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ON THE LACK OF CONVERGENCE OF UNCONDITIONALLY STABLE EXPLICIT RATIONAL RUNGE–KUTTA SCHEMES

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The poor performance of the rational Runge–Kutta (RRK) schemes of Hairer [2, 3] are investigated. By considering two simple model problems, it is demonstrated that this poor performance is in fact due to a lack of convergence. A conceptual model of an unconditionally stable implicit-explicit time-integration scheme is also considered. With the aid of this model, it is possible to establish necessary bounds on the extent of the explicit region for convergence. This demonstrates the limited applicability of such hybrid time-integration schemes.

1. Introduction

Wambecq [1] developed stable rational Runge–Kutta schemes for solving systems of ordinary differential equations (ODEs). These schemes have been adapted to construct unconditionally stable explicit [3] and implicit-explicit [4, 5] time-integration methods for parabolic partial differential equations (PDEs). Hairer [2, 3] investigated the stability properties of these rational Runge–Kutta (RRK) schemes for systems of ODEs. In particular, Hairer established conditions on the parameters of a two-parameter family of RRK schemes for A_0- and I-stability. The A_0-stability suggests that these RRK schemes can be applied to parabolic equations, while the I-stability suggests that RRK schemes can be applied to hyperbolic equations.

The RRK schemes have been implemented for explicit [3] and implicit-explicit [4] time integration of parabolic PDEs. These explicit RRK schemes have also been used in implicit-explicit time integrators for hyperbolic equations [5].

There have been reports of poor performance of the RRK schemes [4, 6], in spite of the fact that the RRK scheme used was second-order accurate, consistent, and unconditionally stable. In this paper, we investigate this poor performance by considering the following simple PDEs:

$$u_t - Cu_x = 0\,, \quad \text{a model hyperbolic equation;} \tag{1.1}$$

$$u_t - Du_{xx} = 0\,, \quad \text{a model parabolic equation}\,. \tag{1.2}$$

By using domain of dependence and region of influence arguments, we establish that the poor performance is, in fact, due to a lack of convergence.

In addition, a simple model of an unconditionally stable implicit-explicit time integrator is considered. With the aid of this model, we establish a necessary bound on the extent of the explicit region for convergence to still be possible. This demonstrates the limited applicability of such hybrid time-integration schemes.

2. The RRK scheme

The two-stage RRK scheme investigated by Hairer [3] for the numerical solution of the system of differential equations

$$\dot{y} = f(y) , \qquad y(t_0) = y_0 , \tag{2.1}$$

is as follows:

$$y^{j+1} = y^j + \Delta t\, e/b^{t} \cdot b , \tag{2.2}$$

where

$$e = 2(g_1^{t} \cdot b)g_1 - (g_1^{t} \cdot g_1)b , \tag{2.3}$$

$$b = \beta g_1 + (1-\beta)g_2 , \tag{2.4}$$

$$g_1 = f(y^j) , \tag{2.5}$$

$$g_2 = f(y^j + \alpha\, \Delta t\, g_1) , \tag{2.6}$$

and α, β are the parameters of the two-parameter family of RRK schemes investigated by Hairer [3]. All of the quantities on the right-hand side of (2.2) are known at the jth time step, so the method is explicit. Wambecq [1] showed that if

$$(1-\beta)\alpha = -\tfrac{1}{2} ,$$

then algorithm (2.2) is second-order accurate.

