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HIGH-ORDER ACCURATE TIME-STEPPING SCHEMES FOR CONVECTION-DIFFUSION PROBLEMS

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Abstract. *A major objective of the study described in the present paper is to achieve a high accuracy in the time integration of transient convection-diffusion problems and to eventually combine this with new methods for space discretization, such as meshless methods. In this way, a uniformly high-order accurate methodology could be made available for the numerical solution of convection-diffusion problems. Both Padé approximations of the exponential function and Runge-Kutta methods are considered for deriving multi-stage schemes involving first time derivatives only, thus easier to implement than standard Taylor-Galerkin schemes which incorporate second and third time derivatives. After a brief discussion of the stability and accuracy properties of the multi-stage schemes and the presentation of illustrative examples, the paper closes with some considerations on the coupling of high-order accurate temporal schemes and meshless methods for the spatial representation.*

1 INTRODUCTION

A great deal of effort has been devoted in recent years to the development of finite element methods for the numerical approximation of transport problems involving convective and diffusive processes. As described by Morton in his recent book [1], many different ideas and approaches have been proposed to overcome the deficiencies of the Galerkin method in highly convective situations.

In the particular case of truly transient problems, which are of interest in the present paper, the basic issue is not merely a question of achieving a stable and accurate spatial approximation, another equally important aspect being to ensure an adequate coupling between the spatial approximation provided by the finite element method and the time discretisation [2]-[5]. For instance, the absence of an adequate coupling between spatial and temporal discretisations is the reason why second-order accurate time-stepping methods, such as the Lax-Wendroff, leap-frog and Crank-Nicolson methods, properly combine with linear finite elements in convection problems only for small values of the time step, thus severely undermining the utility of such time integration schemes in practical applications.

Due to the coupling effects between space and time discretisations, methods for developing time-accurate finite element methods for highly convective unsteady problems must clearly go beyond the concept of properly adding diffusion to the underdiffuse Galerkin method, which was the key to the success in steady state situations. In the transient case, the overall truncation error of numerical schemes clearly incorporates the effects of both the spatial and the temporal discretisations and this must be taken into account when generalising the Galerkin finite element method for truly transient problems. In particular, by contrast with the steady state case, the truncation error in the discretisation of the linear, one-dimensional convection equation cannot be expressed in the form of a diffusion operator. Here, the overall truncation error depends upon the particular time-stepping method used in combination with linear finite elements [1], [3]- [5] and it generally involves both even and odd spatial derivatives of the unknown, thus simultaneously affecting the dissipative and the dispersive properties of the numerical schemes.

In the present paper, a study has been made of high order time-stepping methods with the view of identifying schemes that could possibly be used for a time accurate finite element solution of transient problems describing convective-diffusive transport. Both explicit and implicit methods are considered.

To be easily implemented in combination with C^o finite elements, high-order time-stepping schemes for the convection-diffusion equation should not involve higher-order time derivatives. This is the case for Runge-Kutta methods [6, 7] , as well as for multi-stage schemes emanating from Padé approximations to the exponential function [8, 9]. Schemes involving first time derivatives are indeed easier to implement for solving unsteady convection-diffusion problems than the standard Taylor-Galerkin schemes which imply the substitution of the higher-order time derivatives with spatial derivatives [10]. Moreover, some of the implicit methods to be discussed possess the interesting property of unconditional stability in application to hybrid parabolic-hyperbolic equations and are thus of great interest for solving transient convection-diffusion problems.

Section 2 is devoted to a discussion of multi-stage schemes obtained from Padé approximations to the exponential function. The properties of such schemes are then briefly summarized as regards their stability properties and their phase and damping responses.

Then, Runge-Kutta methods of high order are introduced in Section 3. Both explicit and implicit methods are considered and their stability and accuracy properties are compared with those of corresponding Padé approximations.

Numerical results are then presented in Section 4 to confirm the accuracy and stablility properties of some of the multistage methods considered in the paper.

Finally, Section 5 presents the main conclusions of the present study and indicates the lines of ongoing research in the area of numerical simulation of convection-diffusion phenomena.

2 MULTI-STAGE APPROACH TO PADE APPROXIMATIONS

The task of integrating forward in time the convection-diffusion equation

$$\frac{\partial u}{\partial t} + a \cdot \nabla u = k \nabla^2 u \tag{1}$$

amounts to devise an approximation to the evolution operator

$$E(\Delta t) : u(t^n) \rightarrow u(t^{n+1})$$

which allows to transport the numerical solution at a given time $t^n = n\,\Delta t$ to the next time station $t^{n+1} = t^n + \Delta t$. Now, from the forward Taylor series development

$$\begin{aligned} u^{n+1} &= \left(1 + \Delta t \frac{\partial}{\partial t} + \frac{1}{2!}\Delta t^2 \frac{\partial^2}{\partial t^2} + \frac{1}{3!}\Delta t^3 \frac{\partial^3}{\partial t^3} + \ldots\right) u^n \\ &= \exp\left(\Delta t \frac{\partial}{\partial t}\right) u^n, \end{aligned} \tag{2}$$

one notes that the evolution operator $E(\Delta t)$ is given by the exponential function in the above relationship. It is, therefore, apparent that time-stepping schemes of various orders of accuracy can be devised in the form of Padé approximations [7, 8, 9] to the exponential function. Padé approximations to e^x, where in the present context $x = \Delta t \frac{\partial}{\partial t}$, are shown in Table 1 in which classical explicit and implicit time integration methods are easily recognized.

With the view of integrating convection-diffusion equations forward in time using first time derivatives only, we shall now look at ways of reproducing higher-order Padé approximations through a multi-stage process. Explicit methods will be considered first. Then, multi-stage schemes corresponding to implicit Padé approximations will be examined. The section closes with a summarized account of the accuracy and stability properties of the various multi-stage Padé schemes.

2.1 Explicit multi-stage methods

Padé approximants $R_{n,0}$ in the first row of Table 1 are fully explicit approximations which yield time-stepping schemes of the type:

$$u^{n+1} = E_\Delta\, u^n = u^n + \Delta t\, u_t^n + \tfrac{1}{2}\Delta t^2\, u_{tt}^n + \tfrac{1}{6}\Delta t^3\, u_{ttt}^n + \cdots . \tag{3}$$

To avoid second and higher-order time derivatives which are difficult to express in terms of the spatial derivatives using the governing convection-diffusion equation, a multi-step approach to the explicit schemes derived from the $R_{n,0}$ approximations has been proposed in the literature.

