additional computational time is required for the FFT to be applied over $X_0 + X_1$, and the form of the data added in $X_0$ is appropriate only for that particular problem studied, in which the dependent variable is essentially constant near the left-hand and right-hand boundaries for the problem time of interest. Although thus limited, Gazdag's work demonstrated that pseudo-spectral FFT methods could be adapted to a non-periodic problem, and thereby motivated the present work. Preliminary results on the present work were presented in [8, 9].

## 2. The Technique: Reduction to Periodicity

As a more general artifice that involves no penalty of additional FFT time, consider the following technique which we describe as "reduction to periodicity." Consider an arbitrary distribution of the dependent variable $f_1$ at some time. The $f_1$ distribution is decomposed, in one direction at a time, into the sum of a polynomial $g$ and a residual function $f_2$. The $N$th degree polynomial is chosen so that the residual function $f_2$, when extended as a periodic function, is continuous through the $(N - 1)$ order derivatives at the boundaries. The FFT is applied only to the residual function $f_2$ to obtain its derivatives in the usual way (see e.g. [7]) while the derivatives of the polynomial function $g$ are obtained analytically.

The derivatives of the original (total) function $f_1(x)$ at both boundaries must be known, exactly or approximately, to the order $(N - 1)$. Then the reducing polynomial $g(x)$ is solved so as to match these derivatives in the residual function $f_2(x)$ at the left and right boundaries ($x = 0$ and $x = 1$) as follows. Define

$$f_2(x) = f_1(x) - g(x) \tag{1}$$

where

$$\begin{aligned} g(x) &= a_1 x + a_2 x^2 + \cdots + f_1(0) \\ &= \sum_{k=0}^{N} a_k x^k \end{aligned} \tag{2}$$

and the $a_k$'s are chosen such that

$$f_2^{(n)}(1) - f_2^{(n)}(0) = 0, \qquad 0 \leqslant n \leqslant N - 1 \tag{3}$$

where superscript ($n$) denotes the $n$-th derivative. The solution for $N \leqslant 7$ is given in the Appendix. The general solution is written as follows.

$$a_N = \frac{1}{N!} D_{N-1} \tag{4a}$$

$$a_n = \frac{1}{n!} D_{n-1} - \frac{1}{n} \sum_{k=n+1}^{N} \binom{k}{n-1} a_k, \qquad 0 < n < N, \tag{4b}$$

$$a_0 = f_1(0) \tag{4c}$$

where

$$D_n = f_1^{(n)}(1) - f_1^{(n)}(0) \tag{4d}$$

and the binomial coefficient

$$\binom{k}{n} = \frac{k!}{(k-n)!\,n!} \tag{4e}$$

Note that the definition of $a_0$ is just an arbitrary prescription since the constant term could just as well have been absorbed into the periodic part.

It is perhaps worth emphasizing that this polynomial is *not* a fit of the function $f_1$, but only of the differences of the function $f_1$ and its $(N - 1)$ derivatives at the left and right boundaries, i.e., its departure from smooth periodicity. For example, if $f_1$ is already a periodic and infinitely differentiable function such as a sine wave, then $g = 0$ identically.

The value of the derivatives for $D_n$ at the boundaries must either be given or must be evaluated by one-sided finite difference methods (FDM). Even when FDM are used to evaluate derivatives at the boundaries, we have introduced no discretization error at this point. The decomposition is exact, even for arbitrary values of $a_1$, $a_2$, etc. since these only serve to define $g(x)$. But if these values are good, then $f_2(x)$ will appear to the discrete FFT to be continuous with continuous $(N - 1)$ order derivatives at the quasi-periodic boundaries. Even with $g(x) = 0$, the process is convergent (non-uniformly) but the discontinuities in $f_1(x)$ and its derivatives, when extended periodically, give rise to a "ringing" or Gibbs phenomena in the FFT representation which greatly slows the convergence (e.g. see [3, 10]). The only purpose of the polynomial evaluation is to reduce the "ringing" in the FFT representation of $f_2(x)$.

## 3. Initial Accuracy Tests on Static Functions

In the first phase of these accuracy tests, we tested this technique on several static test functions $f_1$, the most difficult of which was the damped sine wave

$$f_1(x) = e^{ax} \sin(2\pi b x) \tag{5}$$

with $a = -2$ and $b = 3/4$. This function is aperiodic and contains all Fourier components. We evaluated first and second derivatives and compared them to second, fourth, and sixth order FDM applied to both $f_2$ (after the reduction to periodicity) and to $f_1$, using consistently ordered non-centered FDM expressions at and near boundaries. Three methods were used to evaluate $D_n$ in the evaluation of $g$: (1) exact values, (2) FDM values obtained by a "limited second-order" subprogram, and (3) exact values for $D_0$ and $D_1$, and "limited second-order" values for $D_n$ when $n > 1$. The "limited second-order" subprogram was developed to allow second-order accuracy when the mesh spacing is fine enough to assure meaningful evaluation, while assuring a monotonic variation for coarse mesh spacing (like $\Delta x = 1/8$) as is the case with first-order methods. (Since only the difference between derivatives at the left and right boundaries is required, the FDM were rearranged to calculate this difference directly, rather than calculating derivatives at both boundaries and subtracting them. This improved round-off error on the approximately 9-digit PDP-10 computer.)