3. Model hyperbolic equation

3.1. Equation and exact solution

In this section, we consider the application of the RRK scheme (2.2) to perform the time-integration of a space semidiscretization of the model hyperbolic equation

$$\partial U/\partial t = C\, \partial U/\partial x , \quad -\infty < x < \infty , \; t > 0 . \tag{3.1}$$

Applying the method of characteristics to (3.1), we obtain the exact solution:

$$U(x, t) = U(x + Ct, 0)\,. \tag{3.2}$$

3.2. Semidiscretization of the model hyperbolic equation

Consider the central difference spatial discretization of (3.1):

$$\frac{\mathrm{d}u_n}{\mathrm{d}t} = C\Big(\frac{u_{n+1} - u_{n-1}}{2h}\Big) = C\Big(\frac{E - E^{-1}}{2h}\Big)\cdot u_n = A\cdot u_n\,, \tag{3.3}$$

where $u_n(t) \simeq U(x_n, t)$, $x_n = nh$, $n = 0, \pm 1, \ldots$, is a uniform division of the x-axis, $E\cdot u_n = u_{n+1}$ is the spatial shift operator, and $A\cdot := (C/2h)\,(E - E^{-1})\cdot$ is a Toeplitz operator (see e.g. [7]).

3.3. Spectral function of the spatial difference operator $A\cdot$

In order to determine the stability of the RRK scheme (2.2), when applied to the time integration of (3.3), we use the discrete Fourier transform (DFT) pair

$$\bar{u}(\xi, t) = h\sum_{n=-\infty}^{\infty} u_n(t)\,\mathrm{e}^{-\mathrm{i}\xi x_n}\,,\quad u_n(t) = \int_{-\pi/h}^{\pi/h} \bar{u}(\xi, t)\,\mathrm{e}^{\mathrm{i}\xi x_n}\,\frac{\mathrm{d}\xi}{2\pi}\,. \tag{3.4}$$

to determine the spectral function $\hat{A}(\xi)$ of the operator $A\cdot$ (see e.g. [7]). Applying the DFT to (3.3), we obtain

$$(\mathrm{d}\bar{u}\,(\xi, t)/\,\mathrm{d}t) = \hat{A}(\xi)\bar{u}(\xi, t) \quad \text{or} \quad \bar{u}(\xi, t) = \bar{u}(\xi, 0)\,\mathrm{e}^{\hat{A}(\xi)t}\,, \tag{3.5a}$$

where

$$\hat{A}(\xi) = (C\mathrm{i}/h)\sin(\xi h) \tag{3.5b}$$

is the spectral function of the operator $A\cdot$.

3.4. Stability

We use the stability definitions and results given by Hairer [3]. In order to ensure stability of the RRK scheme (2.2) applied to the time integration of the semidiscretization (3.3), we require that $\hat{A}(\xi)\,\Delta t \in D$, where $D \subset \mathbb{C}$ is a stability region of method (2.2). Hairer [3] has shown that the scheme (2.2) is I-stable, i.e., $D = \{\mathrm{i}y \mid y \in \mathbb{R}\}$ is a stability region, if and only if

$$(1 - \beta)\alpha \leq -\tfrac{1}{2}\,. \tag{3.6}$$

If we choose $\beta = 2$ and $\alpha = \tfrac{1}{2}$, then the scheme is I-stable. In this case, it follows from (3.5b) that $\hat{A}(\xi)\,\Delta t \in \{\mathrm{i}y \mid y \in \mathbb{R}\}$ for all Δt, so the scheme is unconditionally stable when applied to (3.3).

3.5. Consistency

By Taylor expansion about the (n, j)th mesh point, it can be shown that with $f(u) = A\cdot u$ in (2.2):

$$\frac{u_n^{j+1} - u_n^j}{\Delta t} = \frac{e_n}{b^{\mathrm{t}} \cdot b} = C\,\frac{\partial u_n^j}{\partial x} + \mathrm{O}(h^2; \Delta t)\,.$$

Consider a sequence of calculations with an increasingly finer mesh. Assume the following relation

$$h = g(\Delta t)\,, \qquad g(0) = 0\,, \tag{3.7}$$

which specifies how the space increment h approaches zero as the time increment Δt approaches zero. It follows that

$$\frac{u_n^{j+1} - u_n^j}{\Delta t} - C\,\frac{\partial u_n^j}{\partial x} = \mathrm{O}(h^2; \Delta t) = \mathrm{O}(g^2(\Delta t); \Delta t) \xrightarrow{\Delta t \to 0} 0\,.$$

Thus the scheme (2.2) yields a consistent time-integration algorithm for (3.3) [8].