As far as $R_{2,0}$ is concerned, a two-step approach has been suggested first by Richtmyer in the finite difference context (see [11]). Here, we write it in the form

$$\begin{aligned} u^{n+\frac{1}{2}} &= u^n + \tfrac{1}{2}\Delta t\, u_t^n \\ u^{n+1} &= u^n + \Delta t\, u_t^{n+\frac{1}{2}} \end{aligned} \tag{4}$$

which emanates from the following factorization of Padé approximation $R_{2,0}$:

$$1 + x + \tfrac{1}{2}x^2 = 1 + x\left(1 + \tfrac{1}{2}x\right) \tag{5}$$

Similarly, for Padé approximation $R_{3,0}$, a three-stage approach has been suggested to produce a third-order method involving first time derivatives only. This corresponds to the following factorization of $R_{3,0}$:

$$\begin{aligned} 1 + x + \tfrac{1}{2}x^2 + \tfrac{1}{6}x^3 &= 1 + x\left(1 + \tfrac{1}{2}x + \tfrac{1}{6}x^2\right) \\ &= 1 + x\left(1 + \tfrac{1}{2}x(1 + \tfrac{1}{3}x)\right) \end{aligned} \tag{6}$$

which produces the three-stage scheme

$$\begin{aligned} u^{n+\frac{1}{3}} &= u^n + \tfrac{1}{3}\Delta t\, u_t^n \\ u^{n+\frac{1}{2}} &= u^n + \tfrac{1}{2}\Delta t\, u_t^{n+\frac{1}{3}} \\ u^{n+1} &= u^n + \Delta t\, u_t^{n+\frac{1}{2}} \end{aligned} \tag{7}$$

This third-order explicit scheme has been employed in references [12] and [13] in the finite element solution of incompressible flow problems.

The above procedure is easily generalized to higher order Padé approximants. For instance, the explicit Padé approximation $R_{4,0}$ can be transformed into a four-stage method through the following factorization:

$$\begin{aligned} 1 + x + \tfrac{1}{2}x^2 + \tfrac{1}{6}x^3 + \tfrac{1}{24}x^4 &= 1 + x\left(1 + \tfrac{1}{2}x + \tfrac{1}{6}x^2 + \tfrac{1}{24}x^3\right) \\ &= 1 + x\left(1 + \tfrac{1}{2}x(1 + \tfrac{1}{3}x + \tfrac{1}{12}x^2)\right) \\ &= 1 + x\left(1 + \tfrac{1}{2}x\left(1 + \tfrac{1}{3}(1 + \tfrac{1}{4}x)\right)\right) \end{aligned} \tag{8}$$

which produces the four-stage explicit method

$$\begin{aligned} u^{n+\frac{1}{4}} &= u^n + \tfrac{1}{4}\Delta t\, u_t^n \\ u^{n+\frac{1}{3}} &= u^n + \tfrac{1}{3}\Delta t\, u_t^{n+\frac{1}{4}} \\ u^{n+\frac{1}{2}} &= u^n + \tfrac{1}{2}\Delta t\, u_t^{n+\frac{1}{3}} \\ u^{n+1} &= u^n + \Delta t\, u_t^{n+\frac{1}{2}} \end{aligned} \tag{9}$$

$R_{n,m}(x)$	$n=0$	$n=1$	$n=2$	$n=3$
$m=0$	1	$1+x$	$1+x+\dfrac{1}{2}x^2$	$1+x+\dfrac{1}{2}x^2+\dfrac{1}{6}x^3$
$m=1$	$\dfrac{1}{1-x}$	$\dfrac{1+\frac{1}{2}x}{1-\frac{1}{2}x}$	$\dfrac{1+\frac{2}{3}x+\frac{1}{6}x^2}{1-\frac{1}{3}x}$	$\dfrac{1+\frac{3}{4}x+\frac{1}{4}x^2+\frac{1}{24}x^3}{1-\frac{1}{4}x}$
$m=2$	$\dfrac{1}{1-x+\frac{1}{2}x^2}$	$\dfrac{1+\frac{1}{3}x}{1-\frac{2}{3}x+\frac{1}{6}x^2}$	$\dfrac{1+\frac{1}{2}x+\frac{1}{12}x^2}{1-\frac{1}{2}x+\frac{1}{12}x^2}$	$\dfrac{1+\frac{3}{5}x+\frac{3}{20}x^2+\frac{1}{60}x^3}{1-\frac{2}{5}x+\frac{1}{20}x^2}$
$m=3$	$\dfrac{1}{1-x+\frac{1}{2}x^2-\frac{1}{6}x^3}$	$\dfrac{1+\frac{1}{4}x}{1-\frac{3}{4}x+\frac{1}{4}x^2-\frac{1}{24}x^3}$	$\dfrac{1+\frac{2}{5}x+\frac{1}{20}x^2}{1-\frac{3}{5}x+\frac{3}{20}x^2-\frac{1}{60}x^3}$	$\dfrac{1+\frac{1}{2}x+\frac{1}{10}x^2+\frac{1}{120}x^3}{1-\frac{1}{2}x+\frac{1}{10}x^2-\frac{1}{120}x^3}$

Table 1: Padé approximations of the exponential function e^x.

As will be seen in Section 3, this method does possess the same stability and accuracy properties as the classical fourth-order explicit Runge-Kutta method.

2.2 Implicit multi-stage methods

We shall now consider implicit multi-stage methods for the convection-diffusion equation emanating from Padé approximations in Table 1 corresponding to $m \neq 0$. Actually, not all implicit methods with $m \neq 0$ are unconditionally stable in application to the linear convection–diffusion equation. As discussed in Section 3, only those approximations which are on or below the diagonal in Table 1, i.e., the $R_{n,m}$ with $m \geq n$, do possess interesting stability properties.

Due to space limitation, we shall limit ourselves to illustate the derivation of multi-stage implicit Padé schemes for the fourth-order approximant $R_{2,2}$ and the sixth-order one $R_{3,3}$. Multi-stage schemes corresponding to other implicit approximants are derived along similar lines [9].

The implicit method corresponding to $R_{2,2}$ reads

$$\left(1 - \frac{x}{2} + \frac{x^2}{12}\right) u^{n+1} = \left(1 + \frac{x}{2} + \frac{x^2}{12}\right) u^n, \tag{10}$$

and produces the well-known fourth-order scheme of Harten and Tal-Ezer [14]:

$$u^{n+1} = u^n + \frac{\Delta t}{2}\left(u_t^n + u_t^{n+1}\right) + \frac{\Delta t^2}{12}\left(u_{tt}^n - u_{tt}^{n+1}\right) \tag{11}$$

To avoid second time derivatives, we rewrite expression (10) in the following factorized form:

$$\left(1 - \frac{x}{2}(1 - \frac{x}{6})\right) u^{n+1} = \left(1 + \frac{x}{2}(1 + \frac{x}{6})\right) u^n \tag{12}$$

from which the following 4-stage method incorporating two explicit stages and two implicit ones can be deduced:

$$\begin{aligned} u^{n+\frac{1}{6}} &= u^n + \frac{\Delta t}{6} u_t^n \\ u^{n+\frac{1}{2}} &= u^n + \frac{\Delta t}{2} u_t^{n+\frac{1}{6}} \\ \tilde{u} &= u^{n+1} - \frac{\Delta t}{6} u_t^{n+1} \\ u^{n+1} &= u^{n+\frac{1}{2}} + \frac{\Delta t}{2} \tilde{u}_t \end{aligned} \tag{13}$$

Note that the two implicit stages in (13) are coupled and thus require a simultaneous solution.