Significantly, the accuracy of this technique of reduction of periodicity was *not* limited to the accuracy of the second-order FDM used to evaluate the $D_n$, over the range of spatial increments tested up to $\Delta x = 1/128$. The purpose of this evaluation of $D_n$ and its use in defining $g$ is not to achieve high "order" but to eliminate the "ringing" in the FFT. The third method for $D_n$, in which $D_1$ is given exactly, is representative of the fluid dynamics problem in the conservation variable $f_1 = u\zeta$, $u$ = velocity and $\zeta$ = vorticity or some other advected property, where $f_1' = 0$ at a no-slip wall or a symmetry line.

In these first-phase tests, we varied $\Delta x = 1/2^p$ from 1/8 to 1/128 (or $p = 3$ to 7) and $N$, the degree of the reducing polynomial, from 1 to 5. In addition, we tested another method of periodically extending $f_1$ by using a mirror image extension as commonly used in the Fourier analysis of non-periodic experimental data. This consists of defining additional data from $x = 1$ to 2 by the equation $f_1(x) = -f_1(2 - x)$, and then applying the FFT from $x = 0$ to 2. However, this method was found to be inferior in all respects to the reducing-polynomial technique for $N > 1$, and not sufficiently accurate for our purposes.

Comparisons were based on three indexes of error: the maximum error over all node points $i$, the mid-range error, and the three-point average mid-range error. The larger error for the new technique occured near the boundaries, as might be expected. The last two indexes were always comparable in magnitude, and are more pertinent to our interest in high Reynolds number fluid dynamics problems.

The total tests for this initial phase of the work thus involved

- 4 methods of reduction to periodicity (3 methods for $D_n$, plus the mirror-image extension),
- 5 values for the degree $N$ of the reducing polynomial $g$,
- 3 orders of FDM (second, fourth, sixth) applied to
- 2 functions (quasi-periodic $f_2$ and aperiodic $f_1$),
- 5 values of $\Delta x$, from 1/8 to 1/128,
- 2 derivatives, $f_1'$ and $f_2''$, and
- 3 error indexes (maximum, mid-range, average mid-range).

Disregarding the tests for the mirror-image extension, all combinations of the above parameters were run. Fortunately, the resulting stacks of computer output can be summarized conveniently and accurately by a few observations about the importance of $N$, and then by comparisons with the high-order FDM.

The degree $N$ of the reducing polynomial $g$ is of critical importance. Subtraction of merely the linear trend ($N = 1$) was completely inadequate. At least $N = 3$ was required for reasonable accuracy of the first derivative $f_1'$, and $N = 4$ for the second derivative $f_1''$. Increasing $N$ from any odd degree $N$ to $N + 1$ did not improve the accuracy of $f_1'$ but did improve $f_1''$. Likewise, increasing from any even degree $N$ to $N + 1$ did not improve $f_1''$ but did improve $f_1'$. This observation applies to the absolute accuracy, not just to the accuracy relative to FDM (see Section 6 below).

When the required higher derivatives at the boundaries are known exactly, the results for $N = 5$ are indeed excellent, being always better than sixth-order FDM. However, this does not correspond to the situation in real fluid dynamics problems wherein the higher derivatives at the boundaries are not known. When evaluating these boundary derivatives by at best second-order FDM, it might appear that the entire representation would be limited to second-order accuracy. However, we found that even for fairly small $\Delta x$ (up to $\Delta x = 1/64$ and even $1/128$ in some cases) the accuracy of this technique with relatively crude FDM evaluation of the boundary derivatives was more accurate than fourth-order FDM.

The various accuracy rankings discussed above are summarized in Tables I–III.

