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# A Pseudospectral Scheme for the Numerical Calculation of Shocks

P. CORNILLE

*Commissariat à l'Energie Atomique,*
*Centre d'Etudes de Limeil, 94190 Villeneuve Saint-Georges, France*

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A pseudospectral numerical scheme is developed in order to calculate the propagation of a shock wave. We use a two-step time-differencing method and a Chebyshev transform method to compute the space derivative. Such a scheme has been used to reduce the oscillations due to Gibb's phenomenon. This numerical method is applied to the solution of the Burgers equation without viscosity term. The accuracy of the numerical solutions is compared to the one given by two finite difference methods.

## 1. INTRODUCTION

Pseudospectral methods have been applied with some success to the solution of initial value problems in fluid dynamics and plasma physics. In a pseudospectral method, an expansion of the dependent variable into a discrete series of orthogonal functions is used to evaluate directly the spatial derivatives, the time differencing being calculated with a finite difference scheme. The accuracy of the space derivative of the dependent variable is of infinite order, provided that all derivatives of the variable are continuous. For variables having continuous derivatives only up to $m$th order, the coefficients in the series decrease as $k^{-(m+1)}$. For a shock wave, the coefficients of the series decrease as $k^{-1}$; therefore, the convergence of the space derivative series is poor: $O(1)$. Moreover, by retaining only the first $N$ terms in the series, oscillations appear in the solution due to Gibb's phenomenon, well studied in classical textbooks [1, p. 186]. For an iterative numerical scheme, these oscillations will grow rapidly as time goes on and destroy the solution to the problem.

The first thing one can do is introduce either explicit or implicit dissipative terms in the numerical scheme to improve the convergence of the space derivative to $O(k^{-1})$. The profile of the shock solution, however, still exhibits important oscillations, though they are reduced by the dissipation. One can instead apply smoothing and filtering techniques either to the function or to the derivative itself.

A few attempts have been made to solve this problem. In this paper, we shall review the different techniques used in the literature to reduce these undesirable oscillations.

The first numerical results were obtained by Gazdag [2] for the numerical solution of the Burgers equation with a viscosity term for an initial step function condition.



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He presented numerical results for different Reynolds numbers from 1 to 5. The computation was performed with 256 modes, and a Taylor expansion of order three was used to calculate the time derivative. The program is time-consuming, since it implies the computation of several space derivatives. Moreover, for Reynolds number 5, one can see the Gibb's oscillations in Gazdag's results. Gazdag [3] presented a new method called a *partially corrected second order Adams–Bashforth Scheme*, where the number of space derivatives to be calculated is reduced to three. Numerical results are shown for the numerical integration of the Vlasov equation. The second approach was presented by Roache [4]. It consists of decomposing the dependent variable $f(x)$ into a sum of a polynomial $g(x)$ and a residual periodic function $h(x)$ calculated with an FFT.

The values of the coefficients in the polynomial expansion $g(x)$ are evaluated with either the given derivatives of the function $f(x)$ at the boundaries or by one-sided finite difference methods. Although oscillations are reduced by the use of a polynomial expansion $g(x)$, they still remain important. Moreover, the case of a shock wave entering or leaving a boundary will not be represented correctly by this technique [4, p. 211].

The third method uses smoothing and filtering techniques. These techniques were first introduced by Majda *et al.* [5], who used them to smooth both the initial conditions and the solution of the problem at each time step. These methods were extended to hydrodynamics problems [6, 7], where both smoothing and filtering were applied every 100 time steps. These techniques are more or less problem-dependent and well suited for moderate shock waves. It is interesting to note several papers [8–10] related to Gibb's phenomenon and Fourier series approach to the Burgers equation.

In this paper we shall study a two-step pseudospectral scheme which drastically and automatically reduces the amplitude of Gibb's oscillations.

## 2. Study of the Truncation Terms

The derivative of a discontinuous function $F(x)$, when evaluated with a truncated Chebyshev polynomial expansion, exhibits two point oscillations of wavelength $\lambda_i = 2\Delta x_i$ over the whole mesh. Since the mesh is nonuniform, the spectrum of these oscillations is large. They can be completely eliminated by using the following filtering for a function $F(x)$: We have

$$F(x) = \sum_{m=0}^{M} c_m a_m T_m(x), \qquad \frac{\partial F}{\partial x} = \sum_{m=0}^{M} c_m b_m T_m(x),$$

with the recurrent relations:

$$b_M = b_{M-1} = 0 \qquad \text{and} \qquad b_{m-1} = b_{m+1} + 2(\sin(\pi m/M)/\sin(\pi/M))\, a_m$$
$$\text{for} \quad 1 \leqslant m \leqslant M-1.$$

It is not difficult, however, to show that the derivative is just the second-order finite difference of the derivative:

$$\frac{\partial F}{\partial x} = \frac{F_{i+1} - F_{i-1}}{x_{i+1} - x_{i-1}} + O(\Delta^2 x).$$

In this case, one cannot expect an accuracy higher than second order, and one loses the advantage of the high accuracy of the pseudospectral method.