Considering now approximation $R_{3,3}$, it produces the time scheme

$$\left(1 - \frac{x}{2} + \frac{x^2}{10} - \frac{x^3}{120}\right) u^{n+1} = \left(1 + \frac{x}{2} + \frac{x^2}{10} + \frac{x^3}{120}\right) u^n, \tag{14}$$

which reads

$$\frac{u^{n+1} - u^n}{\Delta t} = \frac{1}{2}\left(u_t^n + u_t^{n+1}\right) + \frac{\Delta t}{10}\left(u_{tt}^n - u_{tt}^{n+1}\right) + \frac{\Delta t^2}{120}\left(u_{ttt}^n + u_{ttt}^{n+1}\right), \tag{15}$$

Scheme (15) is sixth-order accurate in the time step Δt. To implement such a scheme using first time derivatives only, the following factorization of expression (14) is introduced

$$\left(1-\frac{x}{2}\left(1-\frac{x}{5}(1-\frac{x}{12})\right)\right)u^{n+1} \;=\; \left(1+\frac{x}{2}\left(1+\frac{x}{5}(1+\frac{x}{12})\right)\right)u^{n} \tag{16}$$

This leads to a multi-stage version of $R_{3,3}$ involving three explicit stages

$$\begin{aligned} u^{n+\frac{1}{12}} &= u^n + \frac{\Delta t}{12}u_t^n \\ u^{n+\frac{1}{5}} &= u^n + \frac{\Delta t}{5}u_t^{n+\frac{1}{12}} \\ u^{n+\frac{1}{2}} &= u^n + \frac{\Delta t}{2}u_t^{n+\frac{1}{5}} \end{aligned} \tag{17}$$

followed by three implicit ones

$$\begin{aligned} u^{n+1} - \frac{\Delta t}{12}u_t^{n+1} &= \tilde{u} \\ u^{n+1} - \frac{\Delta t}{5}\tilde{u}_t &= \hat{u} \\ u^{n+1} - \frac{\Delta t}{2}\hat{u}_t &= u^{n+\frac{1}{2}} \end{aligned} \tag{18}$$

Here again, the implicit stages are coupled and require a simultaneous solution

Remarks:

1. When using the above high-order accurate implicit methods in combination with finite elements for spatial discretization, the dimension of the system of semidiscrete equations to be solved at each time station is, as we have seen, very much increased (doubled for the fourth-order method, tripled for the sixth-order one) with respect to traditional second order methods, such as the Crank-Nicolson scheme. However, as shown in Section 4, the high-order time schemes permit the use of larger time-step values for an identical global time accuracy.

2. When dealing with pure convection problems it is generally possible to express the second time derivative of the unknown in terms of spatial derivatives. It follows that multi-stage schemes incorporating both first and second time derivatives can be employed for solving problems describing purely convective transport. In this respect, approximation $R_{2,2}$ can be used directly in pure convection problems, as shown in references [3] and [4] where scheme (11) is directly used in combination with linear elements for spatial discretization.

3. The sixth-order approximation $R_{3,3}$ can also be specialized to deal with pure convection problems. The result of its factorization in the form

$$\left(1-\frac{x}{2}(1-\frac{x}{5}+\frac{x^2}{60})\right)u^{n+1} \;=\; \left(1+\frac{x}{2}(1+\frac{x}{5}+\frac{x^2}{60})\right)u^{n} \tag{19}$$

is a four-stage method including two explicit phases and two implicit ones as follows:

$$
\begin{aligned}
u^{n+\frac{1}{5}} &= u^n + \frac{\Delta t}{5} u_t^n + \frac{\Delta t^2}{60} u_{tt}^n \\
u^{n+\frac{1}{2}} &= u^n + \frac{\Delta t}{2} u_t^{n+\frac{1}{5}} \\
\tilde{u} &= u^{n+1} - \frac{\Delta t}{5} u_t^{n+1} + \frac{\Delta t^2}{60} u_{tt}^{n+1} \\
u^{n+1} &= u^{n+\frac{1}{2}} + \frac{\Delta t}{2} \tilde{u}_t
\end{aligned}
\tag{20}
$$

3 Properties of Padé approximations

3.1 Stability analysis

The spatial discretization of the convection-diffusion equation using finite elements leads to the following system of differential equations to be solved at each station of the time integration procedure:

$$\frac{d\mathbf{u}}{dt} = \mathbf{R}(\mathbf{u}) \tag{21}$$

where $\mathbf{u}$ is the vector collecting the nodal values of the unknown and $\mathbf{R}(\mathbf{u}, t)$ stands for the nodal loads arising from the discretization of the first- and second-order spatial operators.

In order to discuss the stability of any time-integration method applied to eq.(21), we first define the eigenvalues λ of the spatial discretization operator $\mathbf{R}$ as

$$\mathbf{R}(\mathbf{v}) = \lambda \mathbf{v} \tag{22}$$

where $\mathbf{v}$ is the eigenvector associated to the eigenvalue λ.

If $\mathbf{R}(\mathbf{u})$ corresponds to the spatially discrete form of a diffusion operator, the eigenvalues are purely real and negative. On the other hand, if $\mathbf{R}(\mathbf{u})$ arises from the discretization of a convection operator, its eigenvalues are complex with a negative real part if upwind approximations are employed, whereas the real part is zero and the eigenvalues are purely imaginary whenever a central spatial approximation (e.g., the Galerkin projection) is used.

The stability of the method is ensured if and only if the time step is such that the value of the modulus of the amplification factor G is less than unity for all the eigenvalues of the discretization operator $\mathbf{R}$. It can be shown that the amplification factor of a Padé approximation $R_{n,m}$ has the same structure as the approximation itself:

$$G(R_{n,m}) = R_{n,m}(\lambda \Delta t). \tag{23}$$

It follows that Table 1 contains the amplification factors of all Padé approximations considered herein, provided we pose $x = \lambda \Delta t$.

In situations where diffusive effects are small with respect to the convective ones, the eigenvalues of $\mathbf{R}$ are distributed close to the imaginary axis of the $\lambda \Delta t$ complex plane. A time integration method whose stability region encloses the imaginary axis is then necessary. In the frame of explicit methods, the Euler first-order scheme, the stability region of which does not enclose the imaginary axis of the $\lambda\Delta t$ complex plane, has therefore to be rejected in favor, for instance, of higher-order explicit Padé approximations or Runge-Kutta methods. However, even if an explicit method has a stability domain which encloses part of the imaginary axis, the problem of a maximum allowable time step still remains. This is actually the case for all explicit methods.