The principal conclusions of this initial phase of the accuracy tests are as follows. Using exact values for all $D_n$, the technique of reduction to periodicity with a fifth-

TABLE I

Comparison of the Reduction-to-Periodicity Technique to Conventional Finite-Difference Methods[a]

| | |
|---|---|
| (a) Accuracy ranking for $f_1'$ | |
| $N = 2$ | $O(2) < \text{RTP} < O(4)$ |
| 3 | $O(4) < \text{RTP} < O(6)$ |
| 4 | $O(4) < \text{RTP} < O(6)$ |
| 5 | $O(6) < \text{RTP}$ |
| (b) Accuracy ranking for $f_1''$ | |
| $N = 2$ | $O(2) < \text{RTP} < O(4)$ |
| 3 | $O(2) < \text{RTP} < O(4)$ |
| 4 | $O(4) < \text{RTP} < O(6)$ |
| 5 | $O(4) < \text{RTP} < O(6)$ |

[a] The notation $O(2) < \text{RTP} < O(4)$ means that the reduction-to-periodicity technique had an accuracy between second-order and fourth-order FDM; the notation $O(6) < \text{RTP}$ means that the reduction-to-periodicity technique had an accuracy greater than sixth-order FDM. This table is based on the mid-range average error (over three points) for the test function $f_1$ given by Eq. (5). $N$ = degree of the reducing polynomial $g$ in Eq. (4). The mesh spacing was varied from $\Delta x = 1/8$ to $1/128$. Exact values of the boundary derivatives $D_1$, $D_2$, etc., were used to evaluate $g$.

TABLE II

Comparison of the Reduction-to-Periodicity Technique to Conventional Finite-Difference Methods[a]

| | |
|---|---|
| (a) Accuracy ranking for $f_1'$ | |
| $N = 2$ | $O(2) < \text{RTP} < O(4)$ |
| 3 | $O(4) < \text{RTP} < O(6)$ |
| 4 | $O(4) < \text{RTP} < O(6)$ |
| 5 | $O(4) < \text{RTP} < O(6)$ |
| (b) Accuracy ranking for $f_1''$ | |
| $N = 2$ | $O(2) < \text{RTP} < O(4)$ |
| 3 | $O(2) < \text{RTP} < O(4)$ |
| 4 | $O(2) < \text{RTP} < O(4)$ |
| 5 | $O(2) < \text{RTP} < O(4)$ |

[a] Same as Table I, except that the boundary derivatives $D_1$, $D_2$, etc., were evaluated by one-sided second-order FDM.

TABLE III

Comparison of Reduction-to-Periodicity Technique to Conventional Finite-Difference Methods[a]

| | |
|---|---|
| (a) Accuracy ranking for $f_1'$, exact values used for $D_n$ | |
| $N = 3$ | $O(4) < \text{RTP} < O(6)$ |
| 4 | $O(4) < \text{RTP} < O(6)$ |
| 5 | $O(6) < \text{RTP}$ |
| (b) Accuracy Ranking for $f_1'$, with $D_n$ evaluated by $O(\Delta x^2)$ FDM | |
| $N = 3$ | $O(2) < \text{RTP} < O(4)$ |
| 4 | $O(2) < \text{RTP} < O(4)$ |
| 5 | $O(2) < \text{RTP} < O(4)$ |

[a] Same as Tables I and II, except that the comparison is based on the maximum error over all $i$, which occurs at or near the boundaries.

degree reducing polynomial can give mid-range and boundary errors for $f_1'$ better than sixth-order FDM for $\Delta x = 1/8$ to $1/64$, and very comparable to sixth-order FDM for $\Delta x = 1/128$. Using the exact value for $D_1$ and a "limited second order" FDM evaluation of higher $D_n$, the technique can give mid-range and boundary errors between those of fourth and sixth-order FDM. This is the range of interest for high Reynolds number flow calculations (see following section). Results for $f_1''$ are not as good as the above results, especially near the boundaries, and are roughly two orders lower in accuracy; but this is also compatible with considerations at high Re.

## 4. Significance to High Reynolds Number Flows

The technique yields higher-order accuracy for $f_1'$ than for $f_1''$, which is the type of accuracy ranking desirable for high Reynolds number flows. Consider the one-dimensional model equation (in dimensionless variables),

$$\frac{\partial \zeta}{\partial \tau} = -u \operatorname{Re} \frac{\partial \zeta}{\partial x} + \frac{\partial^2 \zeta}{\partial x^2} \tag{6}$$

The first problem that arises for the Reynolds number $\operatorname{Re} \gg 1$ is that second-order FDM do not yield a "balanced" method. When second-order FDM are used for both first and second order spatial derivatives in Eq. (6), then the truncation error from the first-derivative advection term is $O(u \operatorname{Re} \Delta x^2)$, while the truncation error from the second-derivative diffusion term is $O(\Delta x^2)$. For Re sufficiently large, for $u = O(1)$, and for achievable $\Delta x$, the truncation error of $O(u \operatorname{Re} \Delta x^2)$ will be greater than the *entire* diffusion term, so that the actual contribution of the viscous diffusion term is lost in the truncation error of the advection term. Without prior knowledge of the spatial distribution of $\zeta$ (particularly, the relative sizes of $\partial^2\zeta/\partial x^2$ and $\partial\zeta/\partial x$, which are independent for transient and/or multidimensional problems) it is not possible to assess the real import of this lack of a "balanced method" on the accuracy of a particular fluid dynamics solution. However, one plausible criterion to use is that the method be balanced in truncation error, with the *size* (not *order*) of the truncation error from the advection term being approximately equal to that from the diffusion term when $u$, $\partial\zeta/\partial x$ and $\partial^2\zeta/\partial x^2$ are all assumed to be of $O(1)$.