Moreover, in a numerical scheme, this method does not prevent oscillations from growing as time goes on. It is well known that oscillations appear behind the shock when the fluid dynamic equations are solved numerically by second-order finite difference schemes. It has been recognized [11–14] that the presence or absence of oscillations behind the shock in finite difference methods must be attributed to the dissipative or nondissipative character of some truncation terms.

For example, the oscillations given by the Lax–Wendroff scheme are bounded while those of the Leapfrog scheme are not. These oscillations have been generally smoothed out by introducing an explicit dissipative term called pseudoviscosity.

Lerat and Peyret [5] explained that oscillations can be better cancelled by correcting the nondissipative truncation terms. This can be easily done in two-step finite difference schemes.

The profile of a shock wave calculated with a pseudospectral method exhibits oscillations throughout the mesh, not only behind the front as in finite difference methods. Moreover, the accuracy of the scheme will depend on both the time and space truncation terms. In the case of a shock wave, the space series truncation term is important due to the poor convergence of the series.

The similarity of the oscillations in both finite difference and pseudospectral schemes suggests a way to solve this problem by choosing a two-step pseudospectral scheme with implicit dissipation that will drastically reduce the oscillations without losing too much of the accuracy of the pseudospectral scheme.

## 3. Two-Step Pseudospectral Scheme

In order to solve the nonlinear equation

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0, \tag{1}$$

Lerat and Peyret [6, 7] have introduced a class of two-step finite difference schemes $\mathscr{L}_\beta^\alpha$ depending on two parameters $\alpha$ and $\beta$ given by the two equations

$$\begin{aligned} \tilde{U}_i^{n+\alpha} &= (1-\beta)\, U_i^n + \beta U_{i+1}^n - (\alpha\, \Delta t/\Delta x)(F_{i+1}^n - F_i^n), \\ U_i^{n+1} &= U_i^n - (\Delta t/2\alpha\, \Delta x)((\alpha-\beta)\, F_{i+1}^n + (2\beta - 1)\, F_i^n \\ &\quad + (1-\alpha-\beta)\, F_i^n + \tilde{F}_i^{n+\alpha} - \tilde{F}_{i-1}^{n+\alpha}), \end{aligned} \tag{2}$$

with

$$x_i = (i+\beta)\,\Delta x, \qquad t_n = (n+\alpha)\,\Delta t.$$

For some specific values of the parameters $\alpha$ and $\beta$, one can recover some well-known schemes:

(i) two-step Lax–Wendroff scheme, $\mathscr{L}^{1/2}_{1/2}$,

(ii) MacCormack schemes, $\mathscr{L}^{1}_{0}$ and $\mathscr{L}^{1}_{1}$,

(iii) Rubin and Burstein schemes, $\mathscr{L}^{1}_{1/2}$.

### 3.1. *Two-step Pseudospectral Scheme*

By analogy, we introduce a class of two-step pseudospectral schemes written in the form

$$\begin{aligned} \tilde{U}_i^{n+1} &= \frac{1+\alpha}{2}\,U_{i+1}^n + \frac{1-\alpha}{2}\,U_{i-1}^n - \left(\frac{\partial F}{\partial x}\right)_i^n \Delta t \\ U_i^{n+1} &= U_i^n - \left((1-\beta)\left(\frac{\partial F}{\partial x}\right)_i^n + (1+\beta)\left(\frac{\partial \tilde{F}}{\partial x}\right)_i^{n+1}\right)\frac{\Delta t}{2}, \end{aligned} \tag{3}$$

with $-1 \leqslant \alpha \leqslant 1$ and $-1 \leqslant \beta \leqslant 1$.

Such a scheme consists of a predictor time step, where the oscillations of this step are, by a noncentered differencing of the Lax term, out of phase with and of the same amplitude as the ones of the preceding time step, so that they cancel one another when added in the corrector time step.