We have to turn to implicit methods in order to reach unconditional stability. The stability domain then encloses the whole left half-plane of the $\lambda\Delta t$ complex plane, including the imaginary axis. Some implicit Padé approximations do possess the interesting property of unconditional stability or A-stability. As shown in [6, 7], a Padé approximation $R_{n,m}$ is unconditionally stable if it satisfies the condition:

$$m - 2 \leq n \leq m \Longleftrightarrow R_{n,m} \text{ is A-stable} \tag{24}$$

It follows that the implicit Padé approximations

$$R_{0,1},\ R_{1,1},\ R_{0,2},\ R_{1,2},\ R_{2,2},\ R_{1,3},\ R_{2,3},\ R_{3,3}$$

are A-stable and therefore potentially interesting for the time integration of convection-diffusion equations.

3.2 Phase and damping responses

To analyze the accuracy properties of the implicit multi-stage Padé schemes, we consider their application to the linear convection-diffusion equation

$$\frac{\partial u}{\partial t} + a\,\frac{\partial u}{\partial x} = \nu\,\frac{\partial^2 u}{\partial x^2}, \tag{25}$$

using a uniform mesh of linear elements of size h. We then substitute a Fourier mode e^{ikx} into the resulting discrete scheme and, defining the dimensionless wave number $\xi = k\,h$, obtain the amplification factor of the Padé scheme in the form

$$G(R_{n,m}) = f(\xi\,,\, c\,,\, d). \tag{26}$$

Here, $c = a\Delta t/h$ is the Courant number and $d = \nu\,\Delta t/h^2$ the diffusion number. The corresponding quantity for the partial differential equation (25) is

$$G_{exact} = \mathrm{e}^{-(\delta + i\,\omega)} \tag{27}$$

where $\delta = d\,\xi^2$ and $\omega = c\,\xi$ are the exact damping and the exact frequency, respectively. To evaluate the accuracy of the Padé schemes beyond the asymptotic limit $\Delta t \to 0$, we introduce the damping δ_{num} and frequency ω_{num} of the fully discrete schemes through the relation

$$G(R_{n,m}) = \mathrm{e}^{-(\delta_{num} + i\,\omega_{num})} \tag{28}$$

which implies

$$\begin{aligned} \delta_{num} &= -\ln|G(R_{n,m})| \\ \omega_{num} &= \arg\left(G(R_{n,m})\right). \end{aligned} \tag{29}$$

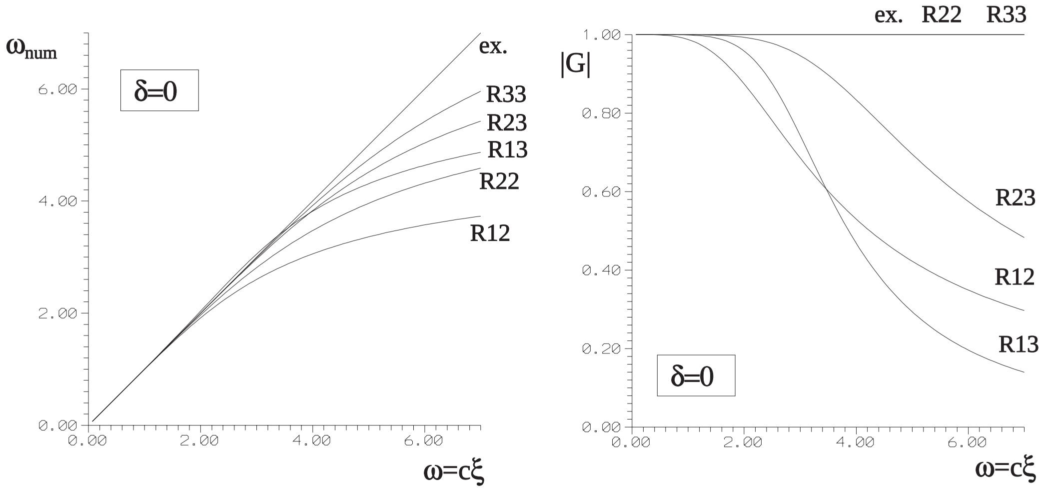


Figure 1: Accuracy of some A-stable Padé approximations for pure convection.

On this basis, the frequency response of the schemes can be characterized by the relative phase error $\Delta = \omega_{num}/\omega - 1$, and their damping response by the damping ratio δ_{num}/δ.

Figures 1 to 3 give a graphical representation of the phase and damping responses of selected implicit Padé schemes. Recall that the amplification factor of the schemes is given by the simple relationship (23). In the case of pure convection (Fig.1), we note that, as expected, the frequency

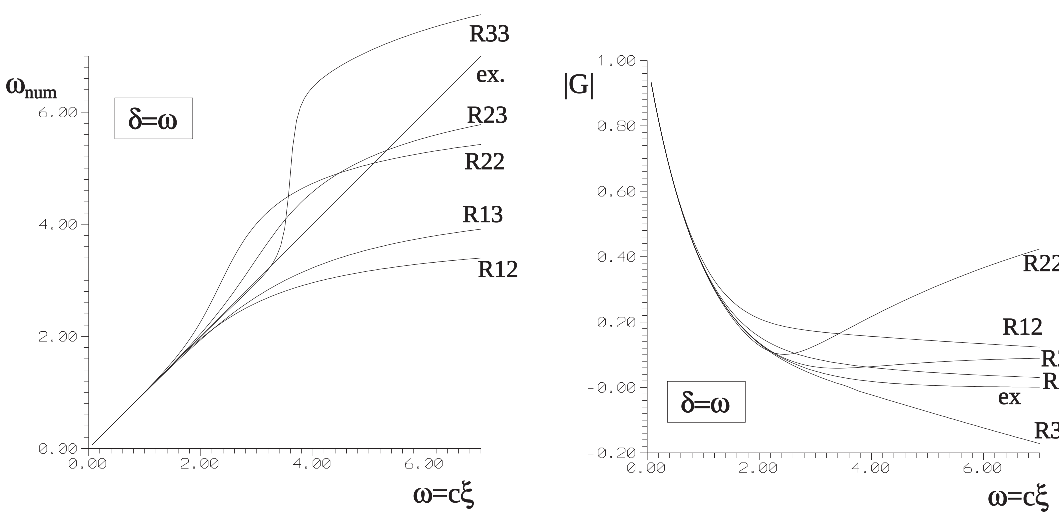


Figure 2: Accuracy of some A-stable Padé approximations for convection-diffusion.

response improves with the temporal accuracy of the multi-stage Padé schemes. We also observe that, for each scheme, there is clearly an accuracy limit. In practice, this means that there is an upper value of the Courant number beyond which there is a clear degradation in the phase accuracy. We also note from Fig. 1 that the off-diagonal approximants yield dissipative schemes, while the $R_{n,n}$ schemes are non-dissipative. As a consequence, such schemes are not ideally suited to deal with pure convection problems if centered (Galerkin) approximations are used for spatial discretization. These methods should therefore be combined with Petrov-Galerkin methods (such as the SUPG [15] or the Galerkin-Least-squares [16] methods) for the spatial representation.