3.6. *Convergence of the approximate solution*

The following convergence argument is similar to that used by Vichnevetsky [9] to prove stability theorems for one-step methods applied to ODEs. This is essentially an application of the Courant–Friedrichs–Lewy condition for the convergence of finite difference schemes.

Consider the advancement of the solution from the jth time step to the $(j+1)$th time step (see Fig. 1). From (2.5), (2.6) it can be seen that the RRK scheme (2.2) uses two stages to advance one step. This means that the right-hand side of (2.1) is evaluated twice, so the domain of computational dependence of the value u_n^{j+1} at (x_n, t_{j+1}) is:

$$[x_n - 2h, x_n + 2h]\,, \tag{3.8}$$

(see Fig. 1).

The analytic solution (3.2) at (x_n, t_{j+1}) can be expressed in terms of the values at the previous time-step as follows:

$$U(x_n, t_{j+1}) = U(x_n + C\,\Delta t, t_j)\,. \tag{3.9}$$

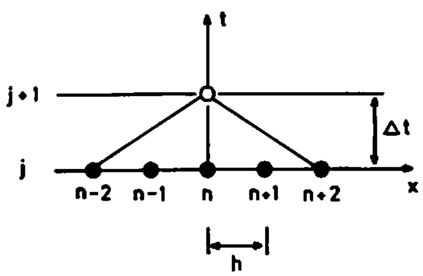

Fig. 1. Domain of computational dependence for the two-stage one-step scheme (2.2). To evaluate u_n^{j+1} (denoted by O), the values u_{n+r}^j with $|r| \leq 2$ (denoted by ●) are used.

From (3.8) and (3.9) it can be seen that if

$$C\,\Delta t > 2h\,,$$

then the analytic solution at (x_n, t_{j+1}) will depend on those values from the previous time step which lie completely outside the region used by the numerical scheme to compute u_n^{j+1}.

It may be argued that u_n^{j+1} is in fact affected by all the values in the vector $\boldsymbol{u}^j$ through the scalar factor $(\boldsymbol{b}^{\mathrm{t}}\cdot\boldsymbol{b})^{-1}$. However, consider a special case in which

$$u_{n-2}^j = u_{n-1}^j = u_n^j = u_{n+1}^j = u_{n+2}^j = 0\,,$$

while $U(x_{n+5}, t_j) = 1$, and where $C\,\Delta t = 5h$. The numerical scheme would then yield $u_n^{j+1} = 0$, whereas $U(x_n, t_{j+1}) = 1$. This situation will persist for any sequence of calculations in which $\Delta t \to 0$ and $h \to 0$ in such a way that

$$\Delta t/h = \text{const} > 2/C\,.$$

We therefore conclude that the numerical scheme (2.2) does not converge for $\Delta t/h > 2/C$ in spite of the fact that it is unconditionally consistent and stable.

4. Model parabolic equation

4.1. Equation and exact solution

In this section we consider the application of the RRK scheme (2.2) to perform the time integration of a space semidiscretization of the pure initial value problem for the heat equation:

$$\begin{aligned} &\partial U/\partial t = D\,\partial^2 U/\partial x^2\,, && -\infty < x < \infty\,,\ t > 0\,,\ D > 0\,,\\ &U(x,0) = U_0(x), && -\infty < x < \infty\,,\ t = 0\,. \end{aligned} \tag{4.1}$$

A formal solution of (4.1) obtained by Fourier transform [10] is:

$$U(x,t) = \int_{-\infty}^{\infty} \left\{ \frac{1}{(4\pi D t)^{1/2}}\, \mathrm{e}^{-(x-x')^2/4Dt} \right\} U_0(x')\,\mathrm{d}x'\,. \tag{4.2}$$

We see that $U(x, t)$ for $t > 0$, no matter how small, depends on the values of $U_0(x)$ at all points. Thus effects travel with an infinite speed.

