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Exponential time differencing methods for nonlinear PDEs

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Abstract

Spectral methods offer very high spatial resolution for a wide range of nonlinear wave equations. Because of this, it should be desirable, for the best computational efficiency, to use also high-order methods in time, but without very strict restrictions on the step size, due to numerical instability.

In this communication, we consider the exponential time differencing fourth-order Runge-Kutta (ETDRK4) method. This scheme was derived by Cox and Matthews in [4] and modified by Kassam and Trefethen in [12]. We have studied its amplification factor and its stability region, which gives us an explanation of its good behavior for dissipative and dispersive problems. In [10], we have applied this method to the nonlinear cubic Schrödinger equation in one and two space-variables. Later, in [11], we have simulated the blow-up of semi-linear diffusion equations.

1. Introduction

The *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 $\phi_k(x), k = 0, 1, \ldots, N$, will be trigonometric for $x-$periodic problems and, otherwise, an orthogonal polynomial of Jacobi type, with Chebyshev polynomials being the most important special case. To determine the expansion coefficients $a_k(t)$, we will focus on the *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. Three books [6], [2] and [16] have been contributed to supplement the classic references [8] and [3].

When a time-dependent PDE is discretized in space with a spectral discretization, 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 problem may be even exacerbated sometimes, for example, when using Chebyshev polynomials (see Chapter 10 of [16] and its references). The linear terms are primarily responsible for the stiffness with rapid exponential decay of some modes (as with a dissipative PDE) or a rapid oscillation of some modes (as with 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 in space and time.

For the sake of space, we only show a numerical simulation for the blow-up of semilinear diffusion equations, referring to [10] for the nonlinear Schrödinger equation.

2. Exponential Time Differencing fourth-order Runge-Kutta Method

The numerical method considered in this communication is an *exponential time differencing* (ETD) scheme. These methods arose originally in the field of computational electrodynamics [15]. Later on, they have recently received attention in [1] and [14], but the most comprehensive treatment, and in particular the ETD with Runge-Kutta time stepping, is in the paper by Cox and Matthews [4].

The idea of the ETD methods is similar to the method of the *integrating factor* (see for example [2] or [16]): we multiply both sides of a differential equation by some integrating factor, then we make a change of variable that allows us to solve the linear part exactly and, finally, we use a numerical method of our choice to solve the transformed nonlinear part.

When a time-dependent PDE in the form

$$u_t = \mathcal{L}u + \mathcal{N}(u,t), \tag{1}$$

where $\mathcal{L}$ and $\mathcal{N}$ are the linear and nonlinear operators respectively, is discretized in space with a spectral method, the result is a coupled system of ordinary differential equations (ODEs):

$$u_t = \mathbf{L}u + \mathbf{N}(u,t). \tag{2}$$

Multiplying (2) by the term $e^{-\mathbf{L}t}$, known as the *integrating factor*, gives

$$e^{-\mathbf{L}t}u_t - e^{-\mathbf{L}t}\mathbf{L}u = e^{-\mathbf{L}t}\mathbf{N}(u,t). \tag{3}$$

Following [1], we integrate (3) over a single time step of length h, getting

$$u_{n+1} = e^{\mathbf{L}h}u_n + e^{\mathbf{L}h}\int_0^h e^{-\mathbf{L}\tau}\mathbf{N}(u(t_n+\tau), t_n+\tau)d\tau. \tag{4}$$

The various ETD methods come from how one approximates the integral in this expression. Cox and Matthews derived in [4] a set of ETD methods based on the Runge-Kutta time stepping, which they called ETDRK methods. In this communication we consider the