### 3.2. *Chebyshev Polynomial Expansion*

We can use a Chebyshev polynomial expansion to evaluate the function $F$ and its derivative. In this case, we have to specify on the interval $(-1, 1)$ the $M+1$ values of the function $F_i(U(x_i, t))$ at the grid points $x_i = \cos(\pi i/M)$. With this choice, we have

$$F_i = \sum_{m=0}^{M} c_m a_m(t)\, T_m(x_i). \tag{4}$$

This expression can be calculated with an FFT by

$$F_i = \sum_{m=0}^{N} c_m a_m \cos\frac{2\pi m i}{N}, \tag{5}$$

with $N = 2M$ and $a_m = 0$ for $M+1 \leqslant m \leqslant N$ $c_m = 0.5$ for $m = 0$, $c_m = 1$ otherwise. The coefficients $a_m$ may be evaluated by the inverse transform of (5)

$$a_m = \frac{4}{N}\sum_{i=0}^{N} c_i F_i \cos\frac{2\pi m i}{N}, \tag{6}$$

with $F_i = 0$ for $M+1 \leqslant i \leqslant N$.

By Eq. (5) and properties of the Chebyshev polynomials, one can calculate an expansion for the derivative:

$$\frac{\partial F}{\partial x} = \sum_{m=0}^{M} c_m b_m T_m(x_n), \tag{7}$$

where the coefficients $b_m$ can be computed from the $a_m$ by using the recurrent relations

$$b_M = 0, \qquad b_{M-1} = Ma_M, \qquad b_{m-1} = b_{m+1} + 2ma_m$$
$$\text{for} \quad 1 \leqslant m \leqslant M-1. \tag{8}$$

### 3.3. *Unconditionally Stable Pseudospectral Scheme*

Gottlieb and Turkel [8] presented a scheme achieving unconditional stability and avoiding the severe condition $\Delta t \leqslant 8/M^2$ for pseudospectral methods using Chebyshev polynomials. The time step $\Delta t$ is in this case limited only by accuracy.

This approach can be illustrated by an example. To solve

$$\frac{\partial U}{\partial t} = a \frac{\partial U}{\partial x} \tag{9}$$

with a Leapfrog pseudospectral scheme, we write

$$U_i^{n+1} = U_i^{n-1} + 2\alpha \, \Delta t \sum_{m=0}^{M-1} E_m^n j m e^{jmi\Delta x} \tag{10}$$

with the stability condition $\Delta t \leqslant 1/|a|(M-1)$. Equation (10) can be rewritten in the form

$$U_i^{n+1} = U_i^{n-1} + 2a/\sigma \sum_{m=0}^{M-1} E_m^n j \sin(m\sigma \, \Delta t) \, e^{jmi\Delta x}. \tag{11}$$

Now the scheme is unconditionally stable provided that the condition $|a/\sigma| \leqslant 1$ is verified.

In this approach the recurrent relations (8) are modified as follows:

$$b_M = 0, \qquad b_{M-1} = \sin(M\sigma \, \Delta t)(a_M/\sigma),$$
$$b_{m-1} = b_{m+1} + 2 \sin(m\sigma \, \Delta t)(a_m/\sigma). \tag{12}$$

## 4. Accuracy, Stability, and Consistency

The question of accuracy, stability, and consistency is more difficult to study for a pseudospectral scheme than for a finite difference scheme [16]. Therefore, we shall now give a heuristic approach to this question. Consider the equation

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0. \tag{13}$$

A second order truncated Taylor series is given by

$$U^{n+1} = U^n + \frac{\partial U}{\partial t}(\Delta t) + \frac{\partial^2 U}{\partial t^2}\frac{\Delta^2 t}{2}. \tag{14}$$

A possible numerical approach of equation (13) is

$$U_i^{n+1} = U_i^n - \left(\frac{\partial F}{\partial x}\right)_i^n \Delta t. \tag{15}$$

Substitution of equation (14) in equation (15) gives the truncation term:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = -\frac{\partial^2 U}{\partial t^2}\frac{\Delta t}{2} + O(\Delta^2 t).$$

Gazdag [2] showed that this method is unstable. Let a positive shock wave propagate in the positive direction $x$; for $\beta = 0$ and $\alpha = -1$, the pseudospectral scheme becomes:

$$\begin{aligned} \tilde{U}_i^{n+1} &= U_{i-1}^n - \left(\frac{\partial F}{\partial x}\right)_i^n \Delta t, \\ U_i^{n+1} &= U_i^n - \left(\left(\frac{\partial F}{\partial x}\right)_i^n + \left(\frac{\partial \tilde{F}}{\partial x}\right)_i^{n+1}\right)\frac{\Delta t}{2}. \end{aligned} \tag{16}$$

This last equation can be written in the form:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = \frac{1}{2}\frac{\partial}{\partial x}(F(U) - F(\tilde{U})) - \frac{\partial^2 U}{\partial t^2}\frac{\Delta t}{2} + O(\Delta^2 t),$$

with

$$\frac{\partial^2 U}{\partial t^2} = U\frac{\partial^2 F}{\partial x^2} + \frac{\partial U}{\partial x}\frac{\partial F}{\partial x} > 0.$$