To achieve this, one can use higher order methods for the advection term. Then for $\Delta x \simeq 1/100$, it may readily be verified that the use of an $O(\Delta x^p)$ method for the diffusion term and an $O(\Delta x^{p+2})$ method for the advection term indicates balance up to $\operatorname{Re} \simeq 10^4$ (see, e.g. [8, 9]). Practically, the Re may go even higher and still allow balance, since the velocity coefficients like $u$ in Eq. (6) will be less than 1 near the separation and reattachment points where the full Navier–Stokes equations are important.

However, the present technique does nothing for the other difficulties associated with high Re fluid dynamics, the oscillatory discretized solutions ("wiggles" [11, pp. 163–165]) and the Nyquist frequency limitation. The oscillations can be removed by using low-ordered methods for the advection term, which aggravates the "balance" problem and deteriorates accuracy, or by nonlinear filtering devices such as those in [12–14]. The Nyquist frequency limitation (e.g., see [9]) means that frequency components higher than the $2\Delta x$ wavelength cannot be resolved with the discrete information available and that these components may be necessary for a qualitatively correct representation. (For some problems, e.g. boundary-layer flows or flows which are nearly parabolic in one direction, the high frequency components *may not* be necessary. For further discussion, see [8, 9, 11].) This appears to be the fundamental difficulty of high Re laminar calculations, and is perhaps insurmountable for any general-purpose algorithm.

For the high Re (hyperbolic) limit, discontinuous solutions are possible. If the boundary conditions are periodic, these problems can still be treated by pseudo-spectral methods, but with some degradation of accuracy [10]. However, the case of of a step discontinuity (e.g., a shock wave) entering or leaving a boundary will not be well represented by the present technique since the higher derivatives used to evaluate the polynomial function $g$ do not exist. Also, like most methods, the present technique does not assure positivity when applied to inherently positive quantities like density.

## 5. Further Accuracy Tests on Static Functions

In the next phase of the work on static functions, the technique was improved by increasing the degree of the reducing polynomial from $N = 5$ to 7, and by increasing the order of accuracy of the FDM used to evaluate derivatives at the boundaries. Two versions of the subroutine used to evaluate these boundary derivatives have evolved. The first, called P7, uses 7-point one-sided FDM (e.g. see [20]) to evaluate the 6 derivatives needed for the seventh-degree reducing polynomial. This calculates the first derivative $D_1$ to sixth order, $D_2$ to fifth order,..., $D_6$ to first order. This distribution of accuracy is suggested by our previous experiments and by the theory of Lyness (see following Section 6). However, for functions which are not very smooth and/or for short word length computers (such as the 9-digit PDP-10 used in this second phase) it does no good, and in fact may deteriorate accuracy, to use sixth-order 7-point FDM for $D_1$. The second subroutine, called P75, uses 5-point FDM for $D_1$ (giving fourth-order accuracy) and for $D_2$, and 7-point FDM for the higher derivatives.

As expected, the use of these higher-order FDM for boundary derivatives increases the accuracy of the overall technique, but the results on static test functions indicate that the improvement is not as significant as hoped for, so that it does not appear possible to approach the accuracy obtained when the exact derivatives are known. The more important improvement is in the use of the seventh-degree polynomial. The accuracy was improved significantly, but not enough to change the ranking compared to fourth and sixth order FDM. For practical reasons, $N = 7$ appears to be the largest value useable (see Appendix).

## 6. Theoretical Justification

Lyness [15] has published a work on what he calls the "Lanczos representation" of a function, which is the same idea for a static function as used here except that the function $g$ is represented as a Bernoulli polynomial. Lyness shows theoretically and for general functions what we had found only experimentally for the particular functions tested—that the degree of the polynomial is very important to the accuracy, that the order of the FDM used at the boundaries is less important, that the use of a fifth-degree polynomial with second-order FDM at boundaries would give $f_1'$ to overall fourth-order accuracy, that the accuracy of the first derivative evaluation would improve as $N$ was increased from $N = 1$ by increments of 2, etc. Lyness' work also suggested that a decreasing order of FDM for the $D_n$ as $N$ increased would be appropriate, and that *some* improvement is to be expected by going to the next higher derivative (i.e., increasing $N$) so long as the error in the required higher derivative is less than $O(1)$. At our request, Lyness also extended his previous work to prove [16] another aspect which we had found experimentally, that second spatial derivatives are two orders less accurate than first spatial derivatives. Because of Lyness' work, the present technique has a firm theoretical basis for static test functions.