ETDRK4 fourth-order scheme, which has the following expression:

$$
\begin{aligned}
a_n &= e^{\mathbf{L}h/2}u_n + \mathbf{L}^{-1}(e^{\mathbf{L}h/2} - \mathbf{I})\mathbf{N}(u_n, t_n), \\
b_n &= e^{\mathbf{L}h/2}u_n + \mathbf{L}^{-1}(e^{\mathbf{L}h/2} - \mathbf{I})\mathbf{N}(a_n, t_n + h/2), \\
c_n &= e^{\mathbf{L}h/2}a_n + \mathbf{L}^{-1}(e^{\mathbf{L}h/2} - \mathbf{I})(2\mathbf{N}(b_n, t_n + h/2) - \mathbf{N}(u_n, t_n)), \\
u_{n+1} &= e^{\mathbf{L}h}u_n + h^{-2}\mathbf{L}^{-3}\{[-4\mathbf{I} - h\mathbf{L} + e^{\mathbf{L}h}(4\mathbf{I} - 3h\mathbf{L} + (h\mathbf{L})^2)]\mathbf{N}(u_n, t_n) \\
&+ 2[2\mathbf{I} + h\mathbf{L} + e^{\mathbf{L}h}(-2\mathbf{I} + h\mathbf{L})](\mathbf{N}(a_n, t_n + h/2) + \mathbf{N}(b_n, t_n + h/2)) \\
&+ [-4\mathbf{I} - 3h\mathbf{L} - (h\mathbf{L})^2 + e^{\mathbf{L}h}(4\mathbf{I} - h\mathbf{L})]\mathbf{N}(c_n, t_n + h)\}.
\end{aligned}
$$

More detailed derivations of the ETD schemes can be found in [4].

Unfortunately, in this form ETDRK4 suffers from numerical instability when $\mathbf{L}$ has eigenvalues close to zero, because disastrous cancellation errors arise. Kassam and Trefethen have studied in [12] those instabilities and have found that they can be removed by evaluating a certain integral on a contour that is separated from zero. The procedure is basically to change the evaluation of the coefficients, which is mathematically equivalent to the original ETDRK4 scheme of [4], although in [5] it has been shown to have the effect of improving the stability of integration in time. Moreover, it can be easily implemented and the impact on the total computing time is small. In fact, we have always incorporated this idea in our *MATLAB*© codes.

The stability analysis of the ETDRK4 method is as follows (see [1], [7] or [4]). For the nonlinear ODE

$$\frac{du}{dt} = cu + F(u), \tag{5}$$

being $F(u)$ the nonlinear part, we suppose that there exists a fixed point u_0; this means that $cu_0 + F(u_0) = 0$. Linearizing about this fixed point, if u is the perturbation of u_0 and $\lambda = F'(u_0)$, then

$$u_t = cu + \lambda u \tag{6}$$

and the fixed point u_0 is stable if $Re(c + \lambda) < 0$.

The application of the ETDRK4 method to (6) leads to a recurrence relation involving u_n and u_{n+1}. Introducing the previous notation $x = \lambda h$, $y = ch$ and using the *Mathematica*© algebra package, we obtain the following amplification factor:

$$\frac{u_{n+1}}{u_n} = r(x, y) = c_0 + c_1 x + c_2 x^2 + c_3 x^3 + c_4 x^4, \tag{7}$$

where

$$
\begin{aligned}
c_0 &= e^y, \\
c_1 &= \frac{-4}{y^3} + \frac{8\,e^{\frac{y}{2}}}{y^3} - \frac{8\,e^{\frac{3\,y}{2}}}{y^3} + \frac{4\,e^{2\,y}}{y^3} - \frac{1}{y^2} + \frac{4\,e^{\frac{y}{2}}}{y^2} - \frac{6\,e^{y}}{y^2} + \frac{4\,e^{\frac{3\,y}{2}}}{y^2} - \frac{e^{2\,y}}{y^2}, \\
c_2 &= \frac{-8}{y^4} + \frac{16\,e^{\frac{y}{2}}}{y^4} - \frac{16\,e^{\frac{3\,y}{2}}}{y^4} + \frac{8\,e^{2\,y}}{y^4} - \frac{5}{y^3} + \frac{12\,e^{\frac{y}{2}}}{y^3} - \frac{10\,e^{y}}{y^3} + \frac{4\,e^{\frac{3\,y}{2}}}{y^3} \\
&\quad - \frac{e^{2\,y}}{y^3} - \frac{1}{y^2} + \frac{4\,e^{\frac{y}{2}}}{y^2} - \frac{3\,e^{y}}{y^2},
\end{aligned}
$$