The first-order Taylor expansion of $U(x)$ in $x$ is

$$U_{i-1}^n = U_i^n - \left(\frac{\partial U}{\partial x}\right)_i^n \Delta x + O(\Delta^2 x).$$

Substitution of this equation in the first equation of (16) gives

$$\tilde{U}_i^{n+1} = U_i^n - \left(\frac{\partial U}{\partial x}\right)_i^n \Delta x - \left(\frac{\partial F}{\partial x}\right)_i^n \Delta t + O(\Delta^2 t) + O(\Delta^2 x).$$

Then we have:

$$\left(\frac{\partial \tilde{U}}{\partial x}\right)_i^{n+1} = \left(\frac{\partial U}{\partial x}\right)_i^n - \left(\frac{\partial^2 U}{\partial x^2}\right)_i^n \Delta x - \left(\frac{\partial^2 F}{\partial x^2}\right)_i^n \Delta t + O(\Delta^2 t) + O(\Delta^2 x).$$

Finally, we get the truncation term of the two-step pseudospectral scheme:

$$\begin{aligned}\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = &\left[U\frac{\partial^2 U}{\partial x^2} + \left(\frac{\partial U}{\partial x}\right)^2\right]\frac{\Delta x}{2} \\ &- \left[\frac{\partial F}{\partial x}\frac{\partial^2 U}{\partial x^2} + \frac{\partial U}{\partial x}\frac{\partial^2 F}{\partial x^2}\right]\Delta x\,\Delta t + O(\Delta^2 x) + O(\Delta^2 t) \qquad (17)\end{aligned}$$

We notice that the right-hand terms of this equation are all positive and that the negative term $-\partial^2 U/\partial t^2$ has been cancelled out. This implies stability. The numerical scheme is consistent if the truncation term goes to zero as $\Delta x$ and $\Delta t$ tend to zero, which is the case here. Moreover, one can see that the accuracy of the numerical scheme is at least $O(\Delta x\,\Delta t)$.

## 5. Computational Results

The pseudospectral scheme three has been tested on Burger's equation, without viscosity term, written in conservative form:

$$\frac{\partial U}{\partial t} + \frac{\partial}{\partial x}\left[\frac{1}{2}U^2\right] = 0. \qquad (18)$$

The numerical results obtained with this scheme are compared with those of the following two finite-difference schemes:

$$\begin{aligned}\tilde{U}_i^{n+(1/1+\beta)} &= \frac{1+\alpha}{2}U_{i+1}^n + \frac{1-\alpha}{2}U_{i-1}^n - \frac{F_{i+1}^n - F_{i-1}^n}{x_{i+1} - x_{i-1}}\frac{\Delta t}{1+\beta}, \\ U_i^{n+1} &= U_i^n - \left[(1-\beta)\frac{F_{i+1}^n - F_{i-1}^n}{x_{i+1} - x_{i-1}}\right. \\ &\quad \left. + (1+\beta)\frac{F_{i+1}^{n+(1/1+\beta)} - F_{i-1}^{n+(1/1+\beta)}}{x_{i+1} - x_{i-1}}\right]\frac{\Delta t}{1+\alpha+\beta}.\end{aligned} \qquad (19)$$

TABLE I

| Table | $M$ | $\Delta t$ | Position of the front at time $t=0$ | Position of the front at time $t=1$ |
|---|---|---|---|---|
| 2 | 32 | $10^{-2}$ | point 17 | point 11/12 |
| 3 | 32 | $10^{-2}$ | point 17 | point 11/12 |
| 4 | 32 | $10^{-2}$ | point 17 | point 11/12 |
| 5 | 32 | $2 \times 10^{-2}$ | point 17 | point 11/12 |
| 6 | 64 | $2.5 \times 10^{-3}$ | point 33 | point 22/23 |

