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A Composite Runge–Kutta Method for the Spectral Solution of Semilinear PDEs

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A new composite Runge–Kutta (RK) method is proposed for semilinear partial differential equations such as Korteweg–de Vries, nonlinear Schrödinger, Kadomtsev–Petviashvili (KP), Kuramoto–Sivashinsky (KS), Cahn–Hilliard, and others having high-order derivatives in the linear term. The method uses Fourier collocation and the classical fourth-order RK method, except for the stiff linear modes, which are treated with a linearly implicit RK method. The composite RK method is simple to implement, indifferent to the distinction between dispersive and dissipative problems, and as efficient on test problems for KS and KP as any other generally applicable method.

Key Words: Runge–Kutta methods; linearly stiff PDE; Fourier collocation; nonlinear waves; Kuramoto–Sivashinsky.

1. INTRODUCTION

Many important partial differential equations (PDEs) involving evolution in time are nonlinear but with a special semilinear structure,

$$\frac{\partial}{\partial t}u(x,t) = N(u) + Lu, \tag{1}$$

where only the linear operator L requires the highest spatial derivatives of u appearing in the equation. Here both x and u may be multidimensional. Examples of this type of PDE include Navier–Stokes, nonlinear Schrödinger (NLS), Korteweg–de Vries (KdV), Kadomtsev–Petviashvili (KP), Kuramoto–Sivashinsky (KS), Gray–Scott, and Cahn–Hilliard. Roughly speaking, these can be divided into equations whose linear part is dispersive (energy-preserving) and those whose linear part is dissipative (energy-losing, at least at some frequencies).

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In many practical cases one can ignore the influence of boundaries on (1) and therefore impose periodic boundary conditions. This choice suggests a discretization in Fourier space for the spatial variables:

$$\frac{d}{dt}\hat{u}(\xi, t) = \hat{N}(\hat{u}) + \hat{L}(\xi)\hat{u}, \quad \xi = \xi_1, \ldots, \xi_n. \tag{2}$$

The evaluation of $\hat{N}$ can be accomplished by transforming $\hat{u}$ to coordinate space, applying nonlinear operations, and transforming back to Fourier space. For instance, the term $2uu_x = (u^2)_x$ would be computed as

$$i\xi\mathcal{F}[(\mathcal{F}^{-1}\hat{u})^2].$$

This operation imposes a cost of two length-n FFTs each time $\hat{N}$ is to be evaluated.

We now consider the solution of (2) as a system of ordinary differential equations (ODEs) in the method of lines. The presence of high-order derivatives in L implies a high power of ξ in $\hat{L}$. At moderately large values of the wavenumber this term will dominate $\hat{N}$ and dictate a very small time step if an explicit ODE method is used. This *stiffness* worsens as the degree of highest derivative increases. For instance, KS (with a u_{xxxx} term) has a $k = O(n^{-4})$ restriction, which is prohibitive. A standard implicit (stiffly stable) method would be able to take much larger time steps, but each step would involve the expensive solution of a system of nonlinear equations.

A number of alternative time-stepping techniques take advantage of the fact that the stiff $\hat{L}$ term is linear (and, in fact, diagonal). Among these are the implicit–explicit or linearly implicit methods [4, 6, 12], split step methods [14], integrating factors method [11], and "exact linear part" (also known as "exponential") time stepping [5]. The approach taken in [7] is a compound method in which different integrators are used for different parts of Fourier space: a standard high-order, explicit, multistep method at the lowest wavenumbers, and stiffly stable, linearly implicit ones at higher wavenumbers where the explicit method fails. This approach is not difficult to implement and was shown to be the most effective of those named here for nonlinear wave equations such as NLS and KdV. It does suffer from a few drawbacks, though:

- As a multistep method, it needs starting values at the beginning of the integration and is unable to handle coefficients which are discontinuous in time.
- Dissipative equations have different stability characteristics and, for optimum performance, require different choices for the component methods than those used in [7].