$$c_3 = \frac{4}{y^5} - \frac{16\,e^{\frac{y}{2}}}{y^5} + \frac{16\,e^{y}}{y^5} + \frac{8\,e^{\frac{3\,y}{2}}}{y^5} - \frac{20\,e^{2\,y}}{y^5} + \frac{8\,e^{\frac{5\,y}{2}}}{y^5} + \frac{2}{y^4} - \frac{10\,e^{\frac{y}{2}}}{y^4}$$
$$+ \frac{16\,e^{y}}{y^4} - \frac{12\,e^{\frac{3\,y}{2}}}{y^4} + \frac{6\,e^{2\,y}}{y^4} - \frac{2\,e^{\frac{5\,y}{2}}}{y^4} - \frac{2\,e^{\frac{y}{2}}}{y^3} + \frac{4\,e^{y}}{y^3} - \frac{2\,e^{\frac{3\,y}{2}}}{y^3},$$
$$c_4 = \frac{8}{y^6} - \frac{24\,e^{\frac{y}{2}}}{y^6} + \frac{16\,e^{y}}{y^6} + \frac{16\,e^{\frac{3\,y}{2}}}{y^6} - \frac{24\,e^{2\,y}}{y^6} + \frac{8\,e^{\frac{5\,y}{2}}}{y^6} + \frac{6}{y^5} - \frac{18\,e^{\frac{y}{2}}}{y^5}$$
$$+ \frac{20\,e^{y}}{y^5} - \frac{12\,e^{\frac{3\,y}{2}}}{y^5} + \frac{6\,e^{2\,y}}{y^5} - \frac{2\,e^{\frac{5\,y}{2}}}{y^5} + \frac{2}{y^4} - \frac{6\,e^{\frac{y}{2}}}{y^4} + \frac{6\,e^{y}}{y^4} - \frac{2\,e^{\frac{3\,y}{2}}}{y^4}.$$

It is important to remark that computing c_1,c_2, c_3 and c_4 by the above expressions suffers from numerical instability for y close to zero. Because of that, for small y, we will use instead their asymptotic expansions:

$$c_1 = 1 + y + \frac{1}{2}y^2 + \frac{1}{6}y^3 + \frac{13}{320}y^4 + \frac{7}{960}y^5 + \mathcal{O}(y^6),$$
$$c_2 = \frac{1}{2} + \frac{1}{2}y + \frac{1}{4}y^2 + \frac{247}{2880}y^3 + \frac{131}{5760}y^4 + \frac{479}{96768}y^5 + \mathcal{O}(y^6),$$
$$c_3 = \frac{1}{6} + \frac{1}{6}y + \frac{61}{720}y^2 + \frac{1}{36}y^3 + \frac{1441}{241920}y^4 + \frac{67}{120960}y^5 + \mathcal{O}(y^6),$$
$$c_4 = \frac{1}{24} + \frac{1}{32}y + \frac{7}{640}y^2 + \frac{19}{11520}y^3 - \frac{25}{64512}y^4 - \frac{311}{860160}y^5 + \mathcal{O}(y^6).$$

3. The semi-linear diffusion equations

Many mathematical models have the property to develop singularities in a finite time T: for instance, the formation of shocks in Burgers' equation without viscosity. Often, this singularity represents an abrupt change in the properties of the models, so it is extremely important for a chosen numerical method to reproduce that change accurately.

In this section, we consider the semi-linear parabolic equation

$$u_t = \Delta u + u^p, \quad p > 1, \quad x \in \mathbb{R}^N, t > 0, \tag{8}$$

with the initial condition

$$u(x,0) = u_0(x), \quad x \in \mathbb{R}^N, \tag{9}$$

where $u_0(x)$ is continuous, nonnegative and bounded.

The local (in time) existence of positive solutions of (8),(9) follows from standard results, but the solution may develop singularities in finite time. In [13], it is proved that there exists a critical exponent $p_c(N) = 1 + \frac{2}{N}$, such that for $1 < p < p_c(N)$, any nontrivial solution of (8),(9) blows up at a finite time T. However, if $p > p_c(N)$, there exist global solutions if the initial value is sufficiently small.

