LOCAL ERROR REDUCTION FOR FIRST ORDER IMPLICIT PSEUDO-SPECTRAL METHODS APPLIED TO LINEAR ADVECTION MODELS

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By using any second or higher order pseudo-spectral method applied to linear non dispersive wave equations, one can experience the appearance in the numerical solution of the celebrated Gibbs phenomenon, located at the discontinuity points. On the contrary, by working out the numerical solution through a first order spectral method such a drawback is avoided. In particular, for stability reasons, we chose to consider the implicit Euler method and experienced that, even through a Richardson's extrapolation of such a method, the numerical solution obtained is always affected by the same phenomenon. In this paper we propose a way to improve the accuracy of the implicit Euler first order pseudo-spectral method by reducing the coefficient of its truncation error leading term via a time one-step extrapolation-like technique.

1. Introduction

Spectral methods are considered to be a valid or at least equivalent alternative to other numerical approaches in working out the solution to a partial differential equation. A very broad and deep treatment of spectral methods is done in various monographies and other books like the ones by Gottlieb and Orszag [1], Vichnevetsky and Bowles [2], Canuto et al. [3], Fonberg [4], Gottlieb and Hestaven [5] beyond the plenty of references quoted therein. For instance, as long as problems in acoustics or optics are concerned, in the book [6, pag.7], LeVeque states that the primary computational difficulty arises from the fact that the domain of interest is many orders of magnitude larger than the wavelength of interest and as a consequence methods with higher order of accuracy are typically used, for example, fourth order finite difference methods or spectral methods.

Dealing with an analytic function, it is proved that, by means of a spectral decomposition, it is possible to achieve a uniform convergence, exponentially increasing with the number of harmonics taken. On the contrary, if we consider functions that are piecewise smooth, even the point-wise convergence is lost and it does arise the celebrated Gibbs phenomenon consisting in a few overshoots located at function discontinuities. As in many practical applications the solution has to be strictly included within a predefined interval, it is obvious that the appearance of the Gibbs phenomenon might make the numerical solution lacking of physical meaning.

Our attention in this paper is devoted to numerically solving the linear advection equation

$$\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v}\, u) = 0 \,, \tag{1}$$

where $u = u(\mathbf{x}, t)$ with $u \in \mathbb{R}$ and the space variables $\mathbf{x} \in \Omega \subset \mathbb{R}^3$, whereas the time variable is t. As long as the advection velocity field $\mathbf{v}$ is concerned, we assume that it is constant. Furthermore, we have a prescribed initial condition and consider only periodic boundary conditions, so that it is straightforward to apply the Fourier decomposition approach.

2. Derivation of pseudo-spectral methods.

By defining the differential spacial operators

$$D = \frac{\partial}{\partial x}, \qquad E = \frac{\partial}{\partial y}, \qquad F = \frac{\partial}{\partial z},$$

we can rewrite the equation (1) as follows

$$\frac{\partial u}{\partial t} + v_1 \mathrm{D}(u) + v_2 E(u) + v_3 F(u) = 0,$$

where v_1, v_2, v_3 are the three constant components of the velocity vector $\mathbf{v}$. The same equation can be rewritten in integral form on the time interval $[t, t + \Delta t]$, as

$$u(\mathbf{x}, t+\Delta t) = u(\mathbf{x}, t) - \int_t^{t+\Delta t} v_1 \mathrm{D}(u) dt - \int_t^{t+\Delta t} v_2 E(u) dt - \int_t^{t+\Delta t} v_3 F(u) dt.$$

In order to obtain a first order implicit scheme by applying a quadrature rule, we can use the end-point rectangle one, so as to get the in time implicit discrete numerical scheme

$$\begin{aligned} u(\mathbf{x}, t + \Delta t) - u(\mathbf{x}, t) = -\Delta t \, \{ & v_1 \mathrm{D}\left[u(\mathbf{x}, t + \Delta t)\right] \\ & + v_2 E\left[u(\mathbf{x}, t + \Delta t)\right] + v_3 F\left[u(\mathbf{x}, t + \Delta t)\right] \} \,. \end{aligned}$$

It is interesting to notice that the resulting integration method have the same discretization error of the quadrature rule considered, because no errors were introduced so far and that this approach is equivalent to integrate directly in time by means of the implicit Euler scheme.