In this paper we propose a composite method similar to that of [7] but based on Runge–Kutta (RK) integrators. This method uses the classical fourth-order integrator (RK4) at low wavenumbers and a third-order, linearly implicit RK method at stiff wavenumbers. As the time step decreases, more modes are treated with RK4, and in the limit standard RK4 is recovered. However, stable time stepping is possible at step sizes much larger than those for RK4, and in practice the method is fourth order over a wide range of step sizes. It is a minor programming change compared to RK4 and overcomes the objections noted here.

In Section 2 we introduce the necessary background on the construction of composite RK methods. In Section 3 we present our specific method for the Fourier collocation of linearly stiff PDEs. In Section 4 we show that the new method performs as well as that of [7] on both dissipative and dispersive problems. In addition no method of the types cited here outperforms it on tests with both types of problems.

2. COMPOSITE RK METHODS AND COMPATIBILITY CONDITIONS

We rewrite the system (2) in the briefer form

$$\dot{y}(t) = f(y(t)) + \lambda y(t). \tag{3}$$

Here y is a vector and λ is a diagonal matrix. Our first step is to partition (3) into

$$\dot{y}(t) = f(y(t), z(t)) + \lambda y(t), \tag{4a}$$

$$\dot{z}(t) = g(y(t), z(t)). \tag{4b}$$

The exact nature of the partitioning will be discussed in Section 3, but for now we simply describe y and z as "fast" (stiff) and "slow" modes. For slow modes the semilinear structure is irrelevant and therefore subsumed under g in (4b). Both y and z are vectors in practice, but we shall regard them as scalars without affecting any of the results.

Each mode is treated with a different RK method. Furthermore, the linear and nonlinear parts of (4a) are treated with different RK methods. The linear method is diagonally implicit, to allow for stiff stability. Thus we express the composite method for advancing from time step n to $n+1$ using step size k as

$$\left.\begin{aligned} Y_i &= y_n + k\sum_{j=1}^{i-1} a_{ij} f(Y_j, Z_j) + k\lambda \sum_{j=1}^{i} \tilde{a}_{ij} Y_j \\ Z_i &= z_n + k\sum_{j=1}^{i-1} \hat{a}_{ij} g(Y_j, Z_j) \end{aligned}\right\} \quad i = 1, \ldots, m,$$

$$y_{n+1} = y_n + k\sum_{i=1}^{m} b_i f(Y_i, Z_i) + k\lambda \sum_{i=1}^{m} \tilde{b}_i Y_i, \tag{5}$$

$$z_{n+1} = z_n + k\sum_{i=1}^{m} \hat{b}_i g(Y_i, Z_i).$$

This is an m-stage RK method. It can be abbreviated in tableau form as

$$\begin{array}{c|cccc|c|cccc} 0 & 0 & & & & 0 & 0 & & & \\ c_2 & a_{21} & 0 & & & \tilde{c}_2 & \tilde{a}_{21} & \tilde{a}_{22} & & \\ \vdots & \vdots & & \ddots & & \vdots & \vdots & & \ddots & \\ c_m & a_{m1} & a_{m2} & \cdots & 0 & \tilde{c}_m & \tilde{a}_{m1} & \tilde{a}_{m_2} & \cdots & \tilde{a}_{mm} \\ \hline & b_1 & b_2 & b_3 & b_4 & & \tilde{b}_1 & \tilde{b}_2 & \tilde{b}_3 & \tilde{b}_4 \end{array} \tag{6a}$$

$$\begin{array}{c|cccc} 0 & 0 & & & \\ \hat{c}_2 & \hat{a}_{21} & 0 & & \\ & \vdots & & \ddots & \\ \hat{c}_m & \hat{a}_{m1} & \hat{a}_{m2} & \ldots & 0 \\ \hline & \hat{b}_1 & \hat{b}_2 & \hat{b}_3 & \hat{b}_4 \end{array} \tag{6b}$$

We will use the usual definition of the "stage level,"

$$c_i = \sum_j a_{ij}, \tag{7}$$

with similar definitions for the tilde and hat coefficients. We now simplify the following discussion by noting that since both $[a_{ij}]$ and $[\hat{a}_{ij}]$ are used for nonstiff, nonlinear terms, we might as well let them be the same method. That is,

$$\hat{a}_{ij} = a_{ij}, \quad \hat{b}_i = b_i, \quad i, j = 1, \ldots, m. \tag{8}$$