The one-dimensional semi-linear parabolic equation is

$$u_t = u_{xx} + u^p, \quad p > 1, \quad x \in \mathbb{R}, t > 0. \tag{10}$$

The critical exponent is $p_c = 3$ and for $1 < p < 3$ the only nonnegative global (in time) solution is $u = 0$. Another question is the asymptotic behavior of the solutions as the blow-up time is approached, for which we refer to [9].

Although problem (10) is not mathematically periodic, we consider that the solution is close to zero at the ends of the interval $[-L, L]$ for L sufficiently large, so it can be regarded as periodic in practice and we can use the Fourier transform. Hence, in the Fourier space we have

$$\widehat{u}_t = -\xi^2 \widehat{u} + \widehat{u^p}, \quad \forall \xi, \tag{11}$$

where ξ is the Fourier wave-number and the coefficients $c = -\epsilon\xi^2 < 0$ span over a wide range of values when all the Fourier modes are considered. For high values of $|\xi|$, the solutions are attracted to the slow manifold quickly because $c < 0$ and $|c| \ll 1$.

In figure 1 we display the boundary stability regions in the complex plane x, for $y = 0, -0.9, -5, -10, -18$, which are similar to figures 3.2, 3.3 and 3.4 of [5]. When the linear part is zero ($y = 0$), we recognized the stability region of the fourth-order Runge-Kutta methods and, as $y \to -\infty$, the region grows. Of course, these regions only give an indication of the stability of the ETDRK4 method.

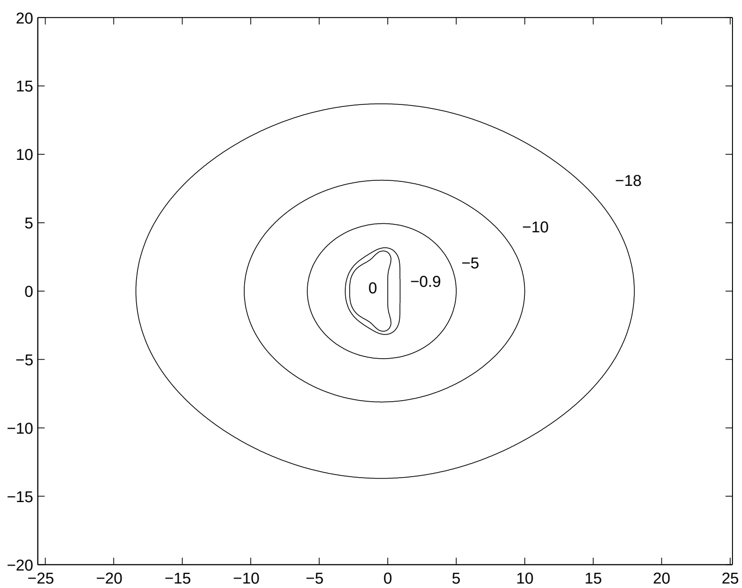

Figure 1: Boundary of stability regions for several negative y

In fact, for $y < 0$, $|y| \ll 1$, the observed boundaries approach to ellipses whose parameters have been fitted numerically with the following expression:

$$(Re(x))^2 + \left(\frac{Im(x)}{0.7}\right)^2 = y^2. \tag{12}$$

Then, the spectrum of the linear operator increases as ξ^2, while the eigenvalues of the linearization of the nonlinear part lay on the imaginary axis and increase as ξ. On the other hand, according to (12), when $Re(x) = 0$, the intersection with the imaginary axis $Im(x)$

increases as $|y|$, i.e., as ξ^2. Since the boundary of stability grows faster than x, the ETDRK4 method should have a very good behavior to solve dissipative equation, which confirms the results of paper [12]. A similar analysis is applicable to other dissipative equations like, for instance, the Kuramoto-Sivashinsky equation or the Allen-Cahn equation of [4] or [12], where $h = 1/4$.

In our first example, we consider $p = 2$ and the initial condition

$$u_0(x) = 6.05\exp(-20x^2), \tag{13}$$

which is symmetric with respect to the origin and has a single maximum at $x = 0$, hence satisfying the hypotheses of [9] under which the asymptotic behavior is known. On the left-hand side of figure 2 we have displayed the evolution of this initial condition from $t = 0$ to $t = 0.95$; a bit later, $u(0,1) \approx 6 \times 10^{10}$. The computer time was about 1.853 seconds.