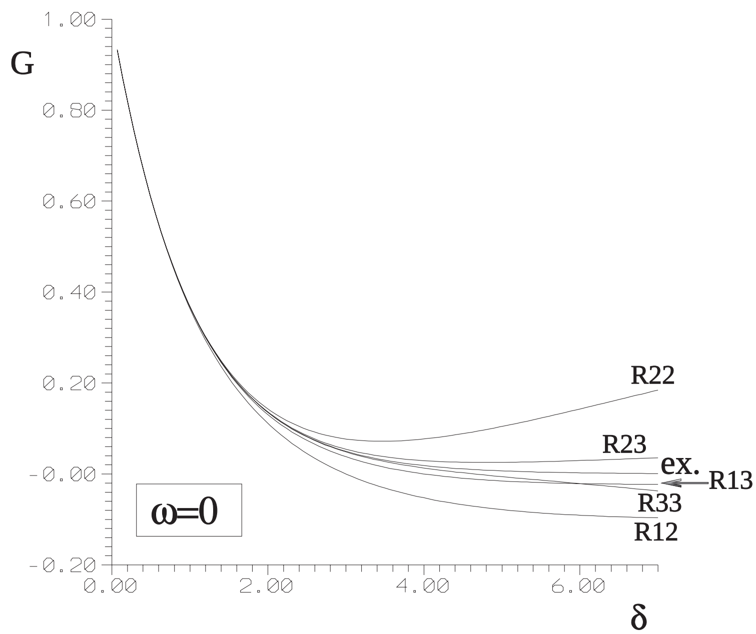


Figure 3: Accuracy of some A-stable Padé approximations for pure diffusion.

Fig. 2 illustrates the frequency and damping responses for a mixed convective-diffusive situation characterized by $\delta = \omega$. We see that all schemes exhibit a very good phase accuracy up to $\omega \simeq 2$ and that there is a systematic accuracy degradation beyond this value. The same applies to the damping response, with all schemes being underdiffusive at elevated frequencies, except $R_{3,3}$ which is overdiffusive.

Finally, for the case of purely diffusive transport, Fig. 3 indicates an accurate response of all schemes up to $\delta = d\,\xi^2 \simeq 2$. This means that, in the range of accurate resolution ($0 \leq \xi \leq \pi/4$), all schemes can be safely operated with a value of the diffusion number d of the order of 3. One also notes that approximants $R_{1,3}$ and $R_{3,3}$ are the most accurate in pure diffusion with an excellent response up to $\delta = 6$.

4 Runge-Kutta methods

The Runge-Kutta methods are multi-stage methods that only make use of the solution u^n at time t^n to compute the next solution u^{n+1}. This is achieved by computing a number k of intermediate values of the time derivative of the unknown u, within the interval $\Delta t = t^{n+1} - t^n$.

Applied to the differential equation

$$\frac{du}{dt} = R(u,t) \tag{30}$$

the most general form of a k-stage Runge-Kutta method is written as follows [6, 7]:

$$\delta_i = \Delta t\, R\left(u^n + \sum_{j=1}^{k} a_{ij}\,\delta_j\,,\; t^n + c_i \Delta t\right) \qquad i = 1,\ldots,k \tag{31}$$

$$u^{n+1} = u^n + \sum_{i=1}^{k} b_i\,\delta_i \tag{32}$$

The associated consistency conditions are (see e.g. [6])

$$c_i = \sum_{j=1}^{k} a_{ij} \qquad \text{and} \qquad \sum_{i=1}^{k} b_i = 1 \tag{33}$$

The widely used explicit Runge-Kutta methods are such that $a_{ij} = 0$ for $j \geq i$. If this condition is not satisfied, the methods are implicit.

4.1 Explicit Runge-Kutta methods

The most popular explicit Runge-Kutta method is the classical fourth-order four-stage scheme:

$$\begin{aligned}
\delta_1 &= \Delta t R\,(u^n\,,\, t^n) \\
\delta_2 &= \Delta t R\left(u^n + \tfrac{1}{2}\delta_1\,,\, t^n + \tfrac{1}{2}\Delta t\right) \\
\delta_3 &= \Delta t R\left(u^n + \tfrac{1}{2}\delta_2\,,\, t^n + \tfrac{1}{2}\Delta t\right) \\
\delta_4 &= \Delta t R\,(u^n + \delta_3\,,\, t^n + \Delta t) \\
u^{n+1} &= u^n + \frac{1}{6}\,(\delta_1 + 2\delta_2 + 2\delta_3 + \delta_4)
\end{aligned} \tag{34}$$

The amplification factor of the above fourth-order Runge-Kutta method is given by:

$$G = 1 + (\lambda\Delta t) + \frac{1}{2!}(\lambda\Delta t)^2 + \frac{1}{3!}(\lambda\Delta t)^3 + \frac{1}{4!}(\lambda\Delta t)^4 \tag{35}$$

The method is effectively fourth-order accurate since G matches $\exp(\lambda\Delta t)$ to the fourth-order term. The associated absolute stability curve is the same as that of Padé approximation $R_{4,0}$ and is shown in Fig.(4). It cuts the real and imaginary axes at -2.78 and $\pm 2\sqrt{2}$, respectively [7]. Since the absolute stability region contains a finite portion of the imaginary axis, the method can be used in convection dominated situations.

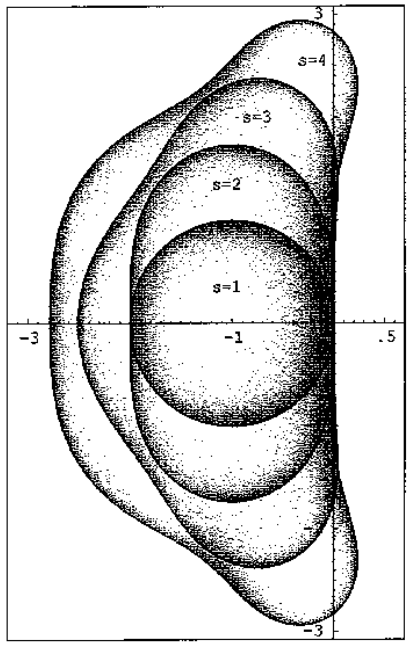


Figure 4: Stability domain of explicit Padé and Runge-Kutta methods of order s.

4.2 Implicit Runge-Kutta methods

Generally, the application of an implicit Runge-Kutta method requires the simultaneous solution of the k equations for the increments δ_i $(i = 1, \ldots, k)$.

Butcher (see e.g. [6]) has deeply investigated k-stage Runge-Kutta methods and shown that, for each value of k, there is one method of order $2k$. Moreover, Crouzeix [7] has demonstrated that such high-order methods are A-stable. This is indeed a very attractive property of implicit Runge-Kutta methods in view of their application in the solution of transient advection-diffusion problems.