As a necessary condition for accuracy of order p, each individual method represented by $[a_{ij}]$ and $[\tilde{a}_{ij}]$ must be an RK method of order at least p. This requirement imposes certain conditions on the individual sets of coefficients. In addition, however, the coefficients of the separate methods are coupled together through certain compatibility requirements. The theory of deriving these requirements is covered extensively in [2, 8, 9]. Because of the assumption (8), the conditions for partitioning compatibility are a superset of those for splitting compatibility (in which more than one derivative of the linear term vanishes). These conditions are similar in form to those for the individual methods. The conditions up to order three are

$$\begin{aligned}
&\sum_{i,j} \tilde{b}_i a_{ij} = \sum_{i,j} b_i \tilde{a}_{ij} = 1, \\
&\sum_i \tilde{b}_i \tilde{c}_i c_i = \sum_i \tilde{b}_i c_i^2 = \sum_i b_i \tilde{c}_i^2 = \sum_i b_i \tilde{c}_i c_i = \frac{1}{3}, \\
&\sum_{i,j} \tilde{b}_i \tilde{a}_{ij} c_j = \sum_{i,j} \tilde{b}_i a_{ij} \tilde{c}_j = \sum_{i,j} \tilde{b}_i a_{ij} c_j = \sum_{i,j} b_i \tilde{a}_{ij} \tilde{c}_j = \sum_{i,j} b_i \tilde{a}_{ij} c_j = \sum_{i,j} b_i a_{ij} \tilde{c}_j = \frac{1}{6}.
\end{aligned} \tag{9}$$

Now we make two final simplifying assumptions:

$$\left.\begin{aligned} \tilde{c}_i &= c_i, \\ \tilde{b}_i &= b_i \end{aligned}\right\} \quad i = 1, \ldots, m. \tag{10}$$

These assumptions are not strictly necessary, and relaxing them might conceivably lead to methods with better stability characteristics (as was the case in [3], for example), but we have not pursued this generalization. With (10) we find that each sum in (9) can be expressed solely in terms of tilde or plain coefficients. Thus to construct an order $p \le 3$ composite method like (5), all we need to find are individual pth-order methods that satisfy (10)—that is, they share the same internal stage levels and final linear combination.

3. A METHOD FOR THE LINEARLY STIFF PDE

We now propose a specific method for the system (2) arising from the Fourier collocation of (1). For the nonstiff, nonlinear integrator represented by $[a_{ij}]$ and $[\hat{a}_{ij}]$ in (6), we choose the standard four-stage RK4 method. Owing to the assumptions in (10), this leaves us to

choose coefficients in the RK method,

$$\begin{array}{c|cccc} 0 & 0 & & & \\ \frac{1}{2} & \tilde{a}_{21} & \tilde{a}_{22} & & \\ \frac{1}{2} & \tilde{a}_{31} & \tilde{a}_{32} & \tilde{a}_{33} & \\ 1 & \tilde{a}_{41} & \tilde{a}_{42} & \tilde{a}_{43} & \tilde{a}_{44} \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array} \tag{11}$$

Because this method is to be applied to stiff terms, it should be stiffly stable. We shall use the usual concept of L-stability; i.e., the numerical solution vanishes in the limit $|\lambda| \to \infty$ in (3). However, it is not possible to achieve both L-stability and fourth-order accuracy in (11) (essentially because we have already forced $\tilde{c}_1 = 0$). Instead we settle for third-order accuracy; as we will see shortly, this choice will have little impact. We choose the third-order, L-stable method given by

$$\begin{array}{c|cccc} 0 & 0 & & & \\ \frac{1}{2} & \frac{1}{6} & \frac{1}{3} & & \\ \frac{1}{2} & \frac{1}{2} & -1 & 1 & \\ 1 & 0 & 0 & \frac{2}{3} & \frac{1}{3} \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array} \tag{12}$$

