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# On the computation of blow-up

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Numerical methods for initial-value problems which develop singularities in finite time are analyzed. The objective is to determine simple strategies which produce the correct asymptotic behaviour and give an accurate approximation of the blow-up time. Fixed step methods for scalar ordinary differential equations are studied first and it is shown that there is a natural embedding of the discrete process in a continuous one. This shows clearly how and why the fixed-step strategy fails. A class of time-stepping strategies that correspond to a time-continuous re-scaling of the underlying differential equation is then proposed; this class is analyzed and criteria established to determine suitable choices for the re-scaling. Finally the ideas are applied to a partial differential equation arising from the study of a fluid with temperature-dependent viscosity. The numerical method involves re-formulating the equation as a moving boundary problem for the peak value and applying the ODE time-stepping strategies based on this peak value.

## 1 Introduction

Many time-evolving differential equations modelling real-world phenomena develop singularities in finite time. Typically the singularity reflects either the break down of some approximations used to derive the model of the real world (as in simple combustion models, e.g. Kapila 1986) or the use of unphysical initial or boundary conditions (as in various models derived from the Navier–Stokes equations by similarity reduction (Childress *et al.* 1989). In the former case it is very important to have precise information about the spatial and temporal scales on which the model breaks down so that the equations can be modified in the simplest possible manner consistent with mathematical considerations (usually asymptotics) and real-world observations. In the latter case, the mechanism of singularity formation is very poorly understood and it is important to have simple numerical schemes to complement analysis.

The numerical analysis of blow-up problems is not a well-developed subject. It is our purpose to construct and evaluate various time-stepping strategies suitable for PDEs by studying in detail the blow-up problem for a scalar ODE. Many numerical methods for time-dependent PDEs can be formulated in terms of the method of lines approach and this justifies our study of the ODE case. We apply our ideas to a concrete PDE in the final section. A simple time-stepping strategy was used by Hocking *et al.* (1972) in their study of bursting in fluid flow and we shall analyse a generalization of this. For computations of the nonlinear Schrodinger equation a re-scaling algorithm related to that in Hocking *et al.* (1972) has been used (LeMesurier *et al.* 1986). The most sophisticated numerical study of blow-up is by Berger & Kohn (1988). They use the scale-invariance of nonlinear parabolic equations to repeatedly refine the spatial and temporal grids, in a coupled fashion, close to the point of formation of the singularity in space–time. This is without doubt the most accurate computation of such a singularity and replicates precisely the known spatial structure of the problem at the blow-up time. However, for many problems there may be no scale-invariant structure or the precise details of the blow-up profile may not be required. For these cases it is useful to have an alternative or simpler numerical approach. In this paper we will concentrate mainly upon the effect of time-discretization. The effects of spatial discretization for PDEs which develop singularities in finite time is considered in Stuart (1989).

We believe that it is important to be able to analyze the asymptotics of the numerical method, for a given time-stepping strategy, in order to show that the asymptotics of the underlying differential equation are correctly reproduced. To be able to do this it is desirable to have a time-stepping procedure which is defined in a simple way in terms of the numerical solution of the differential equation and does not involve *a posteriori* testing to determine whether various tolerances are satisfied at each step; the analysis of the asymptotics of automatic step-size control packages is a difficult subject and studies have only just begun (Griffiths 1987). The procedures we study can be naturally defined in terms of an underlying continuous re-scaling of the problem and this simplifies the analysis considerably; we relate our approach to the work of Griffiths in §3.

For simplicity, our analysis is restricted to one-step methods. In §2 we study fixed step methods for scalar ODEs. We show that there is a natural continuous embedding of the numerical method in which it can be viewed as a bifurcation problem with time as the parameter. This shows clearly how and why fixed step methods, for scalar ODEs with stronger than linear growth rate, break down. By considering $\Delta t$ as an unfolding parameter we show the effect of decreasing the time-step.

We note here that computational results for blow-up problems with fixed time-stepping strategies still appear in the literature (see, for example, Childress *et al.* 1988, §4.2) and we believe that analysis of the simple scalar ODE problem is beneficial in highlighting the pitfalls of such strategies. In §3 we propose a class of variable time-stepping strategies designed to overcome these pitfalls. We analyze the asymptotics of these strategies, again by use of a continuous embedding of the discrete process, and describe criteria which determine the strategy most suited to a particular problem. The classification is based on the growth of the nonlinearity in the differential equation at infinity.

Finally we turn our attention to the parabolic PDE

$$x^q u_t = u_{xx} + f(u),$$

with $q > 0$ and Dirichlet boundary conditions on a finite interval $0 < x < 1$. The equation arises as a qualitative simplification of a model for a fluid with temperature dependent viscosity (Ockendon 1979; Lacey 1984). In §4 we summarize the known theoretical results about the equation and in §5 we describe a numerical method for its solution. Numerical results are then presented. Our analysis in §§2 and 3 suggests the importance of a precise knowledge of the peak value of $u(x, t)$ and we describe a peak-tracking method, coupled with a time-stepping strategy based on the peak value of $u$, to solve the problem. The peak-tracking is crucial to the solution of the PDE since the peak can move arbitrarily close to the boundary (Floater 1989).

Throughout §§2 and 3 we use the following notation to denote a subset of the reals:

**Notation 1.1** For $b \in \Re$, define $B = \{x \in \Re : x \geqslant b\}$.

## 2 Fixed Step Methods for ODEs

In this and the following section we will analyze numerical methods for the scalar differential equation

$$\mathrm{d}u/\mathrm{d}t = f(u), t > 0 \quad \text{and} \quad u(0) = b. \tag{2.1}$$

We require that

$$f(u) \geqslant \bar{f} > 0 \quad \text{for} \quad u \geqslant b. \tag{2.2}$$

With this condition $u(t) \to \infty$ in either finite or infinite time. We assume that $f(u)$ is a $C^1$ function for $u \in B$.

Let $u_n$ denote our approximation to $u(n\,\Delta t)$ for some fixed step size $\Delta t > 0$. We solve (2.1) by the one-step method

$$u_{n+1} = u_n + \Delta t(1-\theta)f(u_n) + \Delta t\theta f(u_{n+1}), n \geqslant 0 \quad \text{and} \quad u_0 = b. \tag{2.3}$$

Here $0 \leqslant \theta \leqslant 1$ and the method is implicit unless $\theta = 0$. Since $u(0) = b$ and the solution of (2.1) and (2.2) is monotonic increasing, we seek solutions $u_{n+1}$ of (2.3) in $B$. We now prove some results which are needed to define a continuous embedding of the numerical method.

**Lemma 2.1** *If there exists a sequence $u_0, u_1, \ldots, u_N$ satisfying* (2.3) *with elements $u_i \in B$, then*

(i) $u_i > u_{i-1}$ for $i = 1, \ldots, N$.
(ii) $u_i \geqslant u_0 + i\,\Delta t\bar{f}$, for $i = 1, \ldots, N$.
(iii) *If $N$ can be arbitrarily large, then $u_i \to \infty$ as $i \to \infty$.*

**Note on Lemma** We have assumed the existence of a sequence of $u_i$'s satisfying (2.3). In general we cannot expect this sequence to be unique. Existence and uniqueness issues are discussed in theorems 2.3 and 2.4.