## 7. Other Similar Techniques

We have already mentioned (in the Introduction) Gazdag's technique of adding an artificial data regime, and its limitations. Also, we mentioned our tests on the "mirror image" data-doubling technique commonly used in the Fourier analysis of non-periodic experimental data; we found this technique to be entirely inadequate. Two other similar approaches should be noted.

Sköllermo [17] subtracted departures from periodicity to develop a high order FFT method for the Poisson equation. In this technique, the derivatives must be known a priori, rather than being evaluated by FDM. Also, knowledge of cross-derivative terms like $\partial^2 f_1/\partial x\, \partial y$ at boundaries are required, and accuracy is limited by corner singularities.

In an earlier paper, Orszag (see [3, p. 316]) considered the improvement from subtracting off the linear trend of data (i.e., $N = 1$ in our terms) from the one-dimensional constant-coefficient advection–diffusion equation. He also mentioned the possibility of subtracting terms to assure continuity of $f_1''$, provided these derivatives are known at the boundaries.

## 8. Accuracy and Stability Tests on Dynamic One-Dimensional Problems

In the initial phase of the one-dimensional tests of a dynamic (time-dependent) problem, we compared the accuracy of the present technique of reduction-to-periodicity with Gazdag's results [7] on Burgers equation, normalized (with $\tau = t/\text{Re}$) as

$$\frac{\partial u}{\partial \tau} = -\,\text{Re}\, u \frac{\partial u}{\partial x} + \frac{\partial^2 u}{\partial x^2} \tag{7}$$

and applied to the step initial condition problem of $u(0, \tau) = u_1$ with $u(x, 0) = 0$ for $x > 0$. This problem has an analytic solution [7] for the quasi-steady-state propagation in terms of the hyperbolic tangent:

$$u = \frac{u_1}{2}\,(1 - \tanh(u_1 \omega\, \text{Re}/4)) \tag{8}$$

where

$$\omega = x - u_1 \operatorname{Re} \tau/2. \tag{9}$$

(Although this solution satisfies (7) exactly, it does not apply to the early transients since it gives $u(0, 0) = u_1/2$ rather than $u_1$. For $\tau > 0$, it gives the correct left-hand boundary condition of $u(0, \tau) = u_1$ only in the limit of $\tau \cdot \operatorname{Re} \equiv t$ large, i.e., it applies only to the quasi-steady-state propagation.) We used both a fixed reference frame for easy comparison with Gazdag's results [7] and a moving reference frame, moving at the speed $u_1/2$ of the far-time solution, for comparison with the fourth-order results of Hirsh [18]. For this case, the Burgers equation is transformed to

$$\frac{\partial u}{\partial t} = -(u - u_1/2) \frac{\partial u}{\partial x} + \frac{1}{\operatorname{Re}} \frac{\partial^2 u}{\partial x^2}. \tag{10}$$

Time differencing was accomplished by the 3-time-level, $O(\Delta t^2)$ Adams–Bashforth method as suggested by Orszag (see [1, p. 253]) and was started with a 2-time-level, $O(\Delta t^2)$ iterative approximation to a Crank–Nicolson method (e.g., see [11]). In [7], a third-order Lax–Wendroff expansion was used for the time differencing. Started from a step initial condition, the "steady-state" pulse propagates at $u_1/2$. Two types of discretization error are manifested in the "steady-state" propagation; errors in the shape of the profile, and errors in the position of the profile. The latter error was removed in [7] by a shift in the time scale, so as to center the coordinate on the pulse. This eliminates the errors due to early transients, which are difficult to interpret for step initial conditions and the quasi-steady analytic solution. We followed the same procedure here. With our time differencing scheme, it happened that the magnitude of the time shift required was comparable to that of [7] but of opposite sign.

The spatial and temporal accuracies achieved using the present technique on this problem were equivalent to Gazdag's results, to the four significant figures published. (See [7, Table 2].) The present technique appears to be more generally applicable and requires an FFT operation on less data, compared to Gazdag's technique. (The time differencing method used in [7] was a third-order Lax–Wendroff expansion, which requires the evaluation of sixth-order spatial derivatives for viscous equations. That method is much more expensive than the present time differencing, but that method has already been superceded by Gazdag's later contribution in [19] of his "partially-corrected Adams–Bashforth" method.)

For comparisons with FDM solutions, we followed Hirsh [18] and set values beyond the computational mesh from the exact solution, thus avoiding the necessity of special one-sided FDM at and near the boundaries. This simplification is applicable only to the test problem, not to the multidimensional fluid dynamics problems of interest, but was felt to be justified since our interest in the high-order FDM is only secondary, for comparison purposes.