The only fourth-order accurate two-stage implicit Runge-Kutta method is given by [7]

$$[a_{ij}] = \begin{bmatrix} \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\ \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \end{bmatrix} \qquad b = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} \qquad c = \begin{pmatrix} \frac{1}{2} - \frac{\sqrt{3}}{6} \\ \frac{1}{2} + \frac{\sqrt{3}}{6} \end{pmatrix} \tag{36}$$

The method then reads

$$\begin{aligned} \delta_1 &= \Delta t\, R\,(u^n + a_{11}\delta_1 + a_{12}\delta_2\,,\, t^n + c_1 \Delta t) \\ \delta_2 &= \Delta t\, R\,(u^n + a_{21}\delta_1 + a_{22}\delta_2\,,\, t^n + c_2 \Delta t) \\ u^{n+1} &= u^n + b_1\delta_1 + b_2\delta_2 \end{aligned} \tag{37}$$

The size of the implicit system associated with this method is double when compared to standard second-order methods, since δ_1 and δ_2 must be simultaneously determined. This is the price to pay to obtain an unconditionally stable fourth-order accurate time integration scheme. As

Implicit RK method	Multistage Padé method	Order	Amplification factor
Gauss	$R_{n,n}$	$2n$	$R_{n,n}(z)$
Radau IA	$R_{n-1,n}$	$2n-1$	$R_{n-1,n}(z)$
Radau IIA	$R_{n-1,n}$	$2n-1$	$R_{n-1,n}(z)$
Lobatto IIIA	$R_{n-1,n-1}$	$2n-2$	$R_{n-1,n-1}(z)$
Lobatto IIIB	$R_{n-1,n-1}$	$2n-2$	$R_{n-1,n-1}(z)$
Lobatto IIIC	$R_{n-2,n}$	$2n-2$	$R_{n-2,n}(z)$

Table 2: Relationship between implicit Runge-Kutta methods and multi-stage Padé schemes.

indicated next, this fourth-order method possesses the same phase and damping properties as Padé scheme $R_{2,2}$.

4.3 Similarities between Runge-Kutta and Padé methods

In the explicit $n-$order algorithms, like the $R_{n,0}$ Padé approximants or the explicit Runge-Kutta methods, the amplification factor $G(z)$, where $z = \lambda \Delta t$ (see eq. (23)), is a polynomial which reads

$$G(z) = 1 + \frac{z}{1!} + \frac{z^2}{2!} + \cdots + \frac{z^n}{n!} + T(z) \tag{38}$$

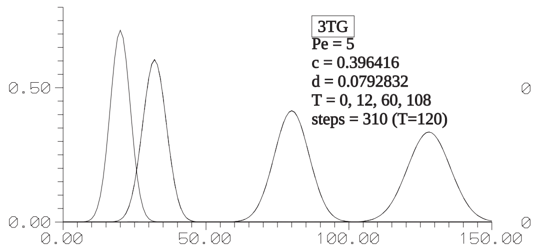
where $T(z) = O(z^{n+1})$. That is,

$$G(z) = R_{n,0}(z) + T(z) \tag{39}$$

The polynomial structure of $G(z)$ in equation (38) indicates why explicit methods cannot be A-stable. In the multistage explicit Padé methods, one has $T(z) = 0$ and the same holds for the explicit n-stage Runge-Kutta methods of order n [6]. Thus, the multistage explicit Padé schemes and the n-stage Runge-Kutta methods of order n are equivalent in application to linear problems. The only difference resides in the numerical implementation of the methods. Recall that the maximum order of a n-stage explicit Runge-Kutta method of order n is 4.

Among the implicit methods, k-stage Runge-Kutta methods of order $2k$ are called the Gauss methods. There are other classical families of implicit Runge-Kutta methods, such as the Radau-IA and Radau-IIA k-stage methods of order $2k-1$, and the Lobatto-IIIA, Lobatto-IIIB and Lobatto IIIC k-stage methods of order $2k-2$ [6, 7]. As indicated in Table 2 from reference [7], the various families of Runge-Kutta methods mentioned above are intimately related to the Padé multi-stage methods in the sense that they possess identical amplification factors.

Another family of implicit Runge-Kutta methods includes the so-called diagonally implicit (DIRK) methods. The great advantage of such methods is the absence of coupling between the various stages ($a_{ij} = 0$ in eq. (31) for $i < j$), which reduces the size of the systems to be solved at each step of the time integration procedure. Unfortunately, the accuracy properties of the DIRK methods in mixed convection-diffusion situations are significantly inferior to those of the classical implicit Runge-Kutta methods and of the implicit Padé schemes.



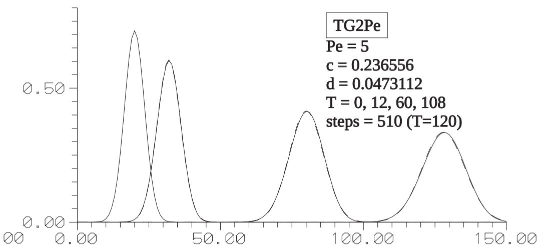


Figure 5: Convection-diffusion of a Gaussian by 3TG [12] and TG2Pe [17] with $Pe = 5$.

5 Numerical examples

Preliminary tests were performed to assess the performance of selected Padé schemes of high order in the solution of advection and advection-diffusion problems.
The selected schemes are $R_{1,2}$, $R_{2,2}$, $R_{2,3}$ and $R_{3,3}$.

Advection-Diffusion of a Gaussian Profile

To illustrate the performance of high-order Padé schemes and compare them to standard explicit schemes, consider first the linear advection-diffusion problem over the spatial interval $[0, 150]$ defined by

$$\begin{aligned} u(x,0) &= \frac{2.5}{\sigma} e^{-\frac{1}{2}X^2} \\ u(0,t) &= 0 \end{aligned} \tag{40}$$

with $X = (x - x_0)/\sigma$, $\sigma = 3.5$ and $x_0 = 20$ for $Pe = 5$ and $x_0 = 60$ for $Pe = 0.1$. We have used a unifrom mesh with $h = 1$.
In Figs. 5 to 10, we compare the profiles of the Gaussian obtained at various time levels with the fourth-order scheme $R_{2,2}$, with the three-stage explicit scheme $R_{3,0}$ (3TG) and with the second order explicit scheme of Peraire [17] (TG2Pe). Two values of the Péclet number were considered, namely $Pe = 0.1$ and $Pe = 5$. The explicit schemes were operated with a time step equal to 90 percent of their critical value, while $R_{2,2}$ used large values of the Courant number c to appraise its accuracy well beyond the stability limit of the explicit schemes. The results indicate that the fourth-order implicit scheme can produce very accurate answers for large values of the time step. The dotted lines in Figs. 5 to 10 correspond to the analytical solution of the problem.