On the other hand, on the right-hand side of figure 2, we have displayed the numerical solution at $t = 0.99$ with continuous line and the estimate from [9] with discontinuous line. The resemblances near the origin are evident.

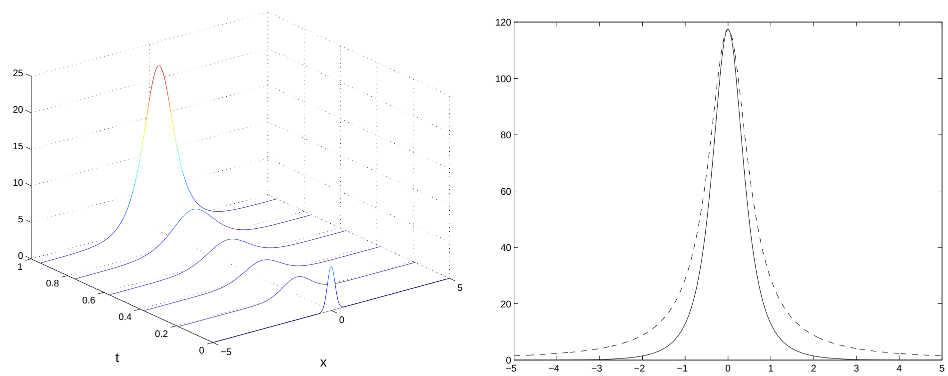

Figure 2: Numerical solution with $u_0(x) = 6.05\exp(-20x^2)$

In the following case, we look for an example where the solution blows up in two points. In figure 3, we represent the numerical solutions for $0 \le t \le 3.5$ with the initial condition

$$u_0(x) = 3\exp(-20(x+4)^2) + \exp(-20(x+1)^2) + 2.05\exp(-10(x-4)^2). \tag{14}$$

On the right-hand side, we have drawn the solution at $t = 3.5$ and the initial condition. In this case we do not know the asymptotic estimates, but in theorem 3 of [9], they have proved an asymptotic behavior close to the Hermite polynomials; in fact, the shape of the plot is similar to that of $-H_4(x)$ (see figure 17.3 of [2]), although we ignore the scale that should be applied.

Bearing in mind the good behavior of our simulation for the one-dimensional problem and the fact that *MATLAB*© also implements higher dimensional discrete Fourier transforms and their inverses (in two variables, we have `fft2` and `ifft2`), we thought that small modifications of our program would allow us to simulate the blow-up for the semi-lineal parabolic equation in two space variables:

$$u_t = u_{xx} + u_{yy} + u^p, \quad p > 1, \quad (x,y) \in \mathbb{R}^2, t > 0. \tag{15}$$

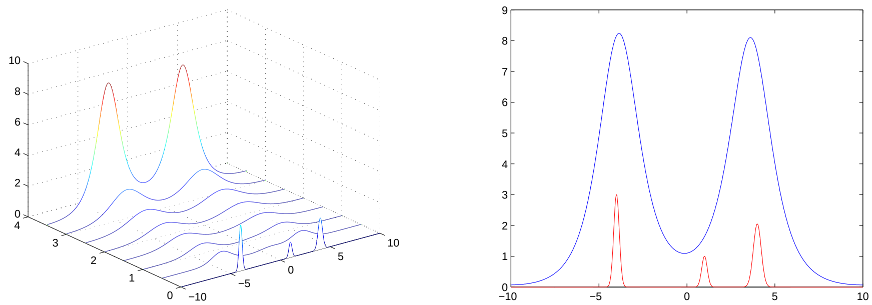

Figure 3: Numerical solution for initial condition (14)

In this case, the critical exponent is $p_c = 2$, so we have taken $p = 1.5$ for our numerical experiments.

For the sake of space, we only display one numerical example. In figure 4, we can observe the evolution of the initial condition

$$u_0(x, y) = 10\exp(-10((x+1)^2 + (y+1)^2) + 10\exp(-10((x-1)^2 + (y-1)^2), \qquad (16)$$

which is symmetric respect to the origin.