4.2. Semidiscretization of the model parabolic equation

Consider the central difference spatial discretization of (4.1):

$$\frac{\mathrm{d}u_n}{\mathrm{d}t} = D\left(\frac{u_{n+1} - 2u_n + u_{n-1}}{h^2}\right) = D\left(\frac{E - 2I + E^{-1}}{h^2}\right)\cdot u_n = B\cdot u_n\,, \tag{4.3}$$

where $B\cdot := D(E-2I+E^{-1})/h^2\cdot$. Otherwise, the notation used here is identical to that defined below (3.3).

4.3. *Spectral function of the spatial difference operator $B\cdot$*

Applying the DFT defined in (3.4) to (4.3), we obtain

$$\bar{u}(\xi,t)=\bar{u}(\xi,0)\,\mathrm{e}^{\hat{B}(\xi)t}\,, \tag{4.4a}$$

where

$$\hat{B}(\xi)=2D(\cos \xi h-1)/h^2 \tag{4.4b}$$

is the spectral function of the operator $B\cdot$.

4.4. *Stability*

Hairer [3] has shown that the scheme (2.2) is A_0-stable, i.e., $D=\{x\in\mathbb{R}\,|\,x\leqslant 0\}$ is a stability region, if and only if

$$(1-\beta)\alpha\leqslant -\tfrac{1}{2}\,.$$

Thus, if we choose $\beta=2$ and $\alpha=\frac{1}{2}$, then the scheme is A_0-stable. In this case, it follows from (4.4b) that $\hat{B}(\xi)\,\Delta t\in\{x\in\mathbb{R}\,|\,x\leqslant 0\}$ for all Δt, so the scheme (2.2) with the above choice of α and β is unconditionally stable when applied to the time integration of (4.3).

4.5. *Consistency*

By Taylor expansion about the (n,j)th mesh point, it can be shown that with $f(u)=B\cdot u$ in (2.2):

$$\frac{u_n^{j+1}-u_n^j}{\Delta t}=\frac{e_n}{b^{\mathrm{t}}\cdot b}=D\,\frac{\partial^2 u_n^j}{\partial x^2}+\mathrm{O}(h^2;\Delta t)\,.$$

Again, consider a sequence of calculations with an increasingly finer mesh defined by (3.7). It follows that

$$\frac{u_n^{j+1}-u_n^j}{\Delta t}-D\,\frac{\partial^2 u_n^j}{\partial x^2}=\mathrm{O}(h^2;\Delta t)=\mathrm{O}(g^2(\Delta t);\Delta t)\xrightarrow{\Delta t\to 0}0.$$

Thus the scheme (2.2) yields a consistent time-integration algorithm for (4.3) [8].

4.6. *Convergence of the approximate solution*

In this section we use a region of influence argument to analyze the convergence of the RRK scheme when used in the time integration of (4.3).

Consider the advancement of the solution from the jth time-step to the $(j+1)$th time step (see Fig. 2). Since the RRK scheme (2.2) uses two stages to advance one step, the region of computational influence of the value u_n^j at (x_n,t_j) is (see Fig. 2):

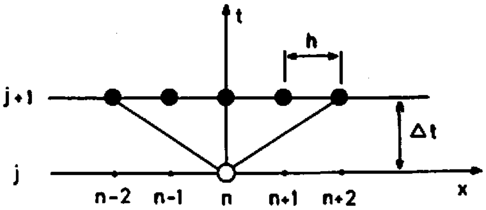

Fig. 2. Region of computational influence for the two-stage one-step scheme (2.2). The value of u_n^j (denoted by ○) affects the values of u_{n+r}^{j+1} with $|r| \leq 2$ (denoted by ●) during the course of the calculation.