This method has simple coefficients, two zeros in the final stage, and only two unique terms on the diagonal. A numerical study indicates that the error constant of this method is close (within a factor less than 2, depending on the norm) to the best achievable. We now rewrite the method (5) with the chosen coefficients and in an explicit form:

$$\begin{aligned} Y_1 &= y_n, \\ Z_1 &= z_n, \\ Y_2 &= \left(1 - \frac{1}{3}k\lambda\right)^{-1}\left(y_n + \frac{1}{2}kf(Y_1, Z_1) + \frac{1}{6}k\lambda Y_1\right), \\ Z_2 &= z_n + \frac{1}{2}kg(Y_1, Z_1), \\ Y_3 &= (1 - k\lambda)^{-1}\left(y_n + \frac{1}{2}kf(Y_2, Z_2) + \frac{1}{2}k\lambda Y_1 - k\lambda Y_2\right), \\ Z_3 &= z_n + \frac{1}{2}kg(Y_2, Z_2), \\ Y_4 &= \left(1 - \frac{1}{3}k\lambda\right)^{-1}\left(y_n + kf(Y_3, Z_3) + \frac{2}{3}k\lambda Y_3\right), \\ Z_4 &= z_n + kg(Y_3, Z_3), \\ y_{n+1} &= y_n + \frac{1}{6}k[f(Y_1, Z_1) + f(Y_4, Z_4) + \lambda(Y_1 + Y_4)] \\ &\quad + \frac{1}{3}k[f(Y_2, Z_2) + f(Y_3, Z_3) + \lambda(Y_2 + Y_3)], \\ z_{n+1} &= z_n + \frac{1}{6}k[g(Y_1, Z_1) + g(Y_4, Z_4)] + \frac{1}{3}k[g(Y_2, Z_2) + g(Y_3, Z_3)]. \end{aligned} \tag{13}$$

All that remains is to specify how the partitioning of modes is to be chosen. As was done in [7], we base the choice on the desired step size. The slow modes represented by z are all those whose linear term fits into the stability region of the slow integrator, RK4. In the notation of (2), in practice we define a slow wavenumber as one satisfying

$$|\hat{L}(\xi)| < \frac{2.8}{k}. \tag{14}$$

This condition is appropriate whether L is dissipative or dispersive. As $k \to 0$, the range of slow modes grows and, for a fixed spatial discretization, the method reduces to standard RK4. The composite method, however, allows us to get fairly accurate results using step sizes well above the stability limit of RK4.

Our method of partitioning takes advantage of the fact that if the solution $u(x, t)$ to the PDE is smooth (more precisely, well resolved), then most of its energy will be at slow wavenumbers and the mere third-order accuracy of (12) will not be very harmful.

4. NUMERICAL RESULTS

We compare the new partitioned RK method (13) for two model equations: the dissipative KS equation,

$$u_t + uu_x + u_{xx} + u_{xxxx} = 0, \tag{15}$$

and the dispersive KP-II equation,

$$(u_t + (3u^2)_x + u_{xxx})_x + 3u_{yy} = 0. \tag{16}$$

In KS we use a Gaussian initial condition (effectively periodic in double precision) and solve for $-16 \le x < 16$, $0 \le t \le 40$, with 256 Fourier modes (see Fig. 1). In KP-II we use a two-phase soliton initial condition in which features travel in an oblique direction, over

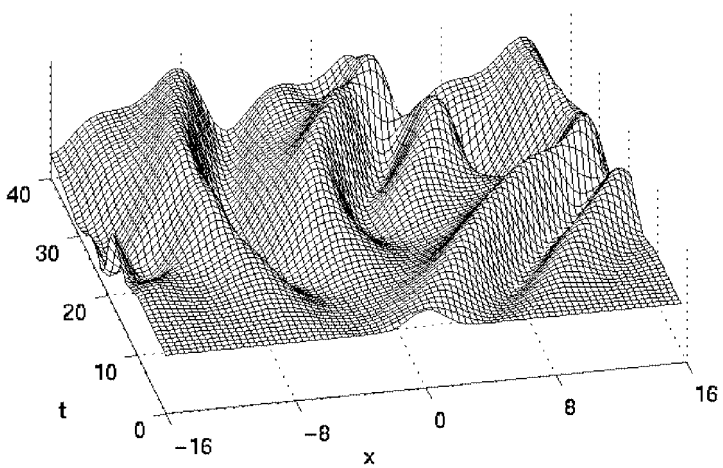

FIG. 1. Solution of KS equation (15) used for method comparisons.