TABLE II

Error Function of $U(x)$ at Time 1 for Initial Conditions 1

| $X$ | M.P.[a] | | L.W.[b] | | M.C.[c] | |
|---|---|---|---|---|---|---|
| 2 | −3 | (−3) | 0 | (−3) | 0 | (−3) |
| 3 | 3 | (−3) | 0 | (−3) | 0 | (−3) |
| 4 | −4 | (−3) | 0 | (−3) | 0 | (−3) |
| 5 | 5 | (−3) | 0 | (−3) | 0 | (−3) |
| 6 | −6 | (−3) | 0 | (−3) | 0 | (−3) |
| 7 | 9 | | 0 | (−3) | 0 | (−3) |
| 8 | −1 | (−2) | 0 | (−3) | 2 | (−3) |
| 9 | 3 | (−2) | 3 | | 4 | (−2) |
| 10 | 1 | (−1) | 2 | | 1.5 | (−1) |
| 11 | 5 | (−1) | 3 | (−1) | 5 | (−1) |
| 12 | −1.7 | (−1) | −7.8 | (−1) | −2.4 | (−1) |
| 13 | −3 | (−2) | 4.8 | (−1) | 2 | (−2) |
| 14 | −7 | (−3) | 4 | (−1) | −2 | (−2) |
| 15 | 1 | (−3) | 3 | (−1) | 5 | (−2) |
| 16 | −3 | (−3) | 3 | (−1) | −7 | (−2) |
| 17 | 0 | (−3) | −5 | (−1) | 5 | (−2) |
| 18 | −2 | (−3) | −5 | (−1) | −6 | (−2) |
| 19 | 0 | (−3) | 4 | (−2) | 5 | (−2) |
| 20 | −2 | (−3) | 4 | (−2) | −4 | (−2) |
| 21 | 0 | (−3) | 2 | (−1) | 2 | (−2) |
| 22 | −2 | (−3) | 2 | (−1) | −2 | (−2) |
| 23 | 0 | (−3) | −2.6 | (−1) | 7 | (−3) |
| 24 | −1 | (−3) | −2.6 | (−1) | −3 | (−3) |
| 25 | 0 | (−3) | 2 | (−1) | 1 | (−3) |
| 26 | −1 | (−3) | 2 | (−1) | −1 | (−3) |
| 27 | 0 | (−3) | −1.3 | (−1) | 3 | (−4) |
| 28 | −6 | (−4) | −1.4 | (−1) | −1 | (−3) |
| 29 | −1 | (−4) | 6 | (−2) | 1 | (−4) |
| 30 | −4 | (−4) | 8 | (−2) | −1 | (−4) |
| 31 | 0 | (−4) | 5 | (−2) | 0 | (−4) |
| 32 | 3 | (−4) | 5 | (−2) | 0 | (−4) |

[a] M.P.: pseudospectral scheme $\alpha = 1, \beta = 0$.
[b] L.W.: Lax–Wendroff scheme $\alpha = 0, \beta = 1$.
[c] M.C.: MacCormack scheme $\alpha = 1, \beta = 0$.

With Lax–Wendroff scheme

$$\alpha = 0 \quad \text{and} \quad \beta = 1;$$

with MacCormack scheme

$$\alpha = 1 \quad \text{and} \quad \beta = 0.$$

The space derivatives of these finite difference schemes are generally calculated over half-mesh increments $x_{i+1/2} - x_{i-1/2}$. The numerical results presented here, however, should be independent of such a choice.

TABLE III

Error Function of $U(x)$ at Time 1 for Initial Conditions 2

| $X$ | M.P.[a] | | L.W.[b] | | M.C.[c] | |
|---|---|---|---|---|---|---|
| 2 | −1 | (−4) | 0 | | 0 | |
| 3 | 1 | (−4) | 0 | | 0 | |
| 4 | −7 | (−5) | 0 | | 0 | |
| 5 | 2 | (−5) | 0 | | 0 | |
| 6 | 4 | (−5) | 0 | | 0 | |
| 7 | −1 | (−4) | 0 | | 8 | |
| 8 | 3 | (−3) | 0 | | 1.5 | (−2) |
| 9 | 6 | (−2) | 4 | (−3) | 9 | (−2) |
| 10 | 3 | (−1) | 5 | (−2) | 3 | (−1) |
| 11 | 7 | (−1) | 3 | (−1) | 6 | (−1) |
| 12 | −7 | (−2) | −1.7 | (−1) | −6 | (−2) |
| 13 | −1 | (−2) | 5 | (−1) | 2 | (−2) |
| 14 | −1 | (−3) | 6 | (−1) | 2 | (−2) |
| 15 | −3 | (−4) | 3 | (−1) | −8 | (−3) |
| 16 | 2 | (−4) | −1.8 | (−1) | −2 | (−3) |
| 17 | −2 | (−4) | −5 | (−1) | −1 | (−4) |
| 18 | 1 | (−4) | −2.7 | (−1) | −3 | (−3) |
| 19 | −1 | (−4) | 4 | (−2) | 7 | (−3) |
| 20 | 1 | (−4) | 2.5 | (−1) | −9 | (−3) |
| 21 | −1 | (−4) | 2 | (−1) | 7 | (−3) |
| 22 | 1 | (−4) | −1 | (−1) | 5 | (−3) |
| 23 | −1 | (−4) | −2.6 | (−1) | 2 | |
| 24 | 1 | (−4) | 0 | (−1) | −2 | |
| 25 | −1 | (−4) | 2 | (−1) | 6 | (−4) |
| 26 | 0 | (−4) | 3 | (−2) | −3 | (−4) |
| 27 | 0 | (−4) | −1.3 | (−1) | 1 | (−4) |
| 28 | 1 | (−4) | −3 | (−2) | −1 | (−4) |
| 29 | 1 | (−4) | 6 | (−2) | 0 | (−4) |
| 30 | 0 | (−4) | 2 | (−2) | −1 | (−4) |
| 31 | 0 | (−4) | −5 | (−2) | 0 | (−4) |
| 32 | 0 | (−4) | −2 | (−2) | 0 | (−4) |