**Proof of Lemma** We prove (i) and (ii) first. From (2.2) and (2.3) we have, since $0 \leqslant \theta \leqslant 1$,

$$u_i \geqslant u_{i-1} + \Delta t(1-\theta)\bar{f} + \Delta t\,\theta\bar{f} = u_{i-1} + \Delta t\bar{f}.$$

This establishes (i) since $\bar{f} > 0$ and (ii) follows by induction. Property (iii) follows automatically from (ii). □

In the following we will find it useful to define a new variable by setting

$$A_n = u_n + \Delta t(1-\theta)f(u_n). \tag{2.4}$$

Thus (2.3) may be written as

$$u_{n+1} = A_n + \Delta t\,\theta f(u_{n+1}). \tag{2.5}$$

We now prove that the $A_n$s form an increasing sequence; this is not immediately obvious since $f(u)$ may be a decreasing function for some values of its argument.

**Lemma 2.2** *Under the same conditions as lemma* 2.1 *we have*

(i) $A_i > A_{i-1}$ for $i = 1, \ldots, N$.

(ii) $A_i \geqslant A_0 + i\Delta t\bar{f}$.

(iii) *If N can be arbitrarily large, then* $A_i \to \infty$ *as* $i \to \infty$.

**Proof of Lemma** We have, by definition,

$$A_i = u_i + \Delta t(1-\theta)f(u_i).$$

Hence, by (2.3), we have
$$\begin{aligned} A_i &= u_{i-1} + \Delta t(1-\theta)f(u_{i-1}) + \Delta t f(u_i) \\ &= A_{i-1} + \Delta t f(u_i) \geqslant A_{i-1} + \Delta t\bar{f}. \end{aligned}$$

The proof is now identical to lemma 2.1 with $A_i$ replacing $u_i$. □

By lemmas 2.1 and 2.2 and equations (2.4) and (2.5) it follows that a solution sequence $\{u_i\}$ satisfying (2.3) can be continuously embedded in a solution branch $X(A)$ of the single parameterized nonlinear equation

$$X = A + F(X), \tag{2.6}$$

for

$$F(X) = \Delta t\,\theta f(X). \tag{2.7}$$

Here we consider $A$ as a continuously varying parameter with $A_0 \leqslant A < \infty$. Note that $A_0 = b + \Delta t(1-\theta)f(b) \geqslant b$. Each element $u_i$ of a sequence of $u_n$'s satisfying (2.3) necessarily corresponds to a solution of (2.6) with $A = A_{i-1}$, where the $A_i$s have properties given in lemma 2.2. By lemmas 2.1 and 2.2, the sequences $\{u_n\}$ and $\{A_n\}$ are monotonic increasing, whilst they exist. Thus there is a bijection between $A \in [A_0, \infty)$ and $t \in [0, \infty)$ if we set, for $A \in [A_n, A_{n+1})$,

$$t = \frac{(A_{n+1} - A)\,t_n + (A - A_n)\,t_{n+1}}{A_{n+1} - A_n}, \tag{2.8}$$

where $t_n = n\,\Delta t$.

Hence equation (2.6) is a simple bifurcation problem for $X$, with $A$ as the bifurcation parameter. The function $X(A)$ can be viewed as a continuous embedding of the sequence $\{u_n\}$ satisfying (2.3); thus $A$ has the role of a time-like variable in the embedding. By answering questions about the existence and multiplicity of solutions $X(A)$, we show clearly when and why the discretization breaks down. We can determine the asymptotic behaviour of solutions of (2.3) for large $n$ by examining the asymptotic behaviour of the single equation (2.6) for large $A$. We will examine three separate cases, determined by the behaviour of $f(u)$ as $u \to \infty$:

Case (a) $\lim_{u\to\infty} [f(u)/u] \to 0$.
Case (b) $\lim_{u\to\infty} [f(u)/u] \to L$, constant.
Case (c) $\lim_{u\to\infty} [f(u)/u] \to \infty$.

Case (c) contains functions for which blow-up in (2.1) occurs in finite time (that is, $u(t) \to \infty$ as $t \to t_b < \infty$); however, not all functions in class (c) necessarily lead to finite time blow-up (consider $f(u) = u\log(u)$, for example).

We are now in a position to prove the following theorem about the solutions of (2.3) for large $n$. Observe that, for $\theta = 0$, (2.3) has a solution for all $n > 0$.

**Theorem 2.3** *For* $0 < \theta \leqslant 1$, *the existence of solutions of* (2.3) *as* $n \to \infty$ *can be classified as follows*:

(i) *For case* (a) *there is a solution* $u_{n+1} \in B$ *for all* $n > 0$.
(ii) *For case* (b) *there is a solution* $u_{n+1} \in B$ *for all* $n > 0$ *if* $\Delta t\,\theta L < 1$.
(iii) *For case* (c) *there exists* $N$ *such that, for all* $n > N$, *there are no solutions* $u_{n+1} \in B$.

**Note on Theorem** It might seem that the non-existence property in (iii) is desirable since case (c) includes differential equations whose solutions cease to exist in finite time. This is not the case for two reasons: firstly, not all equations covered by case (c) have solutions which cease to exist in finite time ($f(u) = u\log(u)$ for example) so that property (iii) is highly undesirable. Secondly, even if the true solution does cease to exist in finite time, the manner in which the discrete solution ceases to exist is of a completely different nature; see theorem 2.4 and example 2.7 below.

**Proof of Theorem** By lemmas 2.1 and 2.2 the question of the existence of solutions of (2.3) in $B$ for all integer $n > 0$ is completely determined by the question of existence of solutions of (2.6) in $B$ for all $A \in [A_0, \infty)$. We define the function $G(X)$ by

$$G(X) = X - A - F(X). \tag{2.9}$$

To prove existence of a solution of (2.6) in $B$ for any given $A$ in the appropriate range, it is sufficient to show that $G(X)$ must change sign, for $b \leqslant X < \infty$. Throughout the following we use the fact that $f(u)$ is a $C^1$ function for $u \in B$.

We have $G(b) = b - A - F(b) < b - A_0 - \Delta t\,\theta \bar{f} \leqslant -\Delta t\,\theta \bar{f} < 0$. Now, for *any* $A \in [A_0, \infty)$,

$$\lim_{X\to\infty} \frac{G(X)}{X} = 1 - \lim_{X\to\infty} \frac{F(X)}{X}.$$

In case (a) we deduce that $G(X) > 0$ for $X$ sufficiently large and thus that a positive solution exists. Thus (i) follows. In case (b) we deduce that $G(X) > 0$ for $X$ sufficiently large provided that $\Delta t\,\theta L < 1$, by (2.7). This establishes (ii).