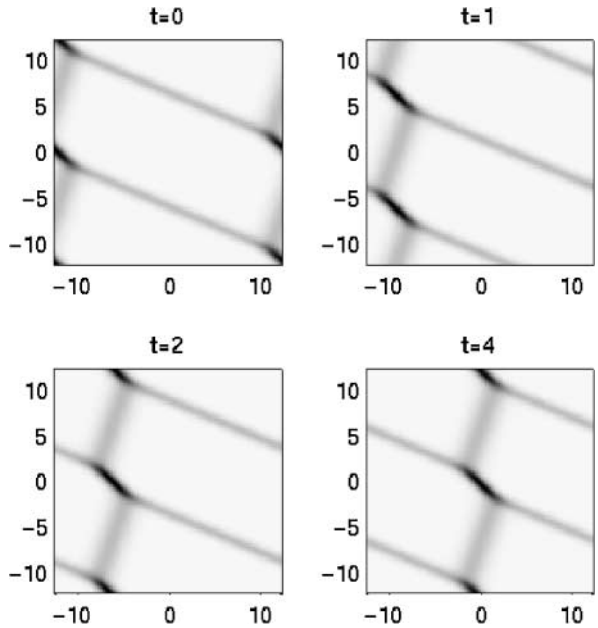

FIG. 2. Soliton solution of KP-II equation (16) used for method comparisons.

a 96×96 grid (see Fig. 2). In both cases we define relative error as the discrete 2-norm of the final error divided by the 2-norm of the initial condition. (The KP final solution is known explicitly; the KS final solution is found by agreement among several time-stepping methods using very small step sizes).

Other methods included for comparison are described next.

IFRK4. Equation (3) is transformed into a new variable using an integrating factor:

$$\frac{dz}{dt} = \frac{d}{dt}(e^{-\lambda t} y) = e^{-\lambda t} f(y(t)) = e^{-\lambda t} f(e^{\lambda t} z(t)). \tag{17}$$

The standard RK4 method is then applied to z. Although there are now time-dependent coefficients, in fact the method depends only on $k\lambda$ and not $t\lambda$. It requires eight FFTs per time step.

CMS42. CMS42 is the combination of linearly implicit multistep methods of orders 4 (slow-to-medium modes) and 2 (fast modes) from [7]. Starting values are found using IFRK4. (For the dissipative KS problem, the method does not need nor use an intermediate 4th/6th order method as described in [7].) It requires two FFTs per time step after starting values are found.

LIRK4. LIRK4 is the five-stage, fourth-order, linearly implicit RK method of [6]. This requires 10 FFTs per time step.

ELP4. ELP4 is the fourth-order "exact linear part" scheme of [5]. After transforming to (17), one solves for z by integrating a polynomial that interpolates past values of $f(y(t))$ (and not $e^{-\lambda t} f(y(t))$ as in a standard multistep method). Starting values are obtained using IFRK4. It then requires two FFTs per time step.

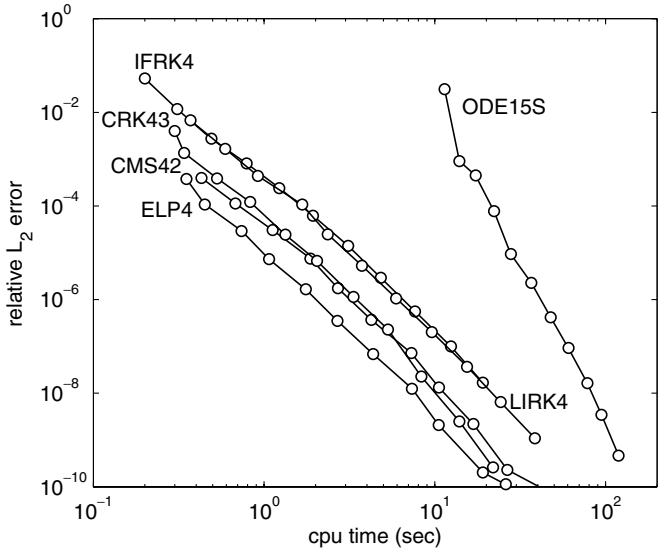

FIG. 3. Comparison of time integration methods for the KS equation.

