Applied Mathematical Sciences, Vol. 4, 2010, no. 38, 1855 - 1868

Explicit Runge-Kutta Time Integrators for One Dimensional Spatially Discrete Semilinear Parabolic Equation

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Abstract

Explosive instabilities in two uniform spatially discrete schemes for a semilinear parabolic equation in one space dimension are studied by intensive numerical simulations. We shows for both schemes that the difficulties of detecting blow-up phenomenons and computing or approximating blow-up solutions for such problem arise at least from the fact the grid spacing must be adequately chosen not only to ensure the similar behaviour between the obtained semidiscretization schemes and the continuous problem but also to ensure a suffisiant upper blow-up time if the continuous one exhibit a blow-up event.

Mathematics Subject Classification: 65M20, 65M12, 35B40

Keywords: Semilinear parabolic equation**,** Runge-Kutta methods, numerical approximations, Blow up phenomenons.

1. Introduction

Many time-dependent nonlinear PDEs that exhibit blow-up phenomenon and that have no known analytical solutions can be solved numerically using appropriate approximations in space and time. When a PDE is first discretized in space, this is the notion of the method of lines (MOL) and the result is a coupled system of nonlinear ordinary differential equations to be solved in place of the differential equations. To get such ODE system, there are several schemes among them one can cite the finite difference, and the finite element approximations. When the obtained ODE system is discretized in time, the result is a set of algebraic equations to be solved in place of the original system. Here also there are several methods which can be used to discretise and solve the ODE system among them we can cite the Runge-Kutta, Adams-Bashford and Taylor-series expansion methods. To obtain accurate numerical solutions for time-dependent nonlinear PDEs which my present blow-up phenomenons, the time integrator is almost as important as the spatial approximation and should not be overlooked.

This paper is devoted to the investigation of the Runge-Kutta methods for solving ODE system that result from an uniform spatial discretisation with finite difference and finite element methods of the following one-dimensionnal semilinear parabolic equation

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

with the initial condition

$$u(x,0) = u_0(x), \quad x \in R, \tag{2}$$

where $u_0(x)$ is continuous, non-negative and bounded.

Parabolic equations like (1) on bounded or unbounded domain appear in several branches of applied mathematics. They have been used to model, for example, chemical reactions and heat transfer and have been studied by several authors. See [3] and the references therein. The local existence (in time) of positive solutions of (1) is followed from standard results, but the solution may develop singularities in finite time. In the case of flat positif initial data, the exact solution to (1) is

$$u_{\text{hom}} = \beta^{\beta}(T_{\text{hom}} - t)^{-\beta} \tag{3}$$

with an exact blow-up time

$$T_{\text{hom}} = \left((p-1)u_0^{p-1}\right)^{-1} \tag{4}$$

where $\beta = (p-1)^{-1}$. Levine studied this problem for a more general positive initial conditions where the solutions are not a priori known and proved the following results [8]. Let $p_c = 3$ be the critical Fujita exponent of (1),

(1) When $1 < p < p_c$, for any non-trivial solution of (1) there exists a finit time T such that

$$\limsup_{t \to T} \left(\sup_{x \in \Re} (u(x,t)) \right) = +\infty.$$

(2) When $p > p_c$, then there exists a global positive solution if the initial values are sufficiently

small. To be precise, for any $k > 0$, δ can be chosen such that problem (1) has a global solution whenever $0 \le u_0(x) \le \delta e^{-k|x|^2}$.

We then say that $u(x,t)$ blows up at a finit time T, which is called the blow-up time of u. Recall however that in the case of a finite space domain and $1 < p$ there exists a global positive solution if the initial values are sufficiently small and a finite time blowup if the initial values are large enough.