The Burgers equation

The main objective of the A-stable implicit methods is to solve nonlinear stiff problems. We use the nonlinear Burgers advection equation with diffusion to show the improvement of the high-order Padé schemes against the standard explicit schemes. We consider the Burgers problem over the spatial interval $[0, 1]$ defined by

$$\begin{aligned} u_t + uu_x &= ku_{xx} \\ u(x,0) &= \sin(\pi x) \\ u(0,t) &= u(1,t) \;=\; 0 \end{aligned} \tag{41}$$

for $Pe = 1$ and $k = 0.001$. We have used a uniform mesh with $h = 0.001$.

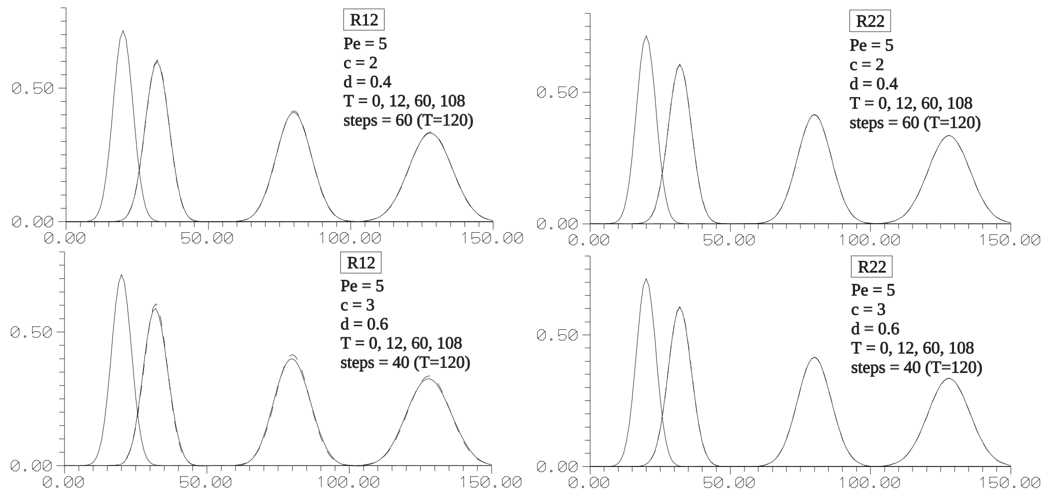


Figure 6: Convection-diffusion of a Gaussian by $R_{1,2}$ and $R_{2,2}$ with $Pe = 5$ at $c = 2$, 3.

In the $R_{2,3}$ and $R_{3,3}$ Padé methods a nonlinear system is solved at each time step by Newton-Raphson iteration. Only two iterations are needed to obtain accuracy over 10^{-4}. Figures 11 and 12 show the results for the implicit and explicit methods. You can see the efficiency of the high order Padé methods in Table 3. The $R_{2,3}$ and the $R_{3,3}$ methods are more than seven times faster than the TG2Pe method, and more than seventeen times faster than the 3TG method. The explicit schemes were operated with a time step equal to 75 percent of their critical value to avoid oscilations, while $R_{2,3}$ and $R_{3,3}$ used large values of the Courant number c.

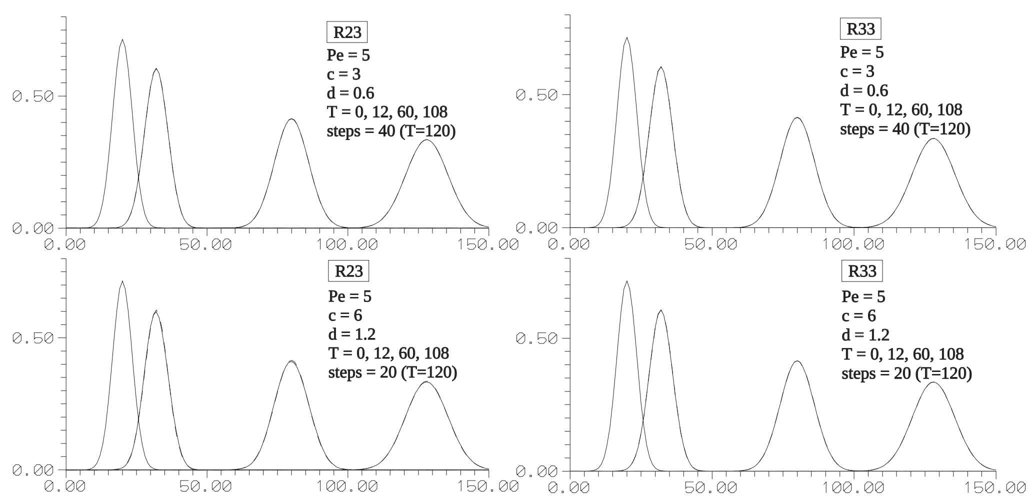


Figure 7: Convection-diffusion of a Gaussian by $R_{2,3}$ and $R_{3,3}$ with $Pe = 5$ at $c = 3$, 6.

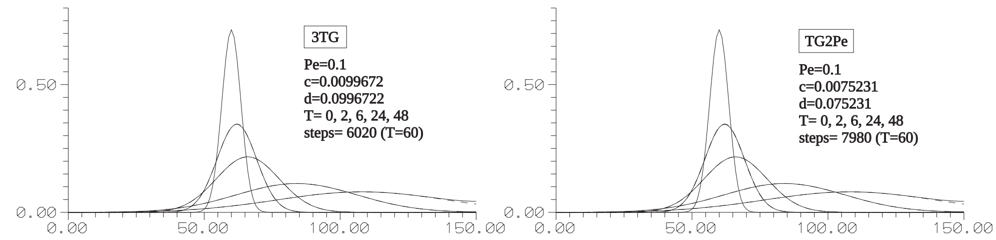


Figure 8: Convection-diffusion of a Gaussian by 3TG [12] and TG2Pe [17] with $Pe = 1$.

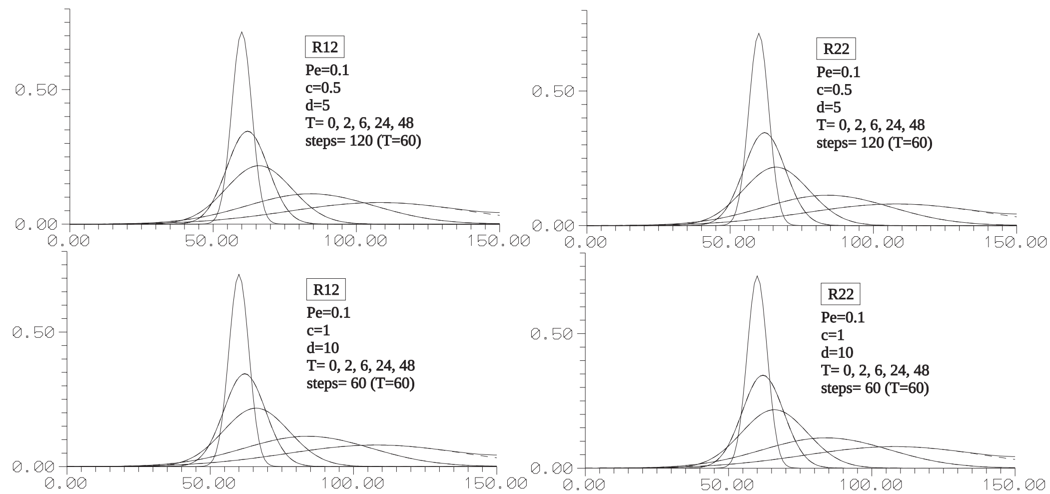


Figure 9: Convection-diffusion of a Gaussian by $R_{1,2}$ and $R_{2,2}$ with $Pe = 1$ at $c = 0.5$, 1.