$$[x_n - 2h, x_n + 2h] . \tag{4.5}$$

As mentioned in the discussion below (4.2), *all* the values of the analytic solution U at time step $j+1$ are affected by the value of the analytic solution at the single node (x_n, t_j). Consider the special case in which

$$u_m^j = U(x_m, t_j) = \begin{cases} 1, & m = n, \\ 0, & m \neq n. \end{cases}$$

The computational scheme yields

$$u_m^{j+1} = 0 \quad \text{for } |m - n| > 2 ,$$

whereas

$$U(x_m, t_{j+1}) \neq 0 \quad \text{for } m < \infty .$$

This situation will persist for any sequence of calculations in which $\Delta t \to 0$ and $h \to 0$ in such a way that

$$h/\Delta t = \text{const} .$$

In fact, the region of computational influence of the point (x_n, t_j) grows at a speed of $2h/\Delta t$, whereas the region of influence of the analytic solution grows at an *infinite speed*.

If we consider a sequence of calculations in which

$$\Delta t = \mathrm{O}(h^{1+\varepsilon}) , \quad \varepsilon > 0 \quad \text{as } \Delta t, h \to 0 , \tag{4.6}$$

then the speed at which the region of computational influence grows will be

$$2(h/\Delta t) = \mathrm{O}(h^{-\varepsilon}) \to \infty \quad \text{as } \Delta t, h \to 0 .$$

So convergence is now possible. The restriction (4.6) limits the magnitude of the time step Δt, so the scheme (2.2) is conditionally convergent in spite of the fact that it is unconditionally consistent and stable.

The above argument can be generalized to any K-stage method in which case the region of computational dependence grows at a rate $K(h/\Delta t)$. For example, the one-step Euler method applied to the time integration of (4.3) has the well-known time-step restriction

$$\Delta t \leq h^2/2D \,,$$

which is compatible with the restriction (4.6). It should be noted that (4.6) is a necessary condition for convergence, but not sufficient.

4.7. Convergence of an implicit-explicit algorithm applied to the model parabolic equation

Liu et al. [4] have advocated the use of an implicit-explicit time-integration algorithm to solve the problem of poor performance of the explicit RRK scheme (2.2). In this section we present a conceptual model of such an algorithm. We demonstrate that convergence is conditional on restricting the size of that part of the mesh which is treated by an explicit unconditionally stable and consistent time-integration scheme. An example of such a scheme is (2.2). We show that the extent of the region which can be *treated explicitly without restricting the time step* depends on the number of function evaluations used by the algorithm.

We consider a time-integration algorithm in which the numerical solution for the nodes $n + r$, where $|r| \leq M$, $r \in \mathbb{Z}$, is advanced using a K-stage explicit scheme, while the remaining nodes $n + r$, where $|r| > M$, $r \in \mathbb{Z}$, are advanced by some implicit scheme, e.g., the Crank–Nicholson method (see Fig. 3). Both schemes are assumed unconditionally stable and consistent.

By employing a similar argument to that in the previous section, we establish a necessary condition for convergence of the implicit-explicit scheme. Consider the special case in which

$$u_m^j = U(x_m, t_j) = \begin{cases} 1, & m = n \,, \\ 0, & m \neq n \,. \end{cases}$$