We again used $O(\Delta t^2)$ Adams–Bashforth time differencing, and compared our FFT results to FDM of order $\Delta x^2$, $\Delta x^4$ (including the standard $\Delta x^4$ method and the compact $\Delta x^4$ method as used by Hirsh) and $\Delta x^6$. We also considered *all* combinations of mixed methods, e.g., our FFT technique on first spatial derivatives with $O(\Delta x^4)$ FDM on the second spatial derivatives, etc.

The results were excellent, in that (1) the present FFT technique with reduction to periodicity is stable for the time dependent problem, and (2) the accuracy is comparable to *sixth-order* FDM methods and to Gazdag's method, even though we used only relatively crude second-order evaluation of $D_n$ near boundaries.

However, neither the present FFT technique nor any of the high order FDM tested solves another problem of high Re flows, that of the spatial oscillations which develop for cell Reynolds numbers $Rc > 2$, where $Rc$ is defined as $Rc = u \operatorname{Re} \Delta x$. (In the moving reference frame, this limit is changed to $Rc > 4$ just because of the Galilean transformation of the advection velocity in Eq. (10), but this has no significance to real fluid dynamics problems.) Such oscillations are also visible in Gazdag's solutions in [7].

It is especially clear in the moving reference frame, Eq. (10), that the problem of the oscillations at $Rc > 2$ is tied in with the Nyquist frequency limitation as previously discussed in Section 4, and can only be removed by filtering of some kind [12–14], thus effectively building-in a fine structure to the solution.

## 9. Operation Count Penalty

The reduction-to-periodicity technique adds to the operation count of the usual pseudospectral FFT method. For $M \equiv 1/\Delta x \gg 1$, the penalties due to the boundary evaluations of $D_n$ and the evaluations of the coefficients $a_n$ are negligible, and the major contribution comes from the evaluation of the reducing polynomial $g$ and its derivatives at each node point. For purposes of comparison, we use the usual asymptotic estimate for the operation count of the FFT over $M$ points, which is [27] $2M \ln M$ "complex operations," defined as a complex multiplication and a complex addition. Using data on the execution times and complex arithmetic operations from a CDC 6600 manual, we find that one "complex operation" is roughly equivalent to $4\frac{1}{2}$ "real operations," defined as a real multiplication and a real addition. For an FFT on real data (corresponding here to the forward FFT on $u$) the operation count can be somewhat reduced [28] by packing real data in complex numbers and operating on $M/2$ points instead of $M$ points, followed by some additional work proportional to $M$. We estimate a representative reduction by a ratio of 2/3 using this packing for the forward FFT on real data. (Using this gives a more conservative engineering estimate of the penalty; i.e., the penalty for our reduction-to-periodicity technique would be slightly better using the simpler FFT operation count.)

For a non-conservation form of an advection-diffusion equation like (7), the evaluation of the spatial derivatives requires the following calculations. The estimate of the real operation count is approximate, and valid for large $M$. The notation $\hat{u}$ denotes the discrete Fourier transform of $u$, and $K$ is the wave number; the calculations required to evaluate the derivatives are described in [7].

| Calculation | Real operation count |
|---|---|
| forward FFT on (real) $u$ to get $\hat{u}$ | $(4\frac{1}{2})(2/3)\,2M \ln M$ |
| divide (complex) $\hat{u}$ by $K$ (real) | $2M$ |
| backward FFT on (complex) $\hat{u}/K$ to get $\partial u/\partial x$ | $(4\frac{1}{2})\,2M \ln M$ |
| divide (complex) $\hat{u}$ by (real) $K^2$ (prestored) | $2M$ |
| backward FFT on (complex) $\hat{u}/K^2$ to get $\partial^2 u/\partial x^2$ | $(4\frac{1}{2})\,2M \ln M$ |
| multiply $\partial u/\partial x$ by Re and $u$, add terms | $2M$ |
| total | $24M \ln M + 6M$ |

The additional operations required by the reduction-to-periodicity technique involve the evaluation of the $N$-th degree polynomial $g$ at $M$ node points and the analytic evaluation of the derivatives of $g$. Note that the evaluation of powers of $x$ in (2) is very expensive but can be pre-stored in one-dimensional arrays.

| Calculation | Operation count |
|---|---|
| evaluate $g$ at each node point | $NM$ |
| evaluate $\partial g/\partial x$ at each node point | $(N-1)M$ |
| evaluate $\partial^2 g/\partial x^2$ at each node point | $(N-2)M$ |
| total | $3(N-1)M$ |

Combining these operation counts for the usual pseudospectral FFT methods and the reduction-to-periodicity technique, we obtain an estimate for the penalty in computer time. For the (worse) case of $N = 7$, we obtain

$$\text{penalty ratio} \simeq \frac{3}{4 \ln M + 1} \tag{11}$$

This gives a 10% penalty at $M = 1024$, 15% at $M = 128$, and 17% at $M = 64$. For a conservation-form equation, the penalty for $M \geqslant 64$ is increased at most 2%. (For $N = 5$, the penalty is reduced by a factor of 2/3.) The value of 15% is thus representative of the penalty for $N = 7$ and the useable range of mesh refinement. This representative penalty of 15% would also apply to the two-dimensional Navier–Stokes equations.