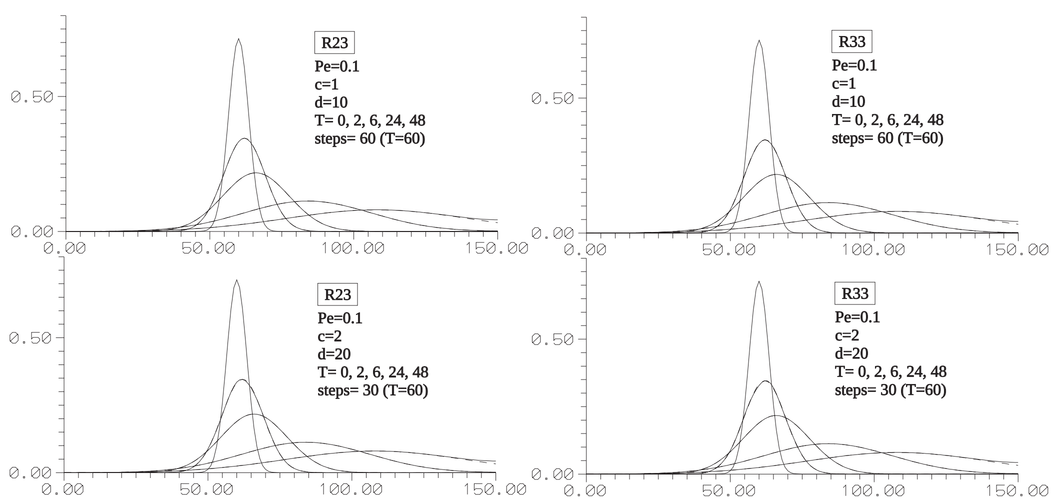


Figure 10: Convection-diffusion of a Gaussian by $R_{2,3}$ and $R_{3,3}$ with $Pe = 1$ at $c = 1$, 2.

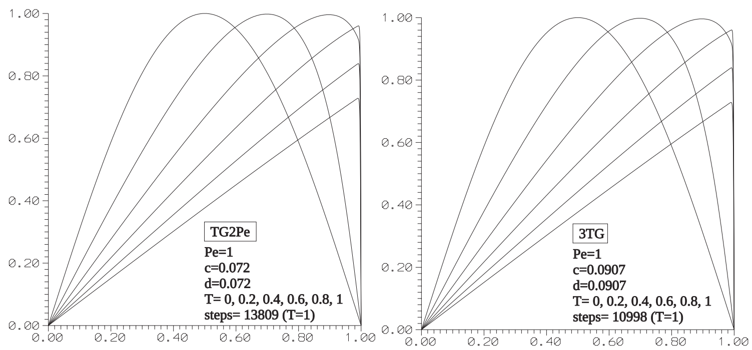


Figure 11: Solution of Burgers equation by 3TG [12] and TG2Pe [17] with $Pe = 1$.

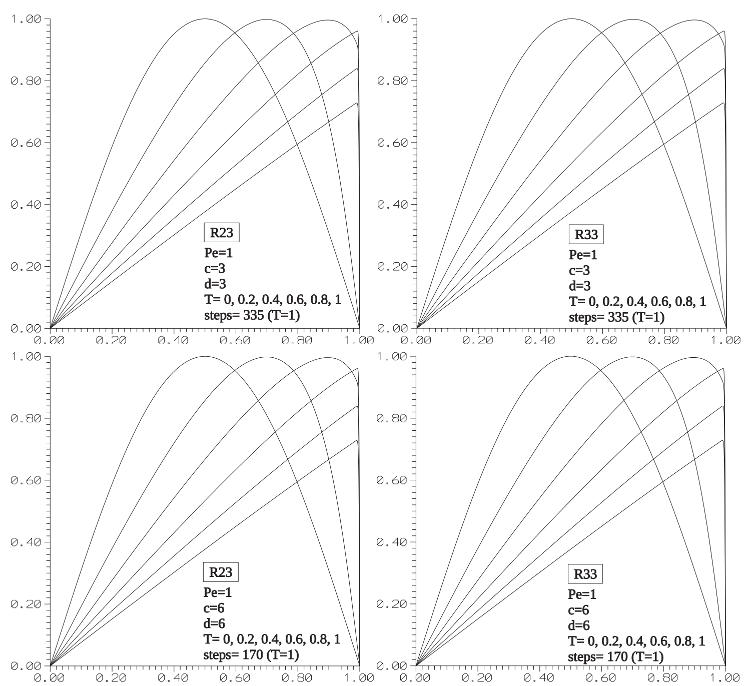


Figure 12: Solution of Burgers equation by $R_{2,3}$ and $R_{3,3}$ with $Pe = 1$ at $c = 3$, 6.

method	c_{max}	d	Δt	CPU	Time steps
TG2Pe	0.072	0.072	0.000072	2215	13809
3TG	0.0907	0.0907	0.0000907	5216	10998
R23	3	3	0.003	537	335
R23	6	6	0.006	280	170
R33	3	3	0.003	572	335
R33	6	6	0.006	306	170

Table 3: Comparison of the Padé and the explicit methods for the Burgers problem.

6 Conclusions

A multi-stage approach to Padé approximations of the exponential function can provide interesting explicit and implicit time-stepping methods of high order. Such methods only involve first time derivatives and are therefore easier to implement than Taylor-Galerkin methods in application to convection-diffusion problems.

Various Runge-Kutta methods were also considered and the intimate relationship between Runge-Kutta methods and multi-stage schemes derived from Padé approximations has been underlined.

Numerical tests have clearly shown that, when compared to traditional second-order time-stepping methods, the higher-order schemes permit the use of larger time-step values to reach a given time accuracy. Indeed the cost per time step of the high-order implicit methods is very much increased with respect to traditional second-order methods.

At this stage, further research efforts should be devoted to ways of improving the spatial accuracy and thereby achieve a uniformly high-order accurate computational method for evolutionary convection-diffusion problems. New methods for spatial discretization, such as meshless methods, are currently being investigated as regards their stability and accuracy properties in application to highly convective transport problems.

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