We now prove (iii). In this case, there exists $X^* > 0$ such that, for $X > X^*$ we have $F(X) \geqslant aX$ for some $a \geqslant 1$. We let

$$\bar{F} = \min_{b \leqslant X \leqslant X^*} F(X) > 0.$$

Then, for $b \leqslant X \leqslant X^*$, we have $G(X) \leqslant X^* - A - \bar{F}$. Thus, for $A > X^* - \bar{F}$ we have $G(X) < 0$ for $b \leqslant X \leqslant X^*$. Also, for $X > X^*$, we have $G(X) \leqslant X - A - aX < 0$, for $A > 0$. Thus, for $A > \max\{X^* - \bar{F}, \epsilon\}$, any $\epsilon > 0$, we have $G(X) < 0$ for all $X \geqslant b$. This implies that (2.5) does not have solutions in $B$ for $A_n$ sufficiently large; hence, by lemma 2.1, equation (2.3) does not have solutions in $B$ for $n$ sufficiently large. □

A desirable property of the equation (2.3) is that it should have a unique solution in $B$. For cases (a) and (b) uniqueness holds if $\Delta t$ is suitably restricted, and $f(u)$ is not highly oscillatory as $u \to \infty$. However, for case (c) uniqueness cannot occur, since (2.3) always possesses an even number of solutions in $B$.

**Theorem 2.4** *For* $0 < \theta \leqslant 1$, *the number of solutions of* (2.3) *in* $B$ *can be classified as follows*:

(i) *In cases* (a) *and* (b) *there is a unique solution in* $B$ *provided that*

$$\sup_{b \leqslant X < \infty} \Delta t\, \theta f'(X) < 1. \tag{2.10}$$

(ii) *In case* (c) *there is an even number of solutions in* $B$ *or none at all.*

**Proof of Theorem** The number of solutions of (2.3) in $B$ for integer $n > 0$ is determined by the number of solutions of (2.6) in $B$ for all $A \in [A_0, \infty)$. Consider $G(X)$ as defined by equation (2.9). Then $G'(X) = 1 - F'(X)$. If condition (2.10) is satisfied then, by (2.7), $G(X)$ is a monotonic increasing function of $X \in B$ for any $A$. Hence the solution of (2.5) is unique in $B$ (if it exists). This establishes (i). In case (c) we have

$$G(b) = b - A - f(b) < b - A_0 - \bar{f} < -\bar{f} < 0 \quad \text{and} \quad G(\infty) < 0$$

so that there must be an even number of solutions of (2.6) in $B$, or none at all. This establishes (ii). □

We now describe some examples which illustrate theorems 2.3 and 2.4. The initial value $b$ is zero in all three examples. All the figures show graphs of solutions $X$ of (2.6) as $A$ is varied. We can identify $A$ with time, through (2.8), and $X$ with a continuous embedding of the solution sequence satisfying (2.3). Thus the pictures are essentially bifurcation diagrams for the numerical solution of (2.1) with time as the parameter. We do not have a precise *numerical* description of time since the identification of $A$ and $t$ via (2.8) depends on the sequence of $A_t$s which we do not know *a priori*; however, by virtue of lemmas 2.1 and 2.2, we know that the plots of $X$ versus $A$ and $X$ (a continuous embedding of $u_n$) versus $t$ will be *topologically equivalent*. We shall study the deformation of these diagrams as we vary the parameter $\Delta t$. In the language of singularity theory we are considering $\Delta t$ as an unfolding parameter.

**Example 2.5** Let $f(u) = \mu e^{-(u-10)^2/10}$. This function falls in category (a). Figure 1 shows the bifurcation diagram for four values of $\Delta t$ chosen so that $\Delta t\, \theta \mu = 8, 4, 2$ and $1$. Consider the largest value of $\Delta t$ described in figure 1 (*a*): the solution $X$ is not unique as a function of time ($A$). The numerical method will pick out a (monotonically increasing) sequence of values of $X$ corresponding to some (monotonically increasing) sequence of values of $A$ (and hence $t$). Near to $A = 5$ the solution generated by the numerical method will undergo rapid transient behaviour as it jumps to the upper branch. This behaviour is spurious and caused by poor temporal resolution. As the temporal mesh is refined this behaviour is eliminated: in figure 1 (*b*) the two fold points coalesce at a cusp catastrophe and in figures 1 (*c*) and 1 (*d*) condition (2.10) is satisfied and the solution is unique.

**Example 2.6** Let $f(u) = \mu(1+u)(11 + 10 \sin(1+u))$. This function does not fall in any of the three categories (a), (b) and (c). However, its behaviour is essentially that in category (b). Figure 2 shows the bifurcation diagram for four values of $\Delta t$ chosen so that $\Delta t\, \theta \mu = 0{\cdot}01$, $0{\cdot}005$, $0{\cdot}0025$ and $0{\cdot}00125$. In figure 2 (*a*) $\Delta t$ is not sufficiently small and non-uniqueness abounds. At every other turning point the numerical solution will undergo spurious transient behaviour as it jumps to the branch above. As the mesh is refined this non-uniqueness is eliminated once condition (2.10) is satisfied.

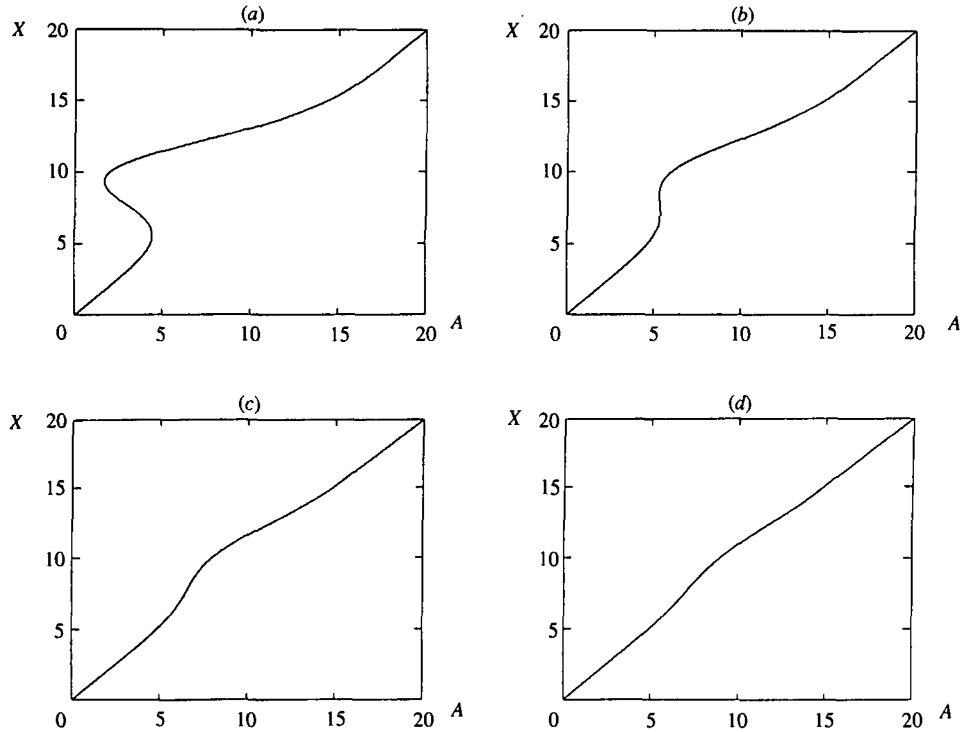


FIGURE 1. *The numerical solution of* (2.1) *and* (2.2); $f(u) = \mu e^{-(u-10)^2/10}$. (*a*) $\Delta t\,\theta\mu = 8{\cdot}0$; (*b*) $\Delta t\,\theta\mu = 4{\cdot}0$; (*c*) $\Delta t\,\theta\mu = 2{\cdot}0$; (*d*) $\Delta t\,\theta\mu = 1{\cdot}0$. $A$ is identified with time, $X$ with the numerical solution of (2.1) and (2.2).