Application of MOL to detect the blow-up phenomenon and compute or approximate the blow-up solutions, times and profiles, for such nonlinear equations leads often to much more difficulties than their linear cousins. Consequently, numerical algorithms for approximating their solution have been intensively studied in past years. For instance semi-discretization in space by finite differences or finite elements leads to an initial-value problem for a system of nonlinear ODEs. Some of the relevant questions in this first step when we want the theoretical solution of this system to display the properties of the blow-up phenomenon are the realisation of the possible truncation of the infinite domain to a finite domain $[-L,L]$, the choice of fixed or adaptive spatial mesh to fit the expected qualitative behavior, and in a more theoretical direction the analysis of convergence. Once the ODE system is obtained, the next step is to discretize the time variable. Others relevant questions when we want the get a good computational solution are the choice of temporal mesh, the choice of time integrator, and also the analysis of convergence.

In [10] the auhor introduce some totally discrete explicit and semi-implicit Euler methods and suggest an adaptive in time step procedure to deal with equation (1) in a bounded spatial domain. Recall that Euler's method is a first-order Runge-Kutta method. Here we shall propose two stage variable step explicit high-order Runge-Kutta methods (blow-up detection and localisation stages) in order to speed the computational of the discrete solution and to reproduce the properties of the continuous one especially when the time t approaches the blow-up time T. Next, we shall check by numerical simulation on uniform spatial meshes whether the classical second order central finite difference spatial discretization scheme [1], CSD, and the modified finite element spatial discretization scheme [11], MSD, used in conjunction with variable step Runge-Kutta integrators are efficients to reproduce the asymptotic behaviour of the continuous solutions. This work is motivated by the fact that for the CSD , the difficulties arise at least from the fact the grid spacing must be adequately chosen not only to ensure the similar behaviour between the obtained semidiscretization scheme and the problem (1) but also to ensure a suffisiant upper blow-up time if (1) exhibit a blow-up event.

The structure of this paper is as follows. In section 2, the proposed Runge-Kutta methods used to solve the studied problem are presented. In section 3, numerical experiments with various initial conditions for the considered problem are reported and compared both from a computational point of view and efficiency. Finally, we summarise our conclusions.

1. The numerical methods

Application of the considered numerical methods on problem (1) requires truncation of the infinite interval to a finit interval $[-L, L]$. For the numerical experiments considered, the constant L must be chosen suffisantly large so that the boundary conditions do not considerably affect the solution behaviour of the continuous problem. Hence, the problem (1-2) may be rewritten as follows

$$\begin{cases} u_t = u_{xx} + s(u,u) & 1 < p,\ x \in [-L, L],\ t > 0, \\ u(\pm L, t) = 0 & t \in [0, \mathrm{T}), \\ u(x,0) = u_0(x) & x \in [-L, L], \end{cases} \tag{5}$$

where $s(x,y) = \left(\frac{x+y}{2}\right)^p$ is the source term.

Let N be a positive integer. The interval $[-L, L]$ is divided into N equal subintervals with grid spacing $h = 2L/N$. The spatial grid points are given by $x_k = \left(\frac{2k}{N} - 1\right)L, k = 1,2,...,N$. The approximate solution to $u(x_k, t)$ is denoted by $u_k(t)$.

2.1 Spatial Discretizations

The first considered classical spatial discretization scheme, CSD, is obtained using a second order central finite difference expression for the second order x-derivative:

$$u_k'(t) = h^{-2}[u_{k+1}(t) - 2u_k(t) + u_{k-1}(t)] + (u_k(t))^p,\ k = 1,2,...,N-1. \tag{6}$$

If one is interested in using (4) as a semidiscretization of the continuous equation, and choose a non negative solution, $u_k(t)$, with

$$h^2 > 2(u_k(0))^{1-p}. \tag{7}$$

then (6) blow up in finite time T (see Theorem 2.1 of [1]) where

$$T \le T_b = \frac{h^2}{2(1-p)} \log\left(1 - \frac{2}{h^2}[u_k(0)]^{1-p}\right). \tag{8}$$

From a numerical point of view, (7) provides a condition on the spatial step size h which ensure explosive behaviour for (5). The difficulties arise here from the fact the choice of h is critical because the grid spacing must be adequately chosen not only to ensure the similar behaviour of (1) and (6) but also to ensure a suffisiant upper blow-up time if (1) exhibit a blow-up event.

