Higher Order Accurate Schemes for a Class of Nonlinear Evolution Equations

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Here we discuss ways to obtain third and fourth order accurate schemes for certain semilinear evolution equations, granted the availablity of schemes of such accuracy for their linear counterparts. Cases of particular interest are those for which FFT methods are available for the linear equations.

1. Equations of nonlinear Schrödinger type

Here we treat evolution equations of the form

$$\frac{\partial u}{\partial t} = Lu + f(u), \tag{1.1}$$

where L is a linear differential operator, generating a semigroup e^{tL}. The paradigm is $L = i\Delta$, but we can also treat variations, such as $L = \Delta$, yielding reaction-diffusion equations. We make use of the integral equation

$$u(t+h) = e^{hL}u(t) + \int_0^h e^{(h-s)L} f\bigl(u(t+s)\bigr)\, ds. \tag{1.2}$$

Applying Simpson's rule to the integral on the right gives

$$u(t+h) \approx e^{hL}u(t) + \frac{h}{6}\Bigl[e^{hL} f\bigl(u(t)\bigr) + 4e^{(h/2)L} f\Bigl(\hat{u}\Bigl(t+\frac{h}{2}\Bigr)\Bigr) + f\bigl(\hat{u}(t+h)\bigr)\Bigr]. \tag{1.3}$$

If $\hat{u}(t+h/2)$ and $\hat{u}(t+h)$ are jth order accurate approximations, then (1.3) is $(j+1)$st order accurate, provided $0 \le j \le 3$.

For example, we can use Strang's splitting method:

$$\hat{u}(t+h) = \Phi^{h/2} e^{hL} \Phi^{h/2} u(t), \tag{1.4}$$

where Φ^t is the solution operator to $\partial u/\partial t = f(u)$. Then (1.4) is second order accurate, and plugging into (1.3) yields a third order accurate scheme.

Another second order accurate scheme is the following, also derived from (1.2):

$$\hat{u}(t+h) = e^{hL}u(t) + \frac{h}{2}\Bigl[e^{hL} f\bigl(u(t)\bigr) + f\bigl(e^{hL}u(t) + he^{hL} f\bigl(u(t)\bigr)\bigr)\Bigr]. \tag{1.5}$$

For a numerical implementation of (1.4), replace Φ^t by the result of a Runge-Kutta difference scheme (or, in rare instances, solve $u' = f(u)$ analytically). If L is a constant coefficient differential operator on the n-dimensional torus $\mathbb{T}^n$, then e^{hL} can be approximated to infinite order via the FFT. Note that in (1.4) you need to (approximately) evaluate the action of e^{hL} only once, while in (1.5) you need to evaluate it twice. In any case, (1.3) involves several additional evaluations of this semigroup action.

We could iterate this procedure to produce a fourth order accurate scheme, but a straightforward iteration would involve evaluating approximations at $t+h/4$ and $t+3h/4$ as well as at the other points. By contrast, the standard Runge-Kutta scheme for ODE miraculously involves fewer evaluations. We can get a close parallel to this Runge-Kutta scheme by the following device.

Let us temporarily assume e^{tL} is a one-parameter *group*, and set $v(t)=e^{-tL}u(t)$. Then (1.1) is equivalent to

$$\frac{\partial v}{\partial t}=\Psi(t,v(t)),\quad \Psi(t,v)=e^{-tL}f(e^{tL}v). \tag{1.6}$$

Applying the Runge-Kutta method to (1.6) gives

$$v(t+h)\approx v(t)+\frac{h}{6}[K_1+2K_2+2K_3+K_4], \tag{1.7}$$

with

$$\begin{aligned} K_1&=\Psi(t,v(t)),\\ K_2&=\Psi\Big(t+\frac{h}{2},v(t)+\frac{h}{2}K_1\Big),\\ K_3&=\Psi\Big(t+\frac{h}{2},v(t)+\frac{h}{2}K_2\Big),\\ K_4&=\Psi(t+h,v(t)+hK_3). \end{aligned} \tag{1.8}$$

Going back to $u(t+h)=e^{(t+h)L}v(t+h)$, we have

$$u(t+h)\approx e^{hL}u(t)+\frac{h}{6}\big[e^{hL}M_1+2e^{(h/2)L}M_2+2e^{(h/2)L}M_3+M_4\big], \tag{1.9}$$

with

$$\begin{aligned} M_1&=f\big(u(t)\big),\\ M_2&=f\Big(e^{(h/2)L}u(t)+\frac{h}{2}e^{(h/2)L}M_1\Big),\\ M_3&=f\Big(e^{(h/2)L}u(t)+\frac{h}{2}M_2\Big),\\ M_4&=f\big(e^{hL}u(t)+he^{(h/2)L}M_3\big). \end{aligned} \tag{1.10}$$

While the Runge-Kutta flavored scheme (1.9)–(1.10) was derived under the hypothesis that e^{sL} is a bounded operator for all real s, note that all the terms on the right side of (1.9)–(1.10) involve e^{sL} only for positive s, so we can hardly fail to conjecture that this yields a valid fourth order accurate scheme for equations of reaction-diffusion type as well as for those of nonlinear Schrödinger type.