**Example 2.7** Let $f(u) = (1+u)^2$. This function falls in category (c) and solutions of (2.1) blow-up in finite time. For the numerical method this strong temporal growth has severe consequences. For *any* non-zero value of $\Delta t\,\theta$ the solutions of the algebraic equations (2.3) are necessarily non-unique (if they exist) and, for large enough $n$, no solutions exist in $B$. This is illustrated in figure 3. Note that the non-existence occurs by a coalescing of the true solution (the lower branch) with a spurious solution introduced by discretization (the upper branch) at a fold point. This non-existence is of entirely different character from that which occurs in the differential equation at the blow-up time.

The continuous embedding of the discrete process shows very clearly what is going on in numerical methods which exhibit grid-scale dynamics: the discrete initial value problem has multiple solutions. Only one of these solutions corresponds to the true trajectory and the numerical method can jump onto a spurious trajectory. In examples 2.5 and 2.6 the jump occurs because the true trajectory ceases to exist for large enough values of $A$ and this occurs by a coalescence of the real trajectory with a spurious one at a turning point. In general this jumping may occur for other reasons associated with the domains of attraction of the solutions for the particular algebraic solver used. The choice of nonlinear algebraic solver is discussed in Iserles (1988).

In example 2.7 this coalescing also occurs, but there is no other solution for the numerical method to select, so that the discrete solution ceases to exist after a finite number of steps.

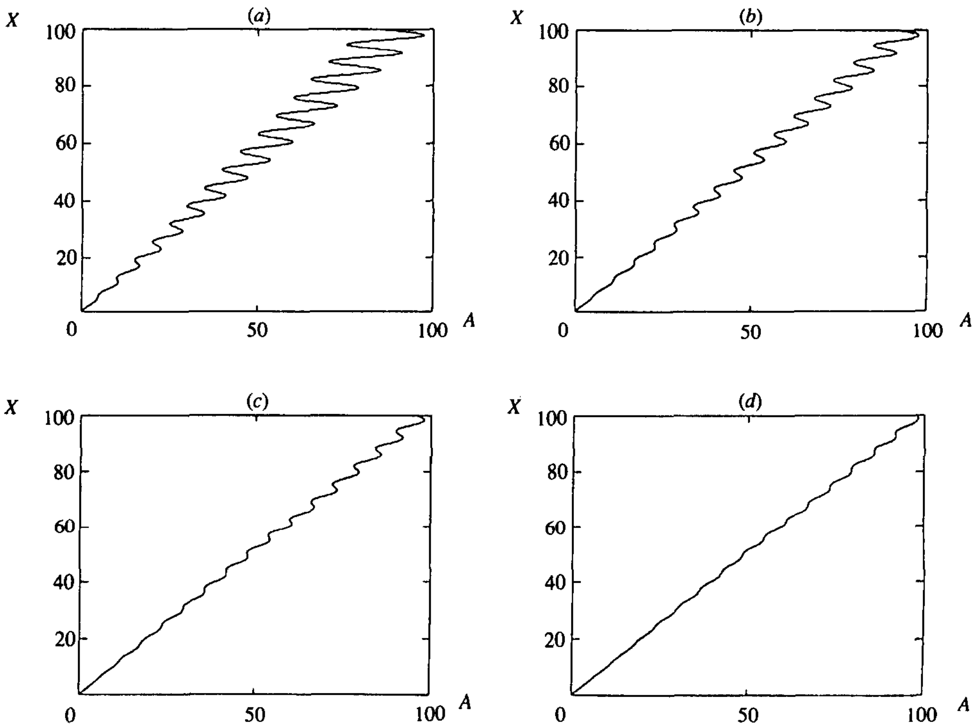


FIGURE 2. *The numerical solution of* (2.1) *and* (2.2); $f(u) = \mu(1+u)(11+10\sin(1+u))$. (*a*) $\Delta t\theta\mu = 0{\cdot}01$; (*b*) $\Delta t\theta\mu = 0{\cdot}005$; (*c*) $\Delta t\theta\mu = 0{\cdot}0025$; (*d*) $\Delta t\theta\mu = 0{\cdot}00125$. $A$ is identified with time, $X$ with the numerical solution of (2.1) and (2.2).

This is typical of nonlinear problems with strong growth. In the remainder of the paper we focus on such problems and examine adaptive time-stepping strategies designed to overcome the multiplicity and non-existence of solutions manifest in example 2.7.

We finish this section with an observation about the explicit case $\theta = 0$. At first glance it might appear that the problems of multiplicity and non-existence arising from case (c) (see theorems 2.3 and 2.4) can be overcome in a straightforward fashion by the use of explicit methods, since (2.3) has a unique solution, for all $n$, if $\theta = 0$. However, the solutions obtained in this case have the undesirable property that in the finite time blow-up case the numerically computed solutions exist for all values of the discrete time $t_n = n\Delta t$. Thus the fixed-step explicit method is totally inadequate at describing highly nonlinear problems, just as its implicit counterpart is.

Figure 4 summarizes the implications of the analysis in this section for the computation of blow-up problems by means of fixed time-stepping routines. The figure shows the true solution (T), which blows up in finite time $t_b = 1$. The curve (I) is a discrete approximation to (T) found by an implicit approximation ($\theta \in (0, 1]$). The solution ceases to exist after finite time; however, this does not occur through blow-up, but by a coalescing of the approximation to the true solution (the lower branch) with a spurious solution introduced by discretization (the upper branch). The curve (E) is an explicit approximation ($\theta = 0$) and the solution exists for all time, even though the true solution ceases to exist at $t = t_b$.