[a] M.P.: pseudospectral scheme $\alpha = 1, \beta = 0$.
[b] L. W.: Lax–Wendroff scheme $\alpha = 0, \beta = 1$.
[c] M.C.: MacCormack scheme $\alpha = 1, \beta = 0$.

These schemes are used with two sets of initial conditions:

$$\begin{aligned} U(x,0) &= 1, \quad \text{for} \quad -1 \leqslant x \leqslant 0, \\ &= 0, \quad \text{for} \quad 0 \leqslant x \leqslant 1. \end{aligned} \tag{I}$$

$$\begin{aligned} U(x,0) &= 1, \quad \text{for} \quad -1 \leqslant x \leqslant 0, \\ &= 0.5, \quad \text{for} \quad x = 0.098, \\ &= 0, \quad \text{for} \quad 0.098 < x \leqslant 1, \end{aligned} \tag{II}$$

and with a boundary condition $U(-1, t) = 1$.

TABLE IV
Error Function of $U(x)$ at Time 1 for Initial Conditions 1

| $X$ | M.P. 1[a] | | M.P. 2[b] | | M.P. 3[c] | |
|---|---|---|---|---|---|---|
| 2 | −3 | (−3) | −1 | (−2) | −1 | (−2) |
| 3 | 3 | (−3) | 1 | (−2) | 1 | (−2) |
| 4 | −4 | (−3) | −1 | (−2) | −1 | (−2) |
| 5 | 5 | (−3) | 1.7 | (−2) | 1.7 | (−2) |
| 6 | −6 | (−3) | −1.8 | (−2) | −1.8 | (−2) |
| 7 | 9 | (−3) | 2 | (−2) | 2 | (−2) |
| 8 | −1 | (−2) | −3 | (−2) | −3 | (−2) |
| 9 | 3 | (−2) | 6 | (−2) | 5 | (−2) |
| 10 | 1 | (−1) | 1 | (−1) | 7 | (−2) |
| 11 | 5 | (−1) | 5 | (−1) | 5 | (−1) |
| 12 | −1.7 | (−1) | −2 | (−1) | −1.7 | (−1) |
| 13 | −3 | (−2) | −4 | (−2) | −6 | (−3) |
| 14 | −3 | (−3) | −1 | (−2) | 6 | (−3) |
| 15 | 1 | (−3) | −1 | (−3) | 2 | (−3) |
| 16 | −2 | (−3) | −2 | (−3) | −7 | (−4) |
| 17 | 0 | (−3) | 0 | (−3) | −6 | (−4) |
| 18 | −2 | (−3) | 2 | (−3) | −6 | (−4) |
| 19 | 0 | (−3) | 0 | (−3) | −5 | (−4) |
| 20 | −2 | (−3) | −9 | (−4) | −6 | (−4) |
| 21 | 0 | (−3) | −1 | (−4) | −4 | (−4) |
| 22 | −2 | (−3) | −7 | (−4) | −4 | (−4) |
| 23 | 1 | (−4) | −1 | (−4) | −3 | (−4) |
| 24 | −1 | (−3) | −5 | (−4) | −3 | (−4) |
| 25 | 1 | (−4) | −1 | (−4) | −2 | (−4) |
| 26 | −7 | (−4) | −4 | (−4) | −2 | (−4) |
| 27 | 0 | (−4) | −1 | (−4) | −2 | (−4) |
| 28 | −6 | (−4) | −4 | (−4) | −2 | (−4) |
| 29 | −1 | (−4) | −1 | (−4) | −2 | (−4) |
| 30 | −4 | (−4) | −3 | (−4) | −2 | (−4) |
| 31 | 0 | (−4) | 0 | (−4) | −1 | (−4) |
| 32 | −3 | (−4) | −3 | (−4) | −1 | (−4) |

[a] M.P. 1: pseudospectral scheme $\alpha = 1, \beta = 0$.
[b] M.P. 2: pseudospectral scheme $\alpha = 1, \beta = 0.1$.
[c] M.P. 3: pseudospectral scheme $\alpha = 0.86, \beta = 0.1$.