By introducing the symbolic operator $\mathrm{R}(\Delta t)$, this scheme can be rewritten more compactly in the form

$$u(\mathbf{x}, t+\Delta t) = \mathrm{R}(\Delta t) u(\mathbf{x}, t) \ , \quad \mathrm{R}(\Delta t) = \frac{1}{\mathrm{I} + \Delta t(v_1 \mathrm{D} + v_2 E + v_3 F)} \ . \quad (2)$$

By indicating with $v(\xi, \eta, \zeta, t) = \texttt{fft}\{u(\mathbf{x}, t)\}$ the spacial FFT of the unknown function $u(\mathbf{x}, t)$, the equation (2) is rewritten in time-spectral domain like this

$$v(\xi, \eta, \zeta, t+\Delta t) = \hat{R}(\Delta t) v(\xi, \eta, \zeta, t) \ , \quad \hat{R}(\Delta t) = \frac{1}{I + i\Delta t(v_1 \xi + v_2 \eta + v_3 \zeta)}$$

where i is the imaginary unit.

More details on the pseudo-spectral algorithm can be found in [7].

3. Numerical approach

The first order discrete numerical scheme at a given time provides the vector $T(\Delta t)$, by indicating with $T(0)$ its value obtained as the discretization parameter Δt tends to zero, we can always write

$$T(0) = T(\Delta t) + \alpha_1 \Delta t + \alpha_2 \Delta t^2 + \alpha_3 \Delta t^3 + \dots + \alpha_m \Delta t^m + \dots ,$$

where it is assumed that the coefficients α_i are independent from Δt. If we refer to the same scheme, but for the reduced time steps $q^k \Delta t$, with $0 < q < 1$, and the exponent $k \geq 0$ and integer, then for each k we can also write

$$T(0) = T(q^k \Delta t) + q^k \alpha_1 \Delta t + q^{2k} \alpha_2 \Delta t^2 + q^{3k} \alpha_3 \Delta t^3 + \dots + q^{mk} \alpha_m \Delta t^m + \dots ,$$

By indicating with $T(k, 0)$ the discrete value $T(q^k \Delta t)$, we can introduce an extrapolation scheme

$$T(k+1, n+1) = T(k, n) + \frac{T(k, n) - T(k+1, n)}{q^w - 1} . \quad (3)$$

As long as the parameter w is equal to the accuracy order owned by the values $T(k, 0)$, such a scheme is just the one by Richardson and the value $T(k, n)$ would have actually an accuracy order increased by the integer n. Otherwise we get an extrapolation-like scheme. Let us now consider the implicit Euler method that is first order accurate, if we extrapolate properly, i.e. by using the value $w = 1$, then for any extrapolated order higher than one, the solution will go on showing the Gibbs phenomenon. On the contrary, by extrapolating once using the value $w = 2$, i.e. we are doing an extrapolation-like technique, we get discrete values that are still first order accurate, but the leading term of the truncation error becomes $q(q-1)\alpha_1\Delta t$, whereas the second one is canceled. If we want to involve the values $T(0,0)$ and a generic $T(k,0)$, then we must modify (3) by using $w = 2k$. In such a case it is easy to prove that for the resulting extrapolated value the leading term becomes $q^k(q^k-1)\alpha_1\Delta t$. As a consequence, being $0 < q < 1$, in any case we get a reduction of the local error. Finally, obtaining always a first order method, there is no point in going on extrapolating beyond the first extrapolation step.

4. Numerical tests

In this section we consider the advection equation in 2D

$$u_t + v_1 \mathrm{D}u + v_2 \mathrm{E}u = 0 \ , \qquad x \in [0, L], \quad y \in [0, L]$$

with the Heavyside function as initial condition jointly to periodic boundary conditions

$$u(x,y,0) = \begin{cases} 0, & \text{for} \quad 0 \le x, y \le L/2 \ , \\ 1, & \text{for} \quad L/2 < x, y \le L \ , \end{cases} \qquad \begin{array}{l} u(x,0,t) = u(x,L,t) \ , \\ u(0,y,t) = u(L,y,t) \ . \end{array}$$

For our numerical calculation we decided to fix a square domain with $L = 10$ and as constant vector field $\mathbf{v} = (1,1)$. As a consequence, at the final time $t_{\max} = 10$, the exact solution will reproduce the initial condition. We carried out two numerical experiments, for the above $2D$ case and the analogous $1D$ case, using $q = 1/2$ and $\Delta t = 0.025$. They consisted in calculating the solution by applying one step of the extrapolation-like technique involving $T(0,0)$ and $T(k,0)$ for $1 \le k \le 5$, so that the obtained solution, $T(k,1)$, can be compared with the one obtained simply by refining the mesh by the same step reduction factor used for each $T(k,0)$. Besides, the FFT was computed involving up to $N = 1024$ harmonics for the $1D$ case, whereas for the $2D$ case it involved $N = 128$ harmonics.