## 10. Stability and Iterative Convergence

We have been unable to prove anything theoretically about the stability of this technique of reduction-to-periodicity. (According to [6], the stability question for spectral methods even without this complication is difficult, and requires a new definition of stability.) However, we have experimentally demonstrated stability and iterative convergence to a steady-state solution for a variety of problems in one and two dimensions. The purpose of these tests is not to present detailed computational results, but only to report that stability and iterative convergence are indeed obtained with this rather complex method for a variety of partial differential equations, boundary conditions, initial conditions, and time-differencing methods.

In one space dimension, the partial differential equations considered were the wave (inviscid) equation, the heat equation with a source term (which converges to a one-dimensional Poisson equation in the steady state), the linearized Butgers equation or advection-diffusion equation, the non-conservation form of the nonlinear Burgers equation (7), and the conservation form of the nonlinear Burgers equation. Boundary conditions considered included the following: fixed left boundary (inflow) and fixed right boundary (stagnation), gradient and extrapolated right boundary (outflow), and sinusoidally varying left boundary (inflow). The initial conditions treated were both impulsive step functions (i.e., one-point pulse change in the right boundary condition) and conditions close to the steady-state solutions. The degree of the reducing polynomial was varied from 1 to 7, and the coefficients were evaluated using up to 7-point FDM [20] at the boundaries. The time differencing schemes used were $O(\Delta t)$ forward-time, $O(\Delta t^2)$ Adams–Bashforth, $O(\Delta t^2)$ "partially-corrected Adams–Bashforth" method due to Gazdag [19], and an $O(\Delta t^4)$ Runge–Kutta scheme.

The impulsive step-function initial condition caused severe errors in the initial transients. Some contribution to this error is apparently characteristic of pseudo-spectral methods and is due to the non-local nature of the spatial approximations, but the situation is aggravated in the present technique by the one-sided FDM evaluation of the boundary derivatives $D_n$.

The Adams–Bashforth method is known to be weakly unstable, which did cause weak oscillations near boundaries in the steady state. These were not very troublesome, but were removed by the use of Gazdag's "partially-corrected Adams–Bashforth" method [19] which is stable and appears in all ways to be preferable to the Adams–Bashforth method. Otherwise, all these time-differencing schemes were stable and iteratively converged to the steady-state solution, with only the usual $\Delta t$-restrictions for pseudo-spectral methods. These restrictions are Courant number $u\,\Delta t/\Delta x < 1/\pi$ (e.g., [5, p. 47]) and diffusion number $\Delta t/\mathrm{Re}\,\Delta x^2 < K/\pi$ [21] where $K \simeq 1$ or 2 for the range of parameters tested here.

The $O(\Delta t^4)$ Runge–Kutta time integration scheme was especially successful. A fourth-order Runge–Kutta time integration has been previously used by Oberkampf and Goh [22] within a semi-discrete "method-of-lines" formulation, and by Bratanow and Ecer [23] within a triangular finite element formulation. (Watanabe and Flood [24] have used an $O(\Delta t^4)$ fully implicit method in one-dimensional calculations which has the advantage of unconditional stability, but which requires nonlinear algebraic solutions by iteration within each time step.) Although the present scheme requires four FFT evaluations for derivatives at each time step compared to one FFT evaluation for the "partially-corrected Adams–Bashforth" method, its critical $\Delta t$ is more than four times as large. (According to Orszag [21], the stability gain for the wave equation is a factor of $2(2)^{1/2} \simeq 2.83$, but our present experience shows this is even greater for the viscous equation.) Oberkampf and Goh [22] also found enhanced stability for their fourth-order Runge–Kutta scheme in the method of lines, as did Bratanow and Ecer [23] in their finite element method. The particular Runge–Kutta scheme which we used (see, e.g., [25]) allows the intermediate calculations to be over-written, so that storage for this scheme requires only one additional storage compared to the $O(\Delta t^2)$ methods. It has proved to be stable with periodic-inflow and continuative-outflow boundary conditions, as well as fixed inflow and outflow conditions. We are now using this scheme of time integration and the reduction-to-periodicity technique for FFT calculations of two-dimensional transient aerodynamics problems.