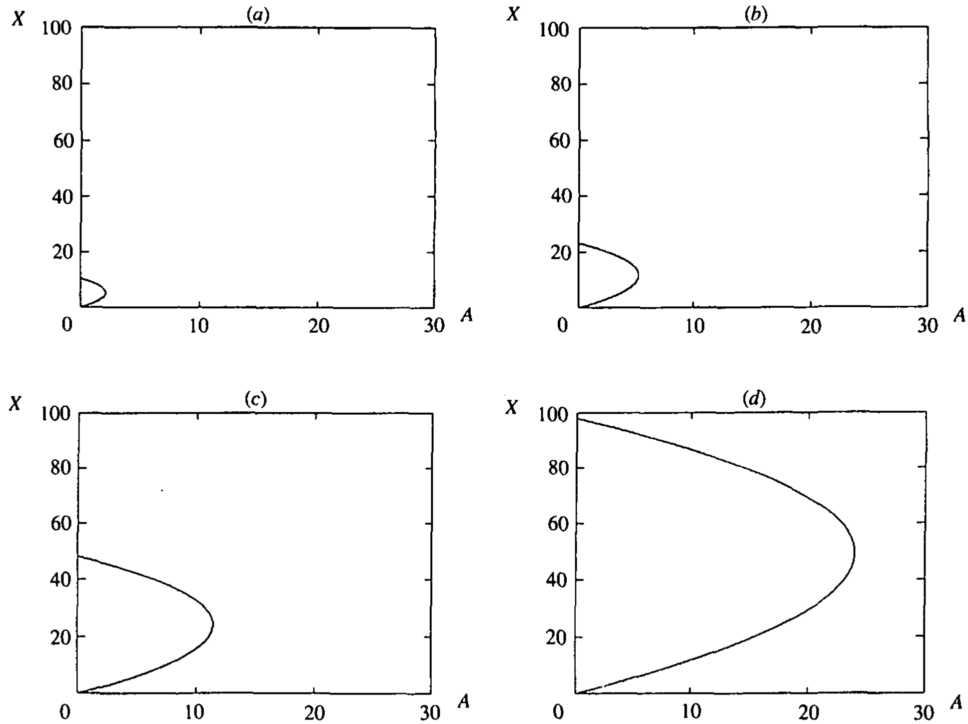


FIGURE 3. *The numerical solution of* (2.1) *and* (2.2); $f(u) = (1+u)^2$. (*a*) $\Delta t\,\theta = 0{\cdot}08$; (*b*) $\Delta t\,\theta = 0{\cdot}04$; (*c*) $\Delta t\,\theta = 0{\cdot}02$; (*d*) $\Delta t\,\theta = 0{\cdot}01$. $A$ is identified with time, $X$ with the numerical solution of (2.1) and (2.2).

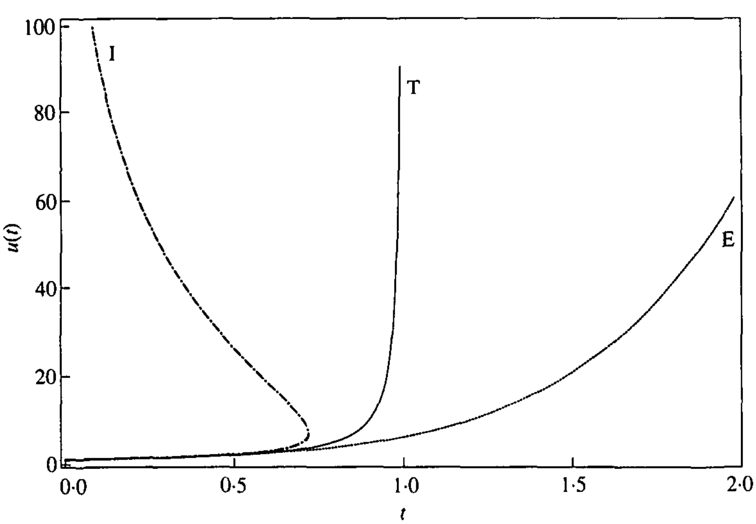


FIGURE 4. Summary of existence theory for fixed step methods for blow-up problems. T = true solution; I = implicit approximation; E = explicit approximation.

## 3 Variable-Step Methods for ODEs

Throughout this section we will study variable step methods for the solutions of equation (2.1), when $f(u)$ is as in case (c); to avoid repetition we will not state this explicitly in the following. In particular we are interested in the case where

$$t_b = \int_0^\infty \frac{\mathrm{d}u}{f(u)} < \infty. \tag{3.1}$$

This is the case for which finite time blow-up occurs, with blow-up time given by $t_b$.

We base our time-stepping strategies on an underlying transformation of the continuous variable $t$. Specifically, we introduce a new time-like variable $s$ with the property that

$$s \to \infty \Leftrightarrow t \to t_b. \tag{3.2}$$

We re-write equation (2.1) as

$$\mathrm{d}u/\mathrm{d}s = H(u)f(u), u(0) = b \tag{3.3}$$

and

$$\mathrm{d}t/\mathrm{d}s = H(u), t(0) = 0. \tag{3.4}$$

We wish to choose $H(u)$ so that the following properties hold. These are properties of $H(u)$ itself, the true solution $u(s)$ and the discrete solution $u_n$, satisfying (3.5) and (3.6).

(I) Property (3.2) holds for the solution $u(s), t(s)$ of (3.3) and (3.4).
(II) For the discretization (3.5) and (3.6), a fixed-stepping strategy in $s$ ($h$ fixed) has a solution $u_{n+1} \in B$ for all $n \geqslant 0$.
(III) The computed solution satisfies $u_n \to \infty$ as $n \to \infty$.
(IV) $H(u) > 0$ for $u \in B$, so that $s(t)$ is a monotonically increasing function, for $t > 0$.
(V) $H(u) \in C^1$ for $u \in B$.

Henceforth we shall assume that properties (IV) and (V) hold. We determine conditions which ensure (I)–(III). For given $f(u)$ satisfying (3.1), there are many different choices of $H(u)$ that will result in the desirable property (I). It is more difficult to ensure (II) and we analyze the discretization (3.5) and (3.6) in some detail to guide our choice for $H(u)$. We shall find that the best choice is determined by the growth of $f(u)$ at infinity. Once existence is established for arbitrary $n > 0$, (III) follows from (IV); see lemma 3.1.

In a recent paper (Griffiths 1987) it is shown that both the error per step and the error per unit step strategies have 'modified equations' interpretations of the form (3.3) and (3.4). Specifically, the former strategy corresponds to $H(u) = |f'(u)f(u)|^{-\frac{1}{2}}$ and the latter to $H(u) = |f'(u)f(u)|^{-1}$. The particular class of problems defined by (3.1) is very special and, rather than using standard error control strategies, we shall take (3.3) and (3.4) to *define* our time-stepping strategy, by taking equally spaced steps in $s$. We shall examine the effect of different choices of the function $H(u)$.

Let $h > 0$ denote a fixed step in the variable $s$. We define the discrete grid by the points $s_n = nh$ and we let $u_n$ and $t_n$ denote our approximations to $u(s_n)$ and $t(s_n)$ respectively. We consider the one-step method defined by

$$u_{n+1} = u_n + hH(u_n)[(1-\theta)f(u_n) + \theta f(u_{n+1})], n > 0 \quad \text{and} \quad u_0 = b \tag{3.5}$$

and

$$t_{n+1} - t_n = hH(u_n), t_0 = 0. \tag{3.6}$$

As in §2, we assume that $0 \leqslant \theta \leqslant 1$ and seek solutions $u_{n+1} \in B$. The method is implicit unless $\theta = 0$. We shall concentrate on the case $\theta \neq 0$. The case $\theta = 0$ is relatively straightforward to analyze since it corresponds to inverting the ODE (2.1) to obtain an ODE for $t(u)$ and applying quadrature on the infinite interval (with the spacing of the step in $u$ determined by the choice of $H(u)$) to determine $t_b$.

The choice of evaluating $H(u)$ in an explicit fashion throughout (3.5) is made for the following reason: our ultimate goal is to gain understanding of time-stepping strategies for PDEs where $H(u)$ will become a functional of the solution (for example, $u$ might be replaced by the maximum norm of $u$ over the spatial variables as in §5) and it is impractical to solve a large *system* of nonlinear equations involving such a functional implicitly since the functional introduces a global coupling of the equations that would destroy any banded or sparse structure arising from the discretization.