Now by substituting the transformation

$$\varepsilon^2 = \frac{2}{h^2}[u_k(0)]^{1-p}. \tag{9}$$

in (8) one can get the following useful form of the upper blow up time bound

$$T_b = -\frac{\log\left(1-\varepsilon^2\right)}{\varepsilon^2} T_{\text{hom}}. \tag{10}$$

From (10) it is clear that $T_b \geq T_{\text{hom}}$.

In the second considered modified spatial discretization scheme, MSD, the spatial discretization is done by a second order nonlinear Galerkin-based method [11] to convert the PDEs to an ODE system :

$$u_k'(t) = h^{-2}\left[u_{k+1}(t) - 2u_k(t) + u_{k-1}(t)\right] + \frac{1}{2}\left[s\left(u_{k+1}(t), u_k(t)\right) + s\left(u_k(t), u_{k-1}(t)\right)\right],\ k = 1,2,\ldots, N-1. \tag{11}$$

Yet there is no known suffisiant theoretical condition, similar to (7), that ensure a blow-up event.

Let $U = \left(u_0(t) u_1(t) \ldots u_N(t)\right)$ be the values of the solution at time t , once we discretise the spatial part of the PDE we get a system of ODE

$$U' = f(U). \tag{12}$$

2.2 Time integrations

Let $U_n = \left(u_0^{(n)} u_1^{(n)} \ldots u_N^{(n)}\right)$ be the values of the numerical approximation of U at time t_n , and let $\tau_n = t_{n+1} - t_n$ be the time increment. For the time-stepping we shall use the modified Euler method (RK2), where the solution U of (12) is approximated by the solution U_n of the following explicit scheme

$$U_{n+1} = U_n + \tau_n\left(w_1 m_1 + w_2 m_2\right). \tag{13}$$

where w_i are weights of the slopes m_i at various points. We also use the classical fourth-order Runge-Kutta method (RK4) and the Runge-Kutta Fehlberg method (RKF45), where the numerical solutions are obtained from the following more general explicit scheme

$$U_{n+1} = U_n + \tau_n\left(w_1 m_1 + w_2 m_2 + w_3 m_3 + w_4 m_4\right). \tag{14}$$

Implementations of these methods using fixed and variable time step for different languages are given in [7]. Here we shall limit ourself to variable-time-step methods since it is well known in the theory of numerical integration of differential equations that fixed-time-step methods are inefficient, [4,5]. In fact, as the blow-up time is approached, the derivative drastically increases and thus smaller and smaller time-steps are required in order to capture the solution with sufficient resolution. The Runge-Kutta implementations of [7] are however of general use and can't fit the expected qualitative behaviour. We shall then propose two stage variable step explicit high-order Runge-Kutta methods (blow-up detection and localisation stages) in order to speed the computational of the discrete solution and to reproduce the properties of the continuous one especially when the time t approaches the blow-up time T .

In the first stage, we are concerned with the blow-up detection event where we use a slightly modified implementation of [7]. The numerical solution is calculated on an uniform time grid $t = m\Delta, m = 0,1,2,...$ using one of the three considered variable step integrators, and at each iteration, these integrators uses the latest obtained variable time step τ_{n_m} as an initial integration step to perform the new iteration. The truncation error is estimated along the solution to adjust the integration step according to aspacified error tolerance. More precisely, if an error violation is detected, the integration will be repeated with one half the previous integration step to improve the accuracy of the solution. Before the next step is taken along the solution, thre is the possibility that the integration step could be increased. Thus, a test is made to determine if the estimated error for each dependent variable is less than 1/4 for RK2 or 1/16 for RK4 or 1/32 for the RKF45 of the error tolerance. If so, the integration step is doubled before the next step along the solution is taken. The computation stops at the m^{th} subinterval, $[m\Delta, (m+1)\Delta]$, when the numerical scheme within the integrator call reduce the step size τ_n below 10^{-16}. The numerical blow-up time detection T_d is then estimated by $T_d = \sum_{j=0}^{n_0 - 1} \tau_j$.