ODE15S. ODE15S is a built-in variable-order stiff integrator for MATLAB[2] based on numerical differentiation formulas. This method was deemed impractical for KP-II due to the need to solve systems with 96^2 variables. Work requirements vary depending on the order of integrator chosen.

Split-step methods were not considered; as was pointed out in [7] for KdV, the nonlinear subproblem is typically difficult enough to make these methods uncompetitive.

The proposed composite RK method (13) is designated CRK43. All methods were implemented in MATLAB and timed using the built-in function cputime. Reasonable efforts were made to write efficient code in each case.

The results for KS and KP-II are shown in Figs. 3 and 4, respectively. In Fig. 5 we also show the power spectrum of the final solution for KS, along with the location of the "fastest slow mode" where the transition from RK4 to the linearly implicit method is made in accordance with (14).

A number of observations can be made:

- The leveling of the curves in the KP-II graph is due to the effect of the fixed spatial resolution. The theoretical point of maximum efficiency for a method is where the convergence curve first meets that floor.
- All the fourth-order methods, including CRK43, converge at essentially the same rate. This supports the claim that the third-order component of CRK43 has little negative effect. Indeed, as can be seen in Fig. 5, this is true even when quite a lot of energy is in slow modes.
- The ELP4 method is the most efficient of those here for KS but is unstable for KP-II. In fact, standard linear stability analysis suggests instability for all nondissipative problems.
- Of methods that were successful on both problems, CRK43 is as efficient as any other method at all accuracy levels, and it gave quite usable results (say, around 1% accuracy) with the least computational effort.

[2] MATLAB is a registered trademark of The MathWorks, Inc.

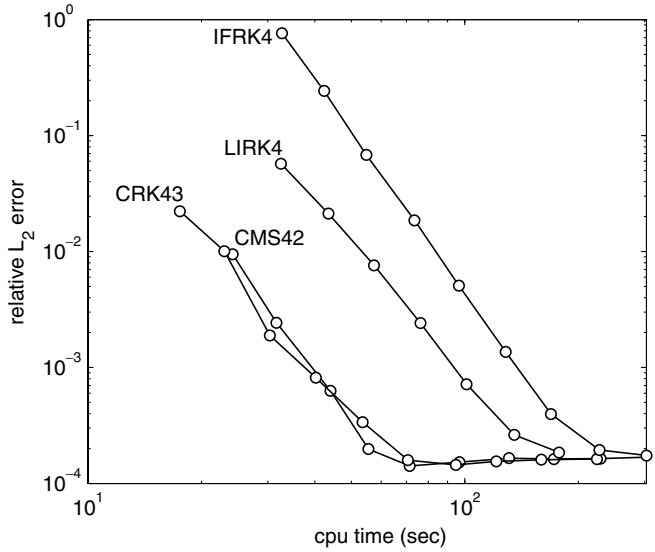

FIG. 4. Comparison of time integration methods for the KP-II equation.

As a demonstration of the ability to handle coefficients that are discontinuous in time, we consider a cubic Schrödinger equation that arises in optical communications [1]:

$$u_t = \frac{i}{2} D(t) u_{xx} + |u|^2 u, \quad -15 \le x \le 15, \quad 0 \le t \le 10. \tag{18}$$

Here $D(t)$ alternates between so-called normal and anomalous dispersion. We have chosen D to be a square wave alternating between values 161 and -159 over a period of 0.2.