In both cases, there is an improvement in slope recovery at the discontinuities. This remark can be appreciated graphically by looking at Fig. 1, for the $1D$ case, and Fig. 2, for the $2D$ case. In order to prove numerically such a result, we can define err_{extra} as the difference between the initial condition and the final time solution obtained by one step of extrapolation-like technique, i.e. $err_{\text{extra}} = |T(0) - T(k,1)|$, whereas analogously err_{ref} is referred to the solution obtained by mesh refining, i.e.

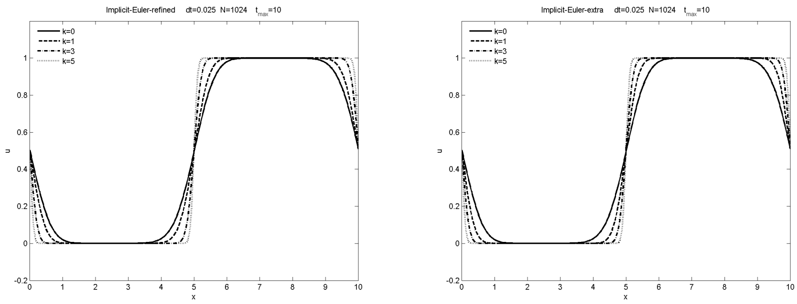

Fig. 1. $1D$ solutions for $k = 0, 1, 3, 5$: on the left, $T(k, 0)$ obtained for mesh refining, whereas on the right, $T(k, 1)$ obtained for extrapolation-like.

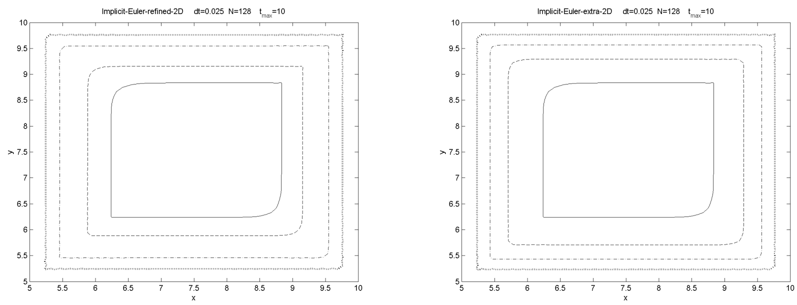

Fig. 2. $2D$ contour plot solution at $u = 0.99$ for $k = 0, 1, 3, 5$: on the left, $T(k, 0)$ obtained for mesh refining, whereas on the right, $T(k, 1)$ obtained for extrapolation-like.

$err_{\rm ref} = |T(0) - T(k, 0)|$. In Table 1, for $1D$ case, and in Table 2, for the $2D$ case, there are reported the $err_{\rm extra}$ and $err_{\rm ref}$ 2-norm values for increasing values of k and it can be seen that also numerically it is proved a real improvement.

It is clear that the higher is the value taken for k the less is the numerical profit in applying the present technique and, as a consequence the maximum profit is achieved by choosing $k = 1$.

5. Conclusions

This work was motivated by a preliminary study concerning the implicit Euler and the second order Adams-Moulton methods, in the ordinary differential context, for more details see Fazio [8]. We have found that, when dealing with discontinuous functions, the Gibbs phenomenon can be avoided

Table 1. $1D$ numerical comparison for increasing k.

k	$\|err_{\text{extra}}\|_2$	$\|err_{\text{ref}}\|_2$	$\|err_{\text{ref}}\|_2 - \|err_{\text{extra}}\|_2$
0	0.047818	0.047818	
1	0.036378	0.040208	0.003830
2	0.032009	0.033808	0.001799
3	0.027628	0.028425	0.000798
4	0.023558	0.023896	0.000338
5	0.019945	0.020083	0.000138

Note: $\Delta t = .025$, N=1024, $t_{\max} = 10$.

Table 2. $2D$ numerical comparison for increasing k.

k	$\|err_{\text{extra}}\|_2$	$\|err_{\text{ref}}\|_2$	$\|err_{\text{ref}}\|_2 - \|err_{\text{extra}}\|_2$
0	0.065722	0.065722	
1	0.048061	0.053928	0.05867
2	0.041443	0.044170	0.02727
3	0.034838	0.036046	0.01208
4	0.028638	0.029163	0.00525
5	0.022861	0.023092	0.00231

Note: $\Delta t = .025$, N=128, $t_{\max} = 10$.

by using a pseudo-spectral method of order one. As a final remark it is clear that the proposed extrapolation-like error reduction technique can be easily extended to $3D$ problems.

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