In order to enhance this estimate, a localisation stage is performed. Here we need to adapt the size of the time step so that we take

$$\tau_n = \min\left(\tau_{n_0}, \frac{\lambda}{p-1} \left(\max_i u_i^{(n)} \right)^{1-p} \right). \tag{14}$$

The parameter λ is initially set to 1 and is reduced or increased by a factor of 2 in the same manner as it is done for the step size τ_n in the event blow-up detection stage. The computation stops when the numerical scheme reduce the step size τ_n below 10^{-16}. The numerical blow-up time is then given by $T^{(n)} = \sum_{j=0}^{n-1} \tau_j$.

3. Numerical experiments

To examine the performance of the suggested methods we consider the three different problems described bellows. The true solution, when it is unknown, is estimated by using the well known Exponential Time Differencing fourth-order Runge-Kutta method, ETDRK4, with $N = 2048$. The error $E_N(u)$ is then calculated as the ∞-norm of the difference between the solution at lower N and the ‘exact’ solution at the larger N. We also use the ETDRK4 method to verify the accuracy of the blow-up time estimate. The ETDRK4 is initially proposed by Cox and Matthews in [12], modified by Kassam and Trefetheny in [2] and successfully applied to problem (1-2) by de la Hoz and Vadillo in [6]. The absolute and relative errors in all considered Runge-Kutta methods are set to 10^{-5} and 10^{-8} respectively, while the parameter Δ is set to 10^{-2}. The error between the 'true' blow-up time, T, and the estimated one, $\hat{T}$, is calculated with the following equation:

$$E_N(T) = \log_{10}\left|T - \hat{T}\right|. \quad (15)$$

The purpose of the next three numerical experiments is to verify numerically for flat-shaped and bell-shaped initial conditions that the proposed Runge-Kutta methods exhibit good properties when their parameters are chosen conveniently.

3.1 The flat-shaped case

To test the solvers on homogenous solutions, we refer to the blow-up equation (1) with $p = 2$. The natural choice of $u(x,0) = 1$ is made. Recall from (3) that the exact solution to (1) is $u(x,t) = (1-t)^{-1}$ with exact blow-up time $T_{\text{hom}} = 1$. Recall from (10) that we have always $T_b \geq T_{\text{hom}}$ and for this example a suffisiant upper blow-up time is satifed for the CSD case.

The problem is first solved on the space interval $-5 \leq x \leq 5$ for times up to $t = 1.2$ with the RK2, RK4 and RKF45 methods. We presente in figures 1 and 2 respectively the error $E_N(T)$ and the computational costs as a function of N. Since these numerical methods gives very similar blow-up detection times, a single error curve for each spatial discretisation scheme appears on figure 1. We observe, for the CSD or the MSD scheme, that the errors $E_N(T)$ decrease with increasing N and reache a somewhat steady state for $N \geq 512$. Clearly, it appears that the CSD outperform the MSD when low values of N are used but give similar performance when the used N is large enough. The limited obtained accuracies for the RK2, RK4 and RKF45 methods are due to the limited space interval $-5 \leq x \leq 5$. To show that the obtained accuracy can be enhanced and the steady state behaviour for $N \geq 512$ can be eliminated by balancing the error due to the boundary effects with the error due to the internal resolution, we repeat the experiments of figure 1 but now using the space interval $-10 \leq x \leq 10$. The results are presented in figures 3 and 4 for the CSD and MSD respectively. Such increase of the spatial interval do not affect the observation concerning the comparison of the performance of the CSD and the MSD schemes, however it lead to an obvious enhancement in accuracy since for a given spatial discretisation scheme and for any fixed value of N a Runge-Kutta method applied on the space interval $-10 \leq x \leq 10$ gives always smaller errors than a Runge-Kutta method applied on the space interval $-5 \leq x \leq 5$. From the point of view of accuracy, the use of RKF45 or RK4 method on the space interval $-10 \leq x \leq 10$ lead now to better results than that of RK2 method; the RK4 method slightly outperform the RKF45 at a cost of a relatively more time demanding; the RK2 is less efficient than the others methods and have always the long computation time. Finally, from a comtutationnal point of view, and for any fixed value of N, the use of CSD with a given Runge-Kutta method is always more efficient than the use of MSD with the same method. We have always noted that the use of RKF45 or RK4 is computationally more efficient than the use of