The initial position of the shock front is set in the middle of the mesh at $x = 0$. The shock wave propagates in the direction $x > 0$ (decreasing point number in the tables). All numerical results are presented at time 1.

All numerical computations were performed with the number of modes and time steps indicated in Table (I). The time steps chosen for these tests are higher than the maximum permissible time step $\Delta t \leqslant 8/M^2$ [9, p. 110], except in Table V, where the numerical scheme is unconditionally stable.

Tables II and III: A comparison of pseudospectral and finite difference schemes for two different sets of initial conditions.

TABLE V

Error Function of $U(x)$ at Time 1 for Initial Conditions 2

| $X$ | M.P. 1[a] | | M.P. 2[b] | | M.P. 3[c] | |
|---|---|---|---|---|---|---|
| 2 | −1 | (−4) | −2 | (−2) | −3 | (−4) |
| 3 | 1 | (−4) | 2 | (−2) | 3 | (−4) |
| 4 | −7 | (−5) | −3 | (−2) | −3 | (−4) |
| 5 | 2 | (−5) | 3 | (−2) | 3 | (−4) |
| 6 | 4 | (−5) | −3 | (−2) | −2 | (−4) |
| 7 | −1 | (−4) | 4 | (−2) | 1 | (−4) |
| 8 | 2 | (−3) | −4 | (−2) | 4 | (−3) |
| 9 | 6 | (−2) | 1 | (−1) | 7 | (−2) |
| 10 | 3 | (−1) | 3 | (−1) | 3 | (−2) |
| 11 | 7 | (−1) | 7 | (−1) | 7 | (−2) |
| 12 | −7 | (−2) | −9 | (−2) | −7 | (−2) |
| 13 | −2 | (−2) | −1 | (−2) | −2 | (−2) |
| 14 | −1 | (−3) | −2 | (−2) | −1 | (−2) |
| 15 | −3 | (−4) | 1 | (−2) | −1 | (−2) |
| 16 | 0 | (−4) | −1 | (−2) | 0 | (−2) |
| 17 | −2 | (−4) | 1 | (−2) | −1 | (−2) |
| 18 | 0 | (−4) | −1 | (−2) | 0 | (−2) |
| 19 | −2 | (−4) | 1 | (−2) | −1 | (−4) |
| 20 | 1 | (−4) | −1 | (−2) | 0 | (−4) |
| 21 | −8 | (−5) | 1 | (−2) | 0 | (−4) |
| 23 | −3 | (−5) | 2 | (−2) | 2 | (−4) |
| 24 | 1 | (−4) | −1 | (−2) | −1 | (−4) |
| 25 | −2 | (−5) | 2 | (−2) | 2 | (−4) |
| 26 | 0 | (−5) | −2 | (−2) | −3 | (−4) |
| 27 | 0 | (−5) | 2 | (−2) | 5 | (−4) |
| 28 | 0 | (−5) | −3 | (−2) | −9 | (−4) |
| 29 | 0 | (−5) | −1 | (−2) | 2 | (−4) |
| 30 | 0 | (−5) | 7 | (−2) | −3 | (−3) |
| 31 | 0 | (−5) | −2 | (−1) | −3 | (−4) |
| 32 | 1 | (−5) | 4 | (−2) | 5 | (−3) |

[a] M.P. 1: pseudospectral scheme without $\sigma$, $\alpha = 1$, $\beta = 0$.
[b] M.P. 2: pseudospectral scheme $\sigma = 1$, $\alpha = 1$, $\beta = 0$.
[c] M.P. 3: pseudospectral scheme $\sigma = 2$, $\alpha = 1$, $\beta = 0$.

Table IV: The influence of the parameters $\alpha$ and $\beta$ on the solution of the problem for an initial step function.

Table V: The results of the pseudospectral schemes in the case of conditional (without) or unconditional (with $\sigma = 1, 2$) stability.

Table VI: The results of the pseudospectral and MacCormack schemes computed with 64 modes.