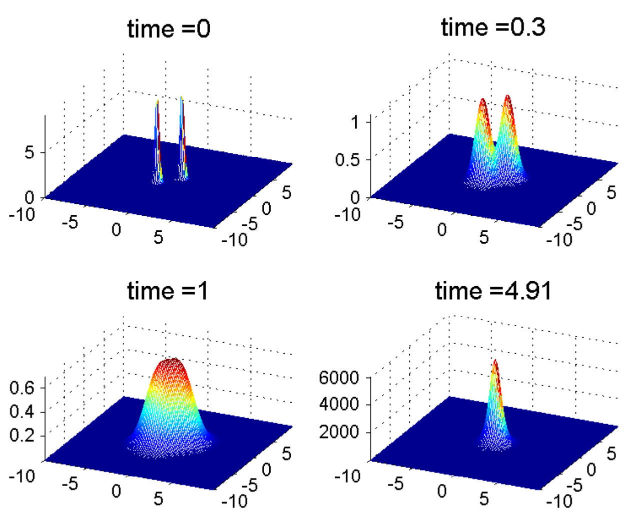

Figure 4: Numerical solution for initial condition (16)

In `http://www.ehu.es/~mepvaarf`, the reader can find the movies corresponding to the previous experiments, as well as the original *MATLAB*© code `etdrk42dchoise.m`, which offers the option to introduce other initial conditions.

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References

[1] G. Beylkin, J.M. Keiser, L. Vozovoi, *A New Class of Time Discretization Schemes for the Solution of Nonlinear PDEs*, J. Comput. Phys. (1998), 147, 362–387.

[2] J.P. Boyd, *Chebyshev and Fourier Spectral Methods. Second Edition (Revised)*, Dover, 2001.

[3] C. Canuto, M.Y. Hussain, A. Quarteroni, T.A. Zang, *Spectral Methods in Fluid Dynamics*, Springer, 1988.

[4] S.M. Cox, P.C. Matthews, *Exponential Time Differencing for Stiff Systems*, J. Comput. Phys. 176 (2002), pp. 430–455.

[5] Q. Du, W. Zhu, *Analysis and Applications of the Exponential Time Differencing Schemes and their Contour Integration Modifications*, BIT Numerical Mathematics (2005), 45, 307–328.

[6] B. Fornberg, *A Practical Guide to Pseudospectral Methods*, Cambridge University Press, 1998.

[7] B. Fornberg, T.A. Driscoll, *A fast spectral algorithm for nonlinear wave equations with linear dispersion*, J. Comput. Phys. (1999), 155, 456–467.

[8] D. Gottlieb, S.A. Orszag, *Numerical Analysis of Spectral Methods: Theory and Applications*, SIAM, 1977.

[9] M.A. Herrero, J.J.L. Velázquez, *Blow-up behavior of one-dimensional semilinear parabolic equations*, Ann. Inst. H. Poincaré (1993), 10, 131–189.

[10] F. de la Hoz, F. Vadillo, *An exponential time differencing method for the nonlinear Schrödinger equation*, Comput. Phys. Commun. 179 (2008), pp. 449–456.

[11] F. de la Hoz, F. Vadillo, *A numerical simulation for the blow-up of semi-linear diffusion equations*, Int. J. Comput. Math. 86 (2009), pp. 493–502.

[12] A. Kassam, L.N. Trefethen, *Fourth-Order Time Stepping for Stiff PDEs*, SIAM J. Sci. Comput. 26 (2005), pp. 1214–1233.

[13] H.A. Levine, *The role of critical exponents in blow-up theorems*, SIAM Review (1990), 32, 262–288.

[14] D.R. Mott, E.S. Oran, B. van Leer, *A Quasi-Steady-State Solver for the Stiff Ordinary Differential Equations of Reaction Kinetics*, J. Comput. Phys. (2000), no. 164, 407–428.

[15] A. Taflove, *Computational Electrodynamics: The Finite Difference Time-Domain Method*, Artech House, Boston, 1995.

[16] L.N. Trefethen, *Spectral Methods in MATLAB*, SIAM, 2000.