RK2; the RKF45 is computationally more efficient than the others algorithms and should be used whenever possible.

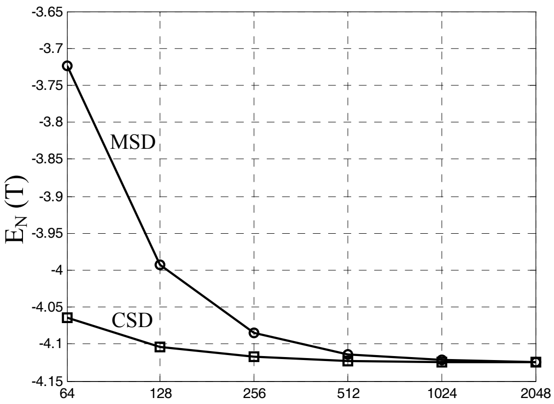


Figure 1 : Accuracy as a function of N for the space interval $-5 \le x \le 5$.

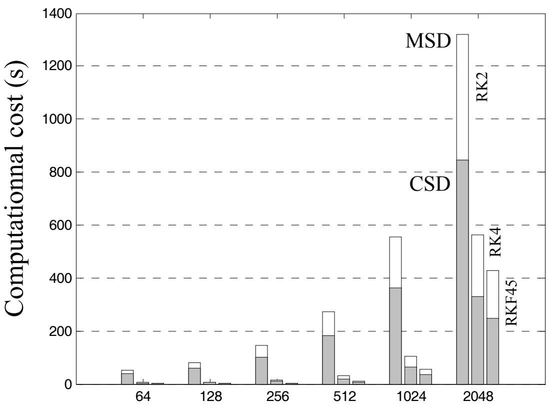
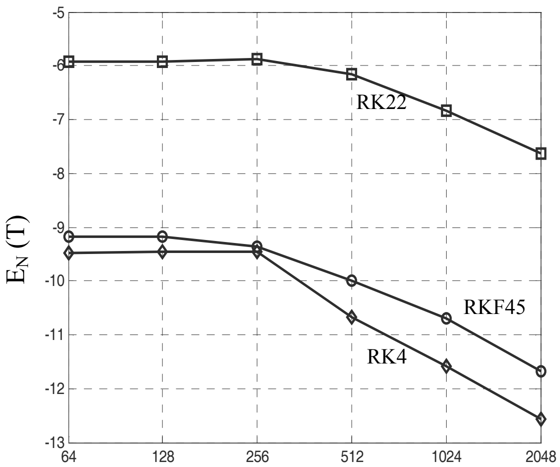


Figure 2 : Costs in secondes as a function of N for the space interval $-5 \le x \le 5$.



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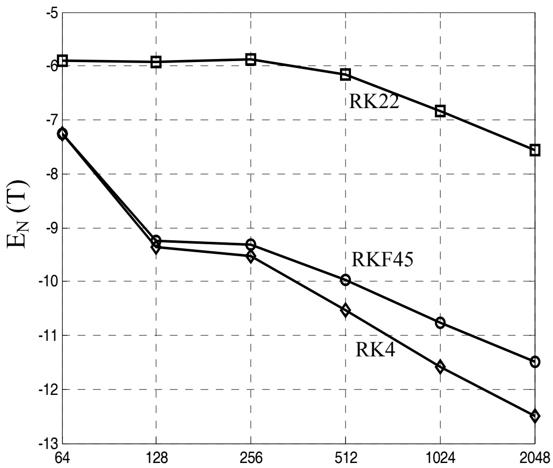

Figure 3 : The CSD accuracy as a function of N for the space interval $-10 \le x \le 10$.