We now discuss various possible choices for the function $H(u)$. Hocking *et al.* (1972) made the observation that $O(1)$ relative changes in $u(t)$, the solution of (2.1), evolve on a time-scale proportional to $u/f(u)$ and that therefore the time-step should be chosen to be small on *that time scale*; the particular nonlinearity they consider has leading order behaviour $\propto u^3$ and the time-step $\Delta t$ is adjusted to keep $\Delta t f(u)/u$ beneath some specified tolerance. In terms of the underlying continuous re-scaling this corresponds to choosing $H(u) = u/f(u)$. By (3.3) this means evolving $u(s)$ satisfying

$$\mathrm{d}u/\mathrm{d}s = u,$$

that is, adapting the time-step so that the solution grows exponentially in the new time-like variable $s$. Clearly this re-scaling results in property (I) on $H(u)$.

We will show that $H(u) = u/f(u)$ has the desired properties (I)–(V) when $f(u)$ has polynomial growth at infinity. However, when the nonlinearity has exponential growth the appropriate choice turns out to be $H(u) = 1/f(u)$, since otherwise (II) is violated. We shall also show that *for all choices* of $H(u)$ the solution $u_{n+1}$ of (3.5) is necessarily non-unique, if it exists. Thus adaptive time-stepping strategies cannot avoid the problem of non-uniqueness inherent in fixed-step strategies: see theorem 3.4.

As in §2, we shall analyze the existence and multiplicity of solutions of (3.5) and (3.6) by defining a continuous embedding of the problem. First we must prove a preparatory lemma; note that the lemma shows that property (III) on $H(u)$ holds once (II) is established. Recall that we assume that properties (IV) and (V) hold.

**Lemma 3.1** *If there exists a sequence $u_0, u_1, \ldots, u_N$ satisfying* (3.5) *with elements $u_i \in B$, then*

(i) $u_i > u_{i-1}$ *for* $i = 1, \ldots, N$.
(ii) $u_i \geqslant u_0 + h\bar{f} \sum_{j=0}^{i-1} H(u_j)$.
(iii) *If $N$ can be arbitrarily large, then $u_i \to \infty$ as $i \to \infty$.*

**Proof of Lemma** By (3.5) we have, since $f(u) \geqslant \bar{f} > 0$ and $H(u) > 0$ for $u \in B$,

$$u_i \geqslant u_{i-1} + hH(u_{i-1})\bar{f}.$$

From this it follows that $u_i > u_{i-1}$ and (ii) follows by induction. By (i) we know that $u_i$ form a monotonically increasing sequence and we deduce that, if $N$ can be arbitrarily large, then

$u_i$ either reaches a limit or tends to infinity with $i$. If it were to approach a limit, say $u^*$, then such a limit would have to be in $B$ and, by (3.5), satisfy

$$u^* = u^* + hH(u^*)f(u^*).$$

However, we know that $H(u) > 0$ and $f(u) \geqslant \bar{f} > 0$ for $u \in B$. Thus a finite limit cannot be attained in $B$. Hence (iii) must be true. □

As a consequence of lemma 3.1 we can continuously embed the solutions of (3.5) in the single equation

$$X = u + hH(u)\left((1-\theta)f(u) + \theta f(X)\right), \tag{3.7}$$

where $u$ is a continuously varying parameter in $B$, and increasing $u$ corresponds to increasing $n$ in (3.5). We can examine the question of existence of solutions of (3.5) for large $n$ by examining the existence of solutions of (3.7) as $u \to \infty$. Furthermore, if the solution $u_i$ of (3.5) and (3.6) exists for all $i$, then $u_i \to \infty$ as $i \to \infty$. Thus we can identify the parameter $b \leqslant u < \infty$ with the variable $0 \leqslant s < \infty$ by defining, for $u \in [u_n, u_{n+1})$

$$s = \frac{(u_{n+1} - u)\, s_n + (u - u_n)\, s_{n+1}}{u_{n+1} - u_n}. \tag{3.8}$$

As for the embedding considered in §2, we do not know the numerical values of $u_i$ *a priori*, so the embedding is not defined numerically. However, we deduce that the graph of $X$ versus $u$ will be topologically equivalent to the graph of $X$ (a continuous embedding of $u_i$) versus $s$. We are particularly interested in determining choices for the re-scaling function $H(u)$ which ensure that equation (3.7) has a solution for all $u > b$ with $h$ fixed. This corresponds to choosing $H(u)$ so that the fixed-step strategy in $s$ gives the correct asymptotic behaviour, namely that the solution exists and blows up as $s \to \infty (t \to t_b)$. We examine this in the following theorem, which gives a sufficient condition for property (II) on $H(u)$ to hold. Property (III) then follows from lemma 3.1. We consider only the case $\theta = 1$ since this simplifies the analysis considerably without altering the nature of the conclusions.

**Theorem 3.2** *Let $\theta = 1$. Then, provided that*

$$\limsup_{X \to \infty} H\left(X - \frac{f(X)}{f'(X)}\right) f'(X) < \infty, \tag{3.9}$$

*there exists $h_c > 0$, independent of $u_n$, such that* (3.5) *has a solution $u_{n+1} \in B$ for all $n \geqslant 0$, for any $h < h_c$.*

**Proof of Theorem** From lemma 3.1 we deduce that the question of existence of solutions of (3.5) in $B$ for all $n$ is equivalent to the question of existence of solutions of (3.7) for all $u \in B$. With $\theta = 1$ equation (3.7) becomes

$$X = u + hH(u)f(X). \tag{3.10}$$

For $u = b$ this equation has at least two solutions $X$ in $B$ for $h$ sufficiently small; this is since $f(u)$ is defined by case (c) in §2. To show that, for some fixed $h > 0$, the equation has a solution for arbitrary $u > b$ it is sufficient to show that the solutions which exist for $u = b$ can be continuously extended to all values $u > b$.

Suppose, for the purpose of contradiction, that the solution $X(u)$ cannot be continuously extended to all values of $u \in B$. Then, by the implicit function theorem, there must exist a pair $X$ and $u$, both in $B$, satisfying (3.10) and

$$1 = hH(u)f'(X). \tag{3.11}$$

At such a point,

$$u = X - \frac{f(X)}{f'(X)}. \tag{3.12}$$

However, if (3.9) holds, then it is possible to choose $h$ *independently* of $u \in B$ so that (3.11) cannot be satisfied with $u$ given by (3.12). This is a contradiction. Thus the solution found for $u = b$ can be continuously extended to all $u \in B$. □

The following result uses theorem 3.2 to determine suitable choices for the time-rescaling function $H(u)$, given different assumptions about the growth at infinity of $f(u)$. By 'suitable' we mean a function $H(u)$ for which property (II) holds; property (III) can then be deduced from lemma 3.1. Properties (I, IV and V) can be established independently. The choice made in Hocking *et al.* (1972) is shown to be suitable for the case of polynomial growth at infinity, but a more severe re-scaling is required when the growth is exponential.