## 11. Demonstration of Stability and Iterative Convergence on a Two Dimensional Problem

As a representative problem for two-dimensional separated flows, we solved the familiar driven cavity problem (e.g., see [15]). The solutions were restricted to a very coarse mesh ($8 \times 8$ cells) and a corresopndingly low Reynolds number, Re $= 5$. The $\psi$–$\zeta$ (stream function and vorticity) system of dependent variables was used with simple $O(\Delta t)$ forward time differencing. The no-slip wall boundary condition on $\zeta$ was evaluated using 5-point (fourth order) and 7-point (sixth order) one-sided FDM [20] for $\partial v_{\text{tangential}}/\partial n$ at the walls. The Poisson equation for $\psi$ was solved in a nested time-like iteration at each time step with a crude convergence criterion during the early transients, since only the steady-state iterative convergence was of interest. It proved to be necessary to under-relax boundary vorticity by a factor of $\frac{1}{2}$ in order to avoid a bounded mild oscillation in the steady-state results. Steady-state iterative convergence was then attained unequivocally, to the 9-digit accuracy of the computer used.

The technique of reduction-to-periodicity is also applicable to arbitrarily stretched coordinates, so long as the transformation applies to $x$ and $y$ independently, and to three space dimensions. The method used for the Poisson equation is not adequate for realistic problems; rather, a high order direct Poisson solver, of $O(\Delta x^4)$ [26] or $O(\Delta x^6)$ is needed to make the method practical. Also, we have yet to demonstrate that the technique works on the cross-derivative terms like $\partial^2 f_1/\partial x\, \partial y$ which are generated by non-orthogonal coordinate transformations.

## 12. Summary

A technique called "reduction to periodicity" has been developed for the use of pseudo-spectral FFT methods in non-periodic time-dependent problems in fluid dynamics. The technique involves the evaluation of a polynomial function which approximates the departure from smooth periodicity of the dependent variable distribution at each time level, with the FFT being applied only to the residual quasi-periodic distribution. The accuracy has been demonstrated in several one-dimensional problems, both on static functions and on dynamic time-dependent problems, linear and nonlinear. The work of Lyness [15] has provided a firm theoretical basis for the accuracy of the one-dimensional representation of static functions. For advection-diffusion equations in typical mesh spacings, the operation count penalty of the technique is roughly 15% compared to the usual pseudospectral FFT method. Stability and iterative convergence have been demonstrated in several one-dimensional problems with first, second, and fourth order time differencing schemes, and in a two-dimensional problem with first-order time differencing.

For practical problems, it is required that high-order derivatives at the boundaries be evaluated by one-sided finite difference methods; however, the accuracy of the overall technique is not limited to the accuracy of these finite difference methods. The technique addresses one of the difficulties associated with high Reynolds number flow calculations, that of obtaining a "balanced" method, and provides an alternative to higher-order finite difference or finite element methods. While quite accurate compared to conventional difference schemes, the technique does not retain the "infinite-order accuracy" of pseudospectral methods based on proper expansions.

## APPENDIX: Expansion of Eqs. (4) for a Seventh-Degree Polynomial

Equations (4) for the coefficients of the reducing polynomial are valid for any degree $N$. However, in practical physical problems, the $(N-1)$ order derivatives at boundaries are not known but must be evaluated by one-sided FDM [20]. As is well known, the evaluation of derivatives of high order by one-sided formulas is adversely affected by minute noise or even by computer rounding errors, due to the large coefficients in the FDM formula. We find that this technique is limited in practice to polynomials of degree $N = 7$. In this case, Eqs. (4) expand as follows.

Given non-periodic data $f_1(x)$, define

$$f_2(x) = f_1(x) - g(x), \tag{A1}$$

$$g(x) = a_1 x + a_2 x^2 + a_3 x^3 + \cdots + f_1(0). \tag{A2}$$

With primes indicating differentiation, let

$$\begin{aligned} D_0 &= f_1(1) - f_1(0) \\ D_1 &= f_1'(1) - f_1'(0) \\ D_2 &= f_1''(1) - f_1''(0), \quad \text{etc.} \end{aligned} \tag{A3}$$

Then, for $g$ a seventh-degree polynomial, we find

$$a_7 = \frac{1}{5040} D_6,$$

$$a_6 = \frac{1}{720} D_5 - \frac{7}{2} a_7,$$

$$a_5 = \frac{1}{120} D_4 - 3a_6 - 7a_7,$$

$$a_4 = \frac{1}{24} D_3 - \frac{5}{2} a_5 - 5a_6 - \frac{35}{4} a_7 ,$$

$$a_3 = \frac{1}{6} D_2 - 2a_4 - \frac{10}{3} a_5 - 5a_6 - 7a_7 ,$$

$$a_2 = \frac{1}{2} D_1 - \frac{3}{2} a_3 - 2a_4 - \frac{5}{2} a_5 - 3a_6 - \frac{7}{2} a_7 ,$$

$$a_1 = D_0 - a_2 - a_3 - a_4 - a_5 - a_6 - a_7 . \qquad \text{(A4)}$$

Polynomials of degree less than 7 are evaluated from these equations by setting higher coefficients equal to zero, e.g., the 5-th degree polynomial is found by setting $a_7 = a_6 = 0$.

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