Figure 4 : The MSD accuracy as a function of N for the space interval $-10 \le x \le 10$.

where the initial condition is the Gaussian function $u_0(x) = M\exp\left(-20x^2\right)$. The solution of this problem experience finit time blow-up. In [9], in a more general framework, it has been shown theoretically under the hypothesis of having a blowup point at $x = 0$, and a symmetric $u_0(x)$ with a single maximum at $x = 0$ that the asymptotic behaviour of a solution of the problem (1) at the blow-up time $T > 0$ is given by

$$\lim_{t \to T} \left(u\left(z\left((T-t)\left|\log(T-t)\right| \right)^{1/2}, t \right) \right) \cdot (T-t)^{\beta} = \beta^{\beta} \left[1 + \frac{(p-1)z^2}{4p} \right]^{-\beta}. \qquad (16)$$

This result holds uniformly on compact sets $|z| \le R$ with $R > 0$ and $\beta = (p-1)^{-1}$. Using the ETDRK4 method, de la Hoz and Vadillo [6] have shown numerically that the blow-up for $M = 6.05$ become pronounced near $t = 1$. They also showed that the resemblances near the origin between the obtained solution at time $t = 0.99$ with the estimate (16) are quite evident. The time step for the ETDRK4 method is set to 0.001.

In the present study, the above problem is first solved on the space interval $-5 \leq x \leq 5$, as in [6], for times up to $t = 1.2$. We presente in figure 5 and figure 6 respectively the accuracy $E_N(u)$and the blow-up detection error $E_N(T)$ of the RK2, RK4 and RKF45 methods for the time $t = 0.95$ as a function of N. Since the different numerical methods gives very similar blow-up detection times, a single error curve for each spatial discretisation scheme appears on the graphs. Here, the MSD accuracy outperform the CSD one, however, they give similar performance when the used N is sufficiently large. For both spatial discretisation, CSD and MSD, we observe that the error $E_N(T)$tend globally to decrease with increasing N. In order to enhance the performance of the numerical method, it is then raisonnable to refine the spatial mesh, but no so mush because of the important increase in computational cost as it can be seen on Table 1. Here also, the RKF45 still computationally more efficient than the others algorithms and should be used whenever possible.

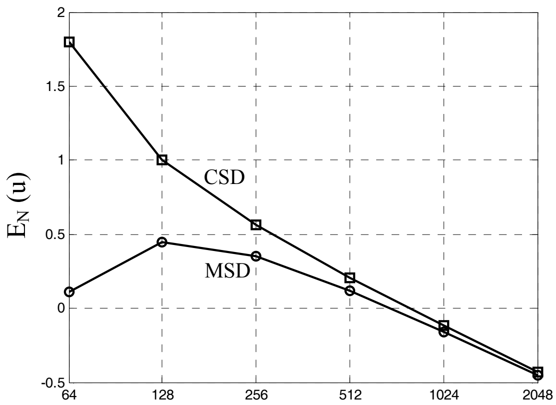

Figure 5 : Accuracy as a function of N for the space interval $-5 \leq x \leq 5$.

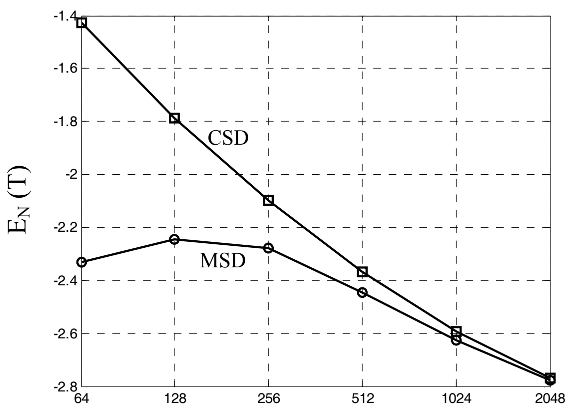

Figure 6 : Blow-up time detection errors as a function of N for the space interval $-5 \leq x \leq 5$.