**Result 3.3** Consider the case $\theta = 1$.

(i) If $f(u) \propto u^p$ as $u \to \infty$, then the choice $H(u) = u/f(u)$ is a suitable re-scaling function.
(ii) If $f(u) \propto \mathrm{e}^u$ as $u \to \infty$, then the choice $H(u) = 1/f(u)$ is a suitable re-scaling function.

**Justification** The justification involves checking that condition (3.9) holds with the given choices for $H(u)$. This is straightforward. □

Having established conditions under which the fixed-stepping strategy in $s$ yields a solution of (3.5) in $B$ for all $n \geqslant 0$ we now turn our attention to equation (3.6) and the numerical approximation of the blow-up time. The numerical blow-up time is given by

$$t_\infty = \sum_{n=0}^{\infty} hH(u_n), \tag{3.13}$$

assuming that the sum exists. Using equation (3.5) this can be re-written as

$$t_\infty = \sum_{n=0}^{\infty} \frac{u_{n+1} - u_n}{(1-\theta)f(u_n) + \theta f(u_{n+1})}. \tag{3.14}$$

The true blow-up time is given by (3.1). Clearly equation (3.14) forms an approximation to the semi-infinite integral (3.1). The accuracy of the approximation is determined by the spacing of the $u_n$ which is itself determined by the choice of the re-scaling function $H(u)$. In the following result we take two representative choices for $f(u)$ and establish convergence of the approximation (3.14) to the true blow-up time (3.1), under suitable choices of $H(u)$ governed by result 3.3. The results prove convergence of the numerical scheme, (3.5) and (3.6), over arbitrarily long intervals in $s$; note that such results are considerably sharper than those which follow from standard estimates – such estimates involve an error constant which grows exponentially with the independent variable $s$.

**Result 3.4** Consider the case $\theta = 1$.

(i) If $f(u) = u^2$ then, with the choice $H(u) = u/f(u)$, the sum (3.14) converges to the integral (3.1) as $h \to 0$.

(ii) If $f(u) = e^u$ then, with the choice $H(u) = 1/f(u)$, the sum (3.14) converges to the integral (3.1) as $h \to 0$.

**Proof**

(i) With $f(u) = u^2$ the integral (3.1) can be evaluated to give $t_b = 1/b$. Here $H(u) = 1/u$ and so (3.5) gives

$$u_{n+1} - u_n = h\frac{u_{n+1}^2}{u_n}.$$

Note that the solution $u_{n+1}$ is non-unique (see theorem 3.5) but that a solution may be found for all $n$ provided that $h < \frac{1}{4}$ (see result 3.3(i)). The required solution is given by the smaller of the two roots and is

$$u_n = C^n u_0, C = \frac{1-(1-4h)^{\frac{1}{2}}}{2h}.$$

Using (3.13) we calculate that

$$t_\infty = \frac{hC}{u_0(C-1)}.$$

Taking the limit shows that $t_\infty \to t_b$ as $h \to 0$.

(ii) With $f(u) = e^u$ the integral (3.1) can be evaluated to give $t_b = e^{-b}$. Here $H(u) = e^{-u}$ and so (3.5) gives

$$u_{n+1} - u_n = h\, e^{u_{n+1}-u_n}.$$

As in part (i) the solution is non-unique, but a solution exists for all $n$ provided that $h < e^{-1}$ (see result 3.3(ii)). The required solution is given by

$$u_n = u_0 + nY = b + nY,$$

where $Y$ is the smaller of the two roots of the equation $Y = h\,e^Y$. Using (3.13) we calculate that

$$t_\infty = \frac{h\,e^Y}{e^b(e^Y-1)}.$$

Thus $t_\infty = Y/e^b(e^Y-1)$ and since $Y \to 0$ as $h \to 0$, we find that $t_\infty \to t_b$ as $h \to 0$. □

In this section we have introduced a new time-like variable $s$ with the property that the finite-time blow-up point $t = t_b$ is transformed to $s = \infty$. The results show that, if the re-scaling function $H(u)$ can be chosen in such a way that (3.9) is satisfied, then a fixed step strategy in $s$ will have a solution for all values of the discrete time, and that there is a precise sense in which this solution trajectory is a continuous extension of the initial value. In addition, the discrete solution tends to infinity as discrete time tends to infinity. Furthermore, we have shown that in two important special cases, the numerical approximation of the blow-up time converges to the true blow-up time as the discretization parameter $h$ tends to zero.

We complete this section with the following cautionary result. The result shows that, even with a careful choice of time-stepping strategy guided by theorem 3.2, numerical methods for blow-up problems introduce a non-uniqueness which is not present in the underlying initial-value problem. Thus particular care is required in the choice of nonlinear algebraic solver to ensure convergence to the correct solution. As before we take $\theta = 1$ since this choice simplifies the analysis without modifying the results.

**Theorem 3.5** *Let $\theta = 1$. Consider a time-stepping strategy chosen with $H(u)$ satisfying* (3.9). *Then there is either an even number of solutions to* (3.5) *in $B$, or no solution in $B$.*

**Proof** It is sufficient to show that (3.10) has either an even number of solutions in $B$ or no solution in $B$, for any value of $u > b$. We use the fact that any solution $X \in B$ of (3.10) must satisfy $X > u$. Thus, for $u \in B$, no solution $X$ of (3.10) can cross the boundary of $B$ as $u$ varies.

Let
$$G(X, u) = hH(u)f(X) + u - X.$$

Then $G(b, b) > 0$ and $G(\infty, b) > 0$, since $f(u)$ is as in case (c), defined in §2 and $H(0) > 0$. Thus, for $u = b$, (3.10) has an either even number of solutions in $B$ or no solution at all in $B$. All of the solutions found for $u = b$ satisfy $X > b$. Since condition (3.9) is satisfied we deduce from the implicit function theorem that the solutions found for $u = b$ remain in $B$ and are continuously extendable to all values of $u > b$; thus the result follows. □

## 4 Application to a Degenerate Parabolic Equation; Theoretical Results

In this section we summarize theoretical results about a degenerate parabolic PDE arising as a qualitative model of a fluid with temperature-dependent vicosity. We emphasize that the equation we study only reflects the qualitative features of the full model: it is one of the simplest parabolic equations in which a degeneracy and a nonlinear source term are present. These theoretical results are presented to motivate the numerical scheme described in the following section.

The model is derived in Ockendon (1979) and the simplifications leading to the equations (4.1)–(4.3) are discussed in Lacey (1984). The problem is to find $u(x, t) \in C^{2,1}((0, 1) \times (0, \tau))$ satisfying, for $q > 0$,

$$x^q u_t = u_{xx} + f(u), (x, t) \in (0, 1) \times (0, \tau), \tag{4.1}$$

$$u(0, t) = u(1, t) = 0, 0 < t < \tau, \tag{4.2}$$

$$u(x, 0) = u_0(x), x \in (0, 1). \tag{4.3}$$

The solution $u(x, t)$ can cease to exist after a finite time $t_b$ at which it becomes infinite. We prove this in theorem 4.1, which is a generalization of proposition 3.1 in Floater (1989). The interesting feature of the blow-up which distinguishes it from non-degenerate problems is that it is possible for the blow-up point to be *at the boundary* $x = 0$; the peak temperature of $u(x, t)$ may occur at a sequence of points which approach arbitrarily closely to $x = 0$ as the blow-up time is approached. For the nonlinearity $f(u) = u^p$, with $1 < p \leqslant 2$ and $q = 1$ this is proved in Floater (1989) and the results are summarized in theorem 4.2.