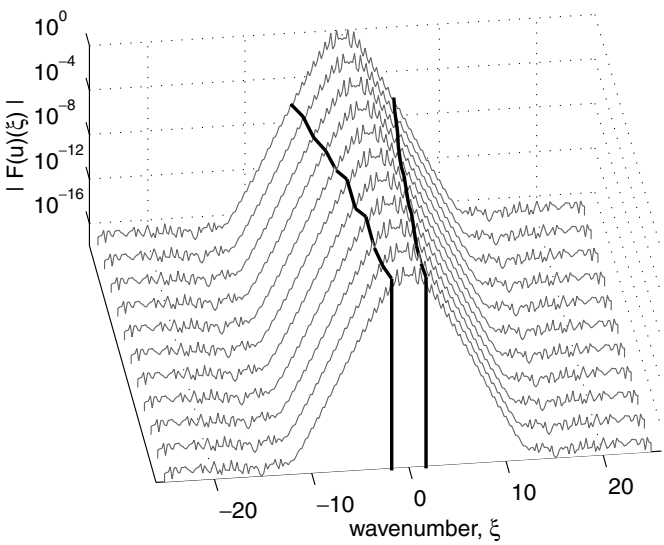

FIG. 5. Power spectrum for the KS solution at $t = 40$. The heavy black lines show where the transition from slow (explicit) to fast (semi-implicit) modes occurs for each of the data points on the CRK43 curve in Fig. 3.

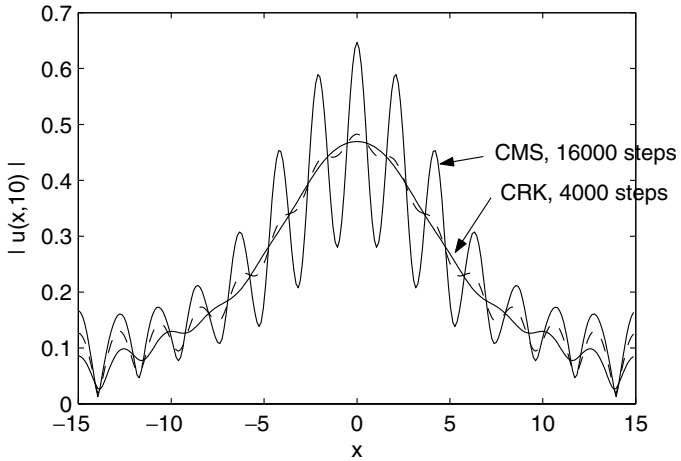

FIG. 6. Solution of Eq. (18) with a discontinuous coefficient. The exact solution (found by refinement) is shown with the dashed line. The composite RK method is less affected by jump discontinuities than the composite multistep method, which formally is no longer fourth-order accurate.

The discontinuities cause problems for multistep methods, which assume smoothness of the solution over several time intervals, but should cause no problem for an RK method as long as time steps align with the jumps. In Fig. 6 we show results using the composite RK (CRK) and CMS methods for equal numbers of nonlinear function evaluations and 256 spatial wavenumbers. The CRK solution is noticeably superior.

5. CONCLUSIONS

A fourth-order composite method built from classical RK4 and a linearly implicit RK formula for stiff modes has proven very effective for the time integration of Fourier collocation discretizations of semilinear PDEs of the type (1). It has the following advantages:

- It produces usable answers at time step sizes that are considerably larger than "black-box" methods (such as ODE15S).
- It is more efficient in practice than the integrating factor and LIRK methods.
- It is equally good without modification for dissipative and dispersive linear terms (unlike CMS42 and ELP4).
- It is self-starting and can be used in the presence of coefficients that are discontinuous in time (unlike CMS42, ELP4, and any other multistep method).
- It requires only modest changes from RK4 and is very easy to implement (compared especially to ELP4, which as described in [5] requires extra programming effort to avoid instabilities in coefficient computations).

Note, though, that the new method (like CMS42) is practical only when the transformed linear term L in (2) is diagonal. For such problems the linearity can be treated essentially on a scalar basis. But if one used, for example, a nonperiodic setting based on Chebyshev polynomials, the corresponding spectral transformation would result in a linear term which is well structured but not diagonal. At this writing we do not see how to cheaply and

stably separate such modes into "fast" and "slow" groups. The IFRK and ELP methods are more clearly salvageable in this case; however, they become much more expensive since they require computation or approximation of matrix exponentials rather than scalar exponentials. (See [5] for an application of ELP to a wavelet-based discretization.) One might want to pursue Krylov-based approximations of matrix exponentials [10, 13] in this context.

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