Table 1: Comparison between the computational cost of the Runge-Kutta methods for the CSD and MSD in the case of the space interval $-5 \leq x \leq 5$.

SD	RK/N	64	128	256	512	1024	2048
	RK2	39,59			61,45		
CSD	RK4				105,66		
	RKF45				195,31		
					390,54		
					923,32		
		3,56			5,43		
		9,44			20,61		
		69,15			367,74		
		0,30			0,69		
		1,23			5,65		
		36,89			279,53		
	RK2	49,32			81,24		
MSD	RK4				145,00		
	RKF45				275,63		
					559,08		
					1327,50		
		4,55			7,44		
		13,59			30,97		
					103,88		
		545,16					
		0,44			0,84		
		1,81			8,47		
		56,24			429,40		

In the second example we have applied the proposed RKF45 method with $N = 256$ to the above problem in order to examine the behaviour of the obtained solution near the estimated blow-up times. We find that the numerical blow-up time is the CSD case is given by $T_h \approx 0.992015$ while it is given in the MSD case by $T_h \approx 0.994737$. The blow-up detection in the CSD take about 1.47s while the blow-up affinement procedure take about 8.17s to get the blow-up time estimate. For the MSD case a slightly more demanding time is needed, about 1.94s for blow-up detection and about 9.81s for blow-up time estimation. In figure 7 we have drawn $-\lg(u_0(t))/\lg(T_h - t)$ versus $-\lg(T_h - t)$ for both CSD and MSD schemes. For the CSD scheme, we can appreciate that the curve, corresponding to $\max u_k = u_0$, has a slop approaching 1 near the blow-up time T_h. This result somewhat seem to be in agreement with the continuous case (see equation 16) where we have $\lim\limits_{t \to T}(u_0(t)) = \beta^{\beta}(T - t)^{-\beta}$ with $C_p = \beta^{\beta} = 1$. Note also that the blow-up rate appears here much more accurate for the CSD scheme than the MSD scheme. If one use the MSD scheme for detection the blow-up event and the CSD scheme for estimating of the blow-up time, better results can then be expected.

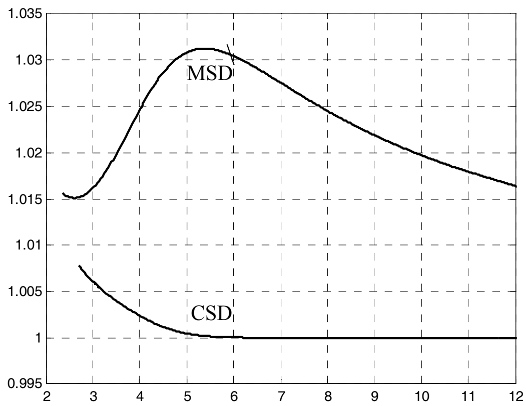

Figure 7 : Blow-up rate of the numerical solution for $N = 256$ and $L = 5$.

3.3 The behaviour at low values of *N*

In the above experiments we have shown for the CSD scheme that the event of blow-up in finite time for the proposed numerical methods can be obtained for N large enough without using the condition (7). This condition appears then to be just a sufficient condition for the Gaussian initial condition $u_0(x) = M\exp\left(-20x^2\right)$ and not a necessary one. When this condition is verified, the quantity ε^2 (see equation 9) and the like-blow-up time for homogenous solution $T_{\text{hom}} = \left((p-1)M^{p-1}\right)^{-1}$ (see equation (4) plays an important role in defining an upper time bound (10) for the numerical blow-up times. The purpose of the present numerical experiment is to study the effect of the CSD and MSD scheme on the numerical blow-up estimate for low values of N. To this end two tests were performed and in both tests the above problem is solved on the space interval $-5 \le x \le 5$ for times up to $t = 1.2s$.

