



Numerical simulations of time-dependent partial differential equations



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ABSTRACT

When a time-dependent partial differential equation (PDE) is discretized in space with a spectral approximation, the result is a coupled system of ordinary differential equations (ODEs) in time. This is the notion of the method of lines (MOL), and the resulting set of ODEs is stiff; the stiffness may be even exacerbated sometimes. The linear terms are the primarily responsible for the stiffness, with a rapid exponential decay of some modes (as in a dissipative PDE), or a rapid oscillation of some modes (as in a dispersive PDE). Therefore, for a time-dependent PDE which combines low-order nonlinear terms with higher-order linear terms, it is desirable to use a higher-order approximation both in space and in time.

Along our research, we have focused on a particular case of spectral methods, the so-called pseudo-spectral methods, to solve numerically time-dependent PDEs using different techniques: an integrating factor, in de la Hoz and Vadillo (2010); an exponential time differencing method, in de la Hoz and Vadillo (2008); and differentiation matrices in the theoretical frame of matrix differential equations, in de la Hoz and Vadillo (2012, 2013a,b). This paper, which is a unified review of those contributions, aims at providing a better understanding of those methods, by illustrating their variety and, more importantly, their power. Furthermore, we also give emphasis to choosing adequate schemes to advance in time.

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1. Introduction

Spectral methods have been shown to be remarkably successful when solving time-dependent partial differential equations (PDEs). The idea is to approximate a solution $u(x, t)$ by a finite sum $v(x, t) = \sum_{k=0}^N a_k(t)\phi_k(x)$, where the function class $\{\phi_k(x)\}$, $k = 0, 1, \dots, N$, is trigonometric for x -periodic problems or, otherwise, consists of orthogonal polynomials of Jacobi type, being Chebyshev polynomials the most important special case. In order to determine the expansion coefficients $a_k(t)$, we have focused on pseudo-spectral methods, where it is required that the coefficients make the residual equal to zero at as many (suitably chosen) spatial points as possible (see [1–5], together with the more classic Refs. [6,7]).

When a time-dependent PDE is discretized in space with a spectral (in particular, pseudo-spectral) approximation, the result is a coupled system of ordinary differential equations (ODEs) in time. This is the notion of the method of lines (MOL), and the resulting set of ODEs is stiff. The stiffness may be even exacerbated sometimes; for instance, when using Chebyshev polynomials (see [5, Chapter 10] and its references). The linear terms are the primarily responsible for the stiffness, with

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a rapid exponential decay of some modes (as in a dissipative PDE), or a rapid oscillation of some modes (as in a dispersive PDE). Therefore, for a time-dependent PDE which combines low-order nonlinear terms with higher-order linear terms, it is desirable to use a higher-order approximation both in space and in time.

This paper is a review of our recent work in the area of pseudo-spectral methods. By writing it, we aim at providing a better understanding of those methods, by illustrating their variety and, more importantly, their power. We also give emphasis to choosing adequate schemes to advance in time. The paper is organized as follows. In Section 2, we summarize the techniques used and the results obtained for the nonlinear Dirac equation [8]. Section 3 is devoted to the nonlinear Schrödinger equation [9]. In Section 4, we explain how to solve two-dimensional advection–diffusion equations by means of differentiation matrices [10]; and we mention briefly other applications of this important type of matrices to other relevant problems [11,12]. Finally, in Section 5, we draw the main conclusions.

Our numerical methods have been implemented in MATLAB®, and the experiments have been carried out in an Intel(R) Core(TM)2 Duo CPU E6850 @ 3.00 GHz. All the codes are available on request (see Appendix A).

2. The nonlinear Dirac equation

In [8], we have presented a new numerical method to simulate the evolution in time of the nonlinear Dirac equation, in one, two and three spatial dimensions. More precisely, this method uses an integrating factor (see for example [1] or [5]) to remove the linear term in the Fourier space; then, the resulting system of ODEs is integrated in time by means of a fourth-order Runge–Kutta scheme.