2. Semilinear wave equations

Here we treat wave equations of the form

$$\frac{\partial^2 u}{\partial t^2} = \Delta u + f(u). \tag{2.1}$$

Say Δ is the Laplace operator on the flat torus $\mathbb{T}^n$, and set $A = \sqrt{-\Delta}$. Then

$$u(t) = \cos tA\, u_0 + \frac{\sin tA}{A} v_0 + \int_0^t \frac{\sin(t-s)A}{A} f\big(u(s)\big)\, ds, \tag{2.2}$$

if $u_0 = u(0,x),\ v_0 = u_t(0,x)$. Using an analogous formula for $u(-t)$ and translating and summing, we get

$$u(t+h) = 2\cos hA\, u(t) - u(t-h) + \int_0^h \frac{\sin(h-s)A}{A} \big[f\big(u(t+s)\big) + f\big(u(t-s)\big)\big]\, ds. \tag{2.3}$$

Applying Simpson's rule to the integral on the right side of (2.3) gives

$$\begin{aligned} u(t+h) \approx{} & 2\cos hA\, u(t) - u(t-h) \\ & + \frac{h}{6}\Big[\frac{\sin hA}{A} f\big(u(t)\big) + 4\frac{\sin(h/2)A}{A} f\Big(\hat{u}\Big(t+\frac{h}{2}\Big)\Big) + f\big(\hat{u}(t+h)\big) \\ & \quad + \frac{\sin hA}{A} f\big(u(t)\big) + 4\frac{\sin(h/2)A}{A} f\Big(\hat{u}\Big(t-\frac{h}{2}\Big)\Big) + f\big(u(t-h)\big)\Big]. \end{aligned} \tag{2.4}$$

The quantities $\hat{u}(t-h/2)$ and $u(t-h)$ are already known (after the first iteration). If these quantities together with $\hat{u}(t+h/2)$ and $\hat{u}(t+h)$ are jth order accurate, then (2.4) is $(j+1)st$ order accurate, provided $0 \le j \le 3$.

For example, we can use a centered difference scheme to get second order accurate $\hat{u}(t+h/2)$ and $\hat{u}(t+h)$, and then (2.4) is third order accurate. We also require higher order accurate approximations of

$$\cos hA, \quad \frac{\sin hA}{A}, \quad \frac{\sin(h/2)A}{A}, \tag{2.5}$$

which can be achieved via the FFT if Δ is the Laplace operator on the torus $\mathbb{T}^n$, with its standard flat metric.

Another approach to (2.1) involves converting it into a system, as follows. Set $v = u_t$. Then (2.1) is equivalent to

$$\frac{\partial}{\partial t}\begin{pmatrix} u \\ v \end{pmatrix} = L\begin{pmatrix} u \\ v \end{pmatrix} + \begin{pmatrix} 0 \\ f(u) \end{pmatrix}, \tag{2.6}$$

where

$$L = \begin{pmatrix} 0 & I \\ \Delta & 0 \end{pmatrix}. \tag{2.7}$$

This has the form (1.1), so the results of §1 are applicable. Note that

$$e^{tL} = \begin{pmatrix} \cos tA & A^{-1}\sin tA \\ -A\sin tA & \cos tA \end{pmatrix}, \quad A = \sqrt{-\Delta}. \tag{2.8}$$

3. Numerical experiments

We have used three numerical methods to approxinate the solution to

$$\frac{\partial u}{\partial t} = -iu_{xx} - 10i|u|^2 u, \quad u(0,x) = e^{-16|x|^2}, \tag{3.1}$$

(periodized to have period 2π in x) over the interval $0 \le t \le 2\pi$. The three numerical methods are:

(A) The Strang splitting method (1.4),

(B) The second order accurate method (1.5),

(C) The fourth order accurate method (1.9)–(1.10).

Here $L = -i\partial_x^2$. We use time steps of size

$$h = \frac{2\pi}{100}, \quad \frac{2\pi}{200}, \quad \frac{2\pi}{500}, \quad \frac{2\pi}{1000}, \tag{3.2}$$

and approximate the action of e^{hL} via the FFT. We present graphs of the computed solutions, at

$$t = \frac{2\pi k}{5}, \quad k = 0, 1, \dots, 5. \tag{3.3}$$

The following observations can be made from these graphs.

All the graphs look the same for $h = 2\pi/500$ and $h = 2\pi/1000$. In fact, graphs made at $h = 2\pi/10000$ also look the same. It seems safe to assume these graphs are accurate.

For $h = 2\pi/100$ and $h = 2\pi/200$, method (C) is noticeably better than methods (A) or (B). Particularly for $h = 2\pi/100$, method (A) (which automatically conserves the L^2-norm) is better than method (B) if the conservation of the L^2-norm of $u(t,\cdot)$ is not enforced. If this conservation is enforced, method (B) becomes about as good as method (A). One can also explicitly enforce L^2-norm conservation in method (C), but it does not lead to noticeable differences in these computations.

Conclusion: Method (C) rules.