We see in Table VI: the higher accuracy obtained with the pseudospectral scheme

TABLE VI

Error Functions of $U(x)$ at Time 1 for Initial Conditions 1

| $X$ | M.P.[a] | | M.C.[b] | | $X$ | M.P.[a] | | M.C.[b] | |
|---|---|---|---|---|---|---|---|---|---|
| 2 | 2 | (−4) | 0 | | 33 | 0 | (−3) | 4 | (−2) |
| 3 | −2 | (−4) | 0 | | 34 | −2 | (−3) | −5 | (−2) |
| 4 | 2 | (−4) | 0 | | 35 | 0 | (−3) | 4 | (−2) |
| 5 | −1 | (−4) | 0 | | 36 | −1 | (−3) | −4 | (−2) |
| 6 | 5 | (−5) | 0 | | 37 | 4 | (−4) | 3 | (−2) |
| 7 | 4 | (−5) | 0 | | 38 | −9 | (−4) | −3 | (−2) |
| 8 | −1 | (−4) | 0 | | 39 | 4 | (−4) | 1 | (−2) |
| 9 | 3 | (−4) | 0 | | 40 | −9 | (−4) | −1 | (−2) |
| 10 | −5 | (−4) | 0 | | 41 | 3 | (−4) | 7 | (−3) |
| 11 | 7 | (−4) | 0 | | 42 | −7 | (−4) | −4 | (−3) |
| 12 | −1 | (−3) | 0 | | 43 | 3 | (−4) | 2 | (−3) |
| 13 | 1 | (−3) | 0 | | 44 | −6 | (−4) | −1 | (−3) |
| 14 | −2 | (−3) | 0 | | 45 | 3 | (−4) | 5 | (−4) |
| 15 | 2 | (−3) | 0 | | 46 | −5 | (−4) | −3 | (−4) |
| 16 | −3 | (−3) | 0 | | 47 | 2 | (−4) | 1 | (−4) |
| 17 | 4 | (−3) | 1 | (−6) | 48 | −4 | (−4) | −4 | (−5) |
| 18 | −6 | (−3) | 1 | (−4) | 49 | 2 | (−4) | 0 | (−5) |
| 19 | 9 | (−3) | 5 | (−3) | 50 | −4 | (−4) | −1 | (−5) |
| 20 | 1 | (−2) | 5 | (−2) | 51 | 2 | (−4) | 0 | (−5) |
| 21 | 2 | (−1) | 2 | (−1) | 52 | −3 | (−4) | 0 | (−5) |
| 22 | 6 | (−1) | 5 | (−1) | 53 | 1 | (−4) | 0 | (−5) |
| 23 | −9 | (−2) | −1 | (−1) | 54 | −3 | (−4) | 0 | (−5) |
| 24 | −2 | (−2) | 2 | (−2) | 55 | 1 | (−4) | 0 | (−5) |
| 25 | 0 | (−3) | 4 | (−2) | 56 | −2 | (−4) | 0 | (−5) |
| 26 | −2 | (−3) | −2 | (−2) | 57 | 1 | (−4) | 0 | (−5) |
| 27 | 1 | (−3) | 1 | (−2) | 58 | −2 | (−4) | 0 | (−5) |
| 28 | −2 | (−3) | −3 | (−2) | 59 | 0 | (−4) | 0 | (−5) |
| 29 | 1 | (−3) | 3 | (−2) | 60 | −2 | (−4) | 0 | (−5) |
| 30 | −2 | (−3) | −4 | (−2) | 61 | 0 | (−4) | 0 | (−5) |
| 31 | 1 | (−3) | 4 | (−2) | 62 | −2 | (−4) | 0 | (−5) |
| 32 | −2 | (−3) | −5 | (−2) | 63 | 0 | (−4) | 0 | (−5) |

[a] M.P.: pseudospectral scheme $\alpha = 1, \beta = 0$.

[b] M.C.: MacCormack scheme $\alpha = 1, \beta = 0$.

between the points 19 and 48. Outside these points, we still have small residual Gibb's oscillations, the magnitude of which is about $10^{-4}$.

The higher accuracy obtained with the pseudospectral scheme is balanced by an increase of a factor of four in computer time. The difference between finite difference and pseudospectral computer times is due solely to the calculation of the space derivatives by the routine DERIV. The operation count could be easily reduced by a factor of four by operating on $M$ modes instead of 2 $M$ modes in the two calls of the FFT, and by writing the FFT in machine language. For the unconditionally stable scheme, the computing time is reduced to twice that of a finite difference method.

## 6. Conclusion

The results presented here show that pseudospectral methods can be applied to the calculation of a shock wave. The accuracy obtained is higher than that of a finite difference method for a given number of mesh points. This scheme with a simple routine DERIV requires more computer time than the one for a finite difference scheme.

For a given precision, however, this scheme should be faster than any finite difference scheme, especially if one used the unconditionally stable pseudospectral scheme.

This scheme can be extended to the case of $n$-dimensional problems with a more important gain in computer time.

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