We deal with the two cases $(p, M) = (2, 16.05)$ and $(p, M) = (3, 6.05)$. For both cases, we have evaluated the blow-up times resulting from using the CSD and the MSD in conjunction with the RKF45 method and plotted the obtained results on figures 8 and 9. The upper time detection bound for the CSD scheme is also plotted on these figures. Recall that the RKF45 method use the same parameters as in the above experiments. It is found that the CSD and MSD schema behave differently for low value of N. While the numerical blow-up time, T_N^{CSD}, for the CSD case increase monotonically with N, the numerical blow-up time associated to the MSD, T_N^{MSD}, attaint a maximum between 24 and 32 before deacreasing monotonically with N. It is also found that the upper bound, T_b, of the CSD case can't be used as an upper bound for T_N^{MSD}, but the blow-up time T_N^{MSD} can be used as an upper bound of T_N^{CSD} where the time T_b is not almost defined. We finally also note that the upper bound T_b become less and less sharp for T_N^{CSD} as N approaches the critical value where the condition (7) become not verified.

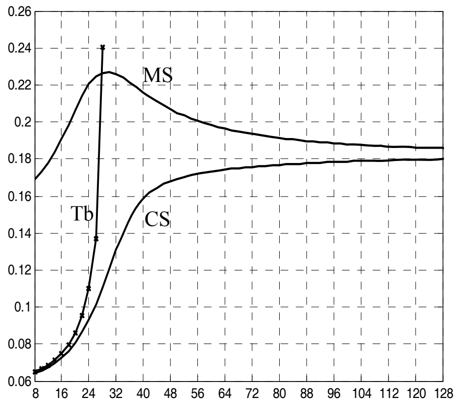

Figure 8 : Evolution of blow-up times with $M = 16.05$ and $p = 2$ as a function of N for the space interval $-5 \le x \le 5$.

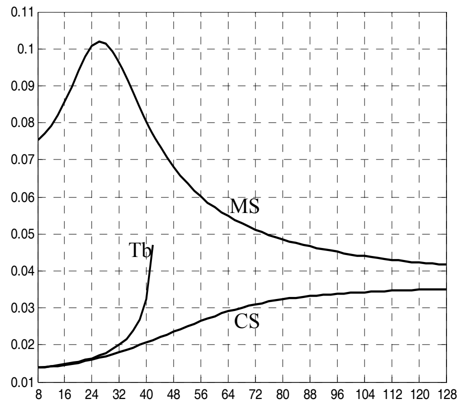

Figure 9 : Evolution of blow-up times with $M = 6.05$ and $p = 3$ as a function of N for the space interval $-5 \le x \le 5$.

4. Conclusion

In this study we have applied the well known high-order Runge-Kutta methods in conjunction with the classical or the modified spatial discretisation scheme. We have presented a slightly modification to their variable time step procedure in order to permit the discrete solution to reproduce the properties of the continuous one when the time approaches the blow-up time. The numerical experiments indicate that these numerical methods can perform well for both the CSD or the MSD scheme when the parameter N is large enough. We have found however that it is preferable to use the MSD for blow-up detection and the CSD for producing the expected qualitative behaviour near the blow-up time. For low values of N, the RKF45 method behave differently when used in conjunction with the CSD or the MSD. While the numerical blow-up time for the CSD case increase monotonically with N, the numerical blow-up time associated to the MSD pass by a maximum between 24 and 32 before deacreasing monotonically with N. We have also observed that the upper bound of the CSD case can't be used as an upper bound for the CSD case. We heve also noted that the upper bound T_b become less and less sharp as N approaches the critical value where the sufficient blow-up condition become not verified.

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Received: November, 2009