The computational scheme (2.2) yields

$$u_m^{j+1} = 0 \quad \text{for}\; |m - n| > 2 \,,$$

whereas

$$U(x_m, t_{j+1}) \neq 0 \quad \text{for}\; m < \infty \,.$$

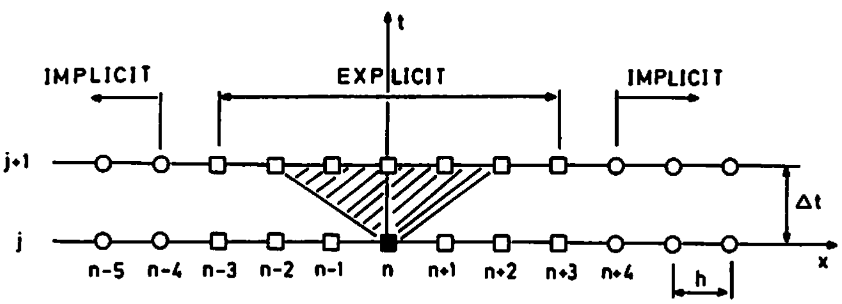

Fig. 3. Conceptual model of an implicit-explicit algorithm. The solution for the nodes $n + r$ with $|r| \leq 3 = M$ (denoted by □) is advanced by the explicit RRK scheme (2.2), while the solution for the nodes $n + r$ with $|r| > 3$ (denoted by ○) is advanced by some implicit scheme. The region of computational influence of the node (n, j) (denoted by ■) for the RRK scheme (2.2) ($K = 2$) is $[x_n - 2h, x_n + 2h]$—see the shaded section.

Again this situation will not improve for any sequence of calculations for which $\Delta t \to 0$ and $h \to 0$ in such a way that

$$h/\Delta t = \text{const}.$$

The region of computational influence of the point (x_n, t_j) grows at a speed $Kh/\Delta t$, whereas the region of influence of the analytic solution grows at an infinite speed. Therefore, we have the same lack of convergence of the scheme as before.

However, if the extent of the explicit region is such that it falls within the region of computational influence, then convergence is possible as the region of computational influence for an implicit scheme grows at an infinite speed. Recall K denotes the number of function evaluations of the explicit integrator. Therefore, if

$$\begin{aligned} &M \leqslant K, \quad \text{convergence is possible}, \\ &M > K, \quad \text{convergence is not possible}. \end{aligned}$$

In fact, by considering a disturbance propagating from one side of the explicit region to the other, it is possible to derive the more stringent necessary condition for convergence

$$2M \leqslant K. \tag{4.7}$$

The result (4.7) agrees with the numerical experiments of Liu et al. [4, Example 3], in which convergence was observed for a problem in which $2M = 2$ and $K = 2$. (Note that the problem they considered is effectively one-dimensional, due to axial symmetry.)

5. Conclusions

We have demonstrated two model problems in which the RRK scheme yields a time integrator which is not convergent, in spite of the fact that it is unconditionally consistent and stable. This would seem to contradict Lax's equivalence theorem [8]. However, Lax's equivalence theorem has only been proved for linear difference schemes and therefore does not guarantee convergence of the RRK difference scheme (2.2), which is nonlinear. In fact, these two model problems provide counterexamples to a conjecture that Lax's theorem could be applied without modification to nonlinear difference schemes.

This paper establishes that the poor performance of the RRK scheme, which has been described as "a loss of accuracy" by Liu et al. [4], is in fact due to a lack of convergence. Since the method is unconditionally stable, the loss of accuracy does not manifest itself in a blow-up of the solution or wild oscillations. Instead, the numerical solution just does not converge to the exact solution. There is evidence (see e.g. [4]) that the RRK scheme does give reasonable results for small time steps—Δt of the order required to stabilize the explicit Euler method. This can be explained by the fact that the RRK scheme for small Δt is approximately linear and so convergence is to be expected by Lax's theorem. Just how small Δt should be in this case is not considered in this paper, although it will almost certainly be problem-dependent.

For an unconditionally stable implicit-explicit algorithm, we were able to establish bounds on the extent of the explicit region in order for convergence to still be possible. Whether this restriction on the explicit region will render such an algorithm impracticable, depends on the particular problem. However, it should be emphasized that we have only established a necessary, not a sufficient, condition for convergence. Thus the algorithm may or may not converge even if a condition such as (4.7) has been established. Therefore, researchers are advised to proceed with caution in view of the fact that it has been demonstrated that Lax's theorem does not hold for nonlinear difference schemes such as (2.2).

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