The nonlinear Dirac (NLD) equation, also known as the (1 + 3)-dimensional NLD equation, is

$$\Psi_t = A_1 \Psi_x + A_2 \Psi_y + A_3 \Psi_z + if(|\psi_1|^2 + |\psi_2|^2 - |\psi_3|^2 - |\psi_4|^2)B\Psi, \tag{1}$$

where $-\infty < x, y, z < +\infty; 0 \leq t \leq T; \Psi \in \mathbb{C}^4$; and A_j and B are 4×4 matrices, defined as

$$A_j = \begin{pmatrix} 0 & -\sigma_j \\ -\sigma_j & 0 \end{pmatrix}, \quad \text{for } j = 1, 2, 3, \quad B = \begin{pmatrix} -I_2 & 0 \\ 0 & I_2 \end{pmatrix}; \tag{2}$$

with σ_j being the Pauli matrices. Moreover, $f(s)$ is a real-valued function of a real variable s ; in particular, we consider the important case

$$f(s) = m - 2\lambda s, \quad m, \lambda \in \mathbb{R}, \tag{3}$$

where λ is a nonlinear parameter. If $0 < \lambda \ll 1$, we are dealing with a weak nonlinear problem.

Let us define a new variable

$$\widehat{\Phi} = M\widehat{\Psi}, \quad \text{where } M = \exp[-i(k_1 A_1 + k_2 A_2 + k_3 A_3)t] \begin{pmatrix} P & Q \\ Q & P \end{pmatrix},$$

where P and Q , which depend on the number of spatial variables, are given in [8]. In the Fourier space, the linear term does not appear, so we get the system of ODEs

$$\widehat{\Phi}_t = if(|(\mathcal{F}^{-1}(M^{-1}\widehat{\Phi}))_1|^2 - |(\mathcal{F}^{-1}(M^{-1}\widehat{\Phi}))_2|^2)MBM^{-1}\widehat{\Phi}, \tag{4}$$

which is solved by a fourth-order classic Runge–Kutta scheme.

The nonlinear Dirac equation in (1 + 1)-dimensions has two exact solutions, which are used as a test in our numerical experiments. The first one is a standing wave solution given in [8, Eq. (11)]. The second one represents a solitary wave traveling with speed v ; that solution is

$$\Psi^{ss}(x, t) = (\psi_1^{ss}(x, t), \psi_2^{ss}(x, t))^T, \tag{5}$$

where

$$\begin{aligned} \psi_1^{ss}(x, t) &= \sqrt{\frac{\gamma + 1}{2}} \psi_1^{sw}(\tilde{x}, \tilde{t}) + \text{sign}(v) \sqrt{\frac{\gamma - 1}{2}} \psi_2^{sw}(\tilde{x}, \tilde{t}), \\ \psi_2^{ss}(x, t) &= \sqrt{\frac{\gamma + 1}{2}} \psi_2^{sw}(\tilde{x}, \tilde{t}) + \text{sign}(v) \sqrt{\frac{\gamma - 1}{2}} \psi_1^{sw}(\tilde{x}, \tilde{t}), \end{aligned}$$

with $\gamma = 1/\sqrt{1 - v^2}$, $\tilde{x} = \gamma(x - vt)$, and $\tilde{t} = \gamma(t - vx)$. When $v > 0$, the wave travels from left to right and, when $v < 0$, from right to left. When $v = 0$, it does not move, and, hence, we have a standing wave.

On the other hand, Hong and Li in [13] proved three conservation laws, for the charge \mathcal{Q} , the linear momentum \mathcal{P} , and the energy \mathcal{E} . They are defined as follows:

$$\mathcal{Q}(\Psi)(t) = \int_{\mathbb{R}} (|\psi_1(x, t)|^2 + |\psi_2(x, t)|^2) dx,$$

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