In theorem 4.3 we derive a condition on the formation of interior zeros of $u_x(x, t)$ as time evolves. This condition is helpful in our numerical simulations, which are based on tracking the peak value of $u$. It appears difficult to show that if $u_0$ has only one critical point (where $u_{0x} = 0$) then $u(x, t)$ has only one critical point for any $t > 0$. However, under the assumption that $u_0''+f(u_0) \geqslant 0$, we can prove that no new peak forms to the right of the initial one.

Having established that blow-up *can* occur at the boundary, an important question is to determine *when* it actually does occur there. As theorem 4.2 shows, this depends on two factors: the initial condition and the relationship between the strength of the source term and the effect of degeneracy. The effect of the initial data is intuitively obvious, since if $u_0(x)$ attains its maximum near $x = 0$, it has more chance of blowing up at $x = 0$. The balance between the source term and the degeneracy can be interpreted as follows: the stronger the degeneracy, the more rapidly the peak is pulled towards $x = 0$; on the other hand, the stronger the source term the more quickly the solution blows up. The bound on $p$ for blow-up at the boundary is determined by this balance: $p > 1$ ensures that blow-up occurs, whilst $p \leqslant q+1$ ensures that the solution does not blow-up before the peak reaches the boundary. Numerically we are interested in testing the sharpness of the upper bound on $p$, together with testing the necessity of the condition on the initial data.

**Theorem 4.1** *Let $\phi(x) \geqslant 0$ be the principal eigenfunction satisfying*

$$\phi_{xx}+\lambda x^q \phi = 0, \phi(0) = \phi(1) = 0,$$

*with corresponding eigenvalue $\lambda$. Take $\phi$ to be normalized so that $\int_0^1 x^q \phi \, dx = 1$. Define $U(t) = \int_0^1 x^q \phi(x) u(x,t) \, dx$. Assume that*

(i) *$f(u)$ is a strictly positive, convex function.*
(ii) *$f(U)-\lambda U > 0$, for all $U \geqslant U(0)$.*
(iii) *$\int_{U(0)}^{\infty} dU/[f(U)-\lambda U] = t^* < \infty$.*

*Then the solution $u(x,t)$ of* (4.1)–(4.3) *blows up in finite time $t_b < t^*$.*

**Proof** Multiply (4.1) by $\phi(x)$ and integrate over $x \in (0,1)$, using parts twice on the second term. This gives

$$\int_0^1 x^q \phi u_t \, dx = \int_0^1 \phi_{xx} u \, dx + \int_0^1 \phi f(u) \, dx.$$

Using the defining equation for $\phi$ we obtain

$$\begin{aligned} \frac{dU}{dt} &= -\lambda U + \int_0^1 \phi f(u) \, dx, \\ &\geqslant -\lambda U + \int_0^1 x^q \phi f(u) \, dx. \end{aligned}$$

By the convexity of $f(u)$ we may apply Jensen's inequality (Gradsteyn & Ryzhik 1981; 12.411) to obtain

$$\frac{dU}{dt} \geqslant -\lambda U + f(U).$$

Integrating this differential inequality, using (ii) and (iii), establishes that $U(t)$ becomes unbounded in finite time. Hence $u(x,t)$ must become unbounded at, at least, one point. This completes the proof. □

**Theorem 4.2**

(i) *There exists a unique classical solution of* (4.1)–(4.3) *which either exists for all* $0 \leqslant t < \infty$ *or becomes unbounded in finite time* $t_b < \infty$.

(ii) *Suppose that*

$$\left[\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{u_0(x)}{x}\right) \leqslant 0\right]$$

*for all* $x \in (0, 1)$ *and that* $f(u) = u^p$ *for any* $p$ *such that* $1 < p \leqslant q+1$. *If* $u(x, t)$ *blows up in finite time, then the only blow-up point is* $x = 0$.

**Proof** Part (i) is proved in Floater (1989) for $f(u) = u^p$ and can be easily adapted to more general $f(u)$ – see also Floater (1988). Part (ii) is proved in Floated (1989).

In theorem 4.3 we use the following notation, which we also employ in §5. Suppose that $u_{0x}(x) > 0$ for $0 < x < a$ and $u_{0x}(x) < 0$ for $a < x < 1$. Define $s(t)$ to be the continuous curve such that $s(0) = a$ and $u_x(s(t), t) = 0$.

**Theorem 4.3** *Suppose that* $u_0'' + f(u_0) \geqslant 0$. *Then, for all* $t > 0$ *and* $x > s(t)$, $u_x(x, t) < 0$.

**Proof** Set $w(x, t) = u_x(x, t)$ in the region $S = \{(x, t): t > 0, s(t) < x < 1\}$. Differentiating (4.1) gives

$$x^q w_t - w_{xx} - f'(u)\, w = -q x^{q-1} u_t < 0.$$

The fact that $u_t > 0$ follows from the maximum principle applied to $u_t(x, t)$; see Floater (1989). At the boundaries of $S$ we have $w(s(t), t) = 0$, $w(1, t) < 0$ (by the strong maximum principle applied to $u(x, t)$) and $w(x, 0) < 0$ for $a < x < 1$. Hence, by the maximum principle, $w < 0$ in $S$, as required. □

## 5 Application to a Degenerate Parabolic Equation; Numerical Method and Results

In this section we decribe a numerical method for the solution of (4.1)–(4.3). Theorems 4.1 and 4.2 indicate that equations (4.1)–(4.3) form a very delicate problem since not only does the solution blow up, but it is possible for the peak value to approach arbitrarily close to the boundary $x = 0$. By virtue of the boundary condition (4.2), this suggests that a boundary layer forms at $x = 0$ with thickness which becomes arbitrarily small as the blow-up time is approached. As discussed in the previous section, an important question is to determine the balances between the strength of nonlinearity $f(u)$ and the degeneracy $x^q$ which determine when blow-up actually occurs at the boundary.

We propose treating equations (4.1)–(4.3) as a moving boundary problem, with the peak value of $u(x, t)$ determining the position of the boundary. Thus we introduce a peak-tracking numerical method. This decision is made for two reasons:

(i) The main theoretical interest in equations (4.1)–(4.3) is in the possibility of blow-up occurring at the boundary $x = 0$, since it is this feature that distinguishes it from non-degenerate problems. A fixed grid numerical method cannot track the position of the peak value close to the boundary $x = 0$ since it is naturally limited to placing the peak at least one grid point from the boundary, in addition to losing important spatial resolution between the peak value of $u$ and the boundary at $x = 0$. By re-formulating the problem as a moving boundary problem for the position of the peak, and using a suitable co-ordinate transformation, we essentially introduce an automatic mesh-refinement that places a reasonable number of mesh points between the boundary $x = 0$ and the position of the peak.

(ii) The analysis in §§2 and 3 indicates the care required in choosing a time-stepping strategy, even for the scalar ODE (2.1). For the PDE we propose the use of time-stepping strategies based on the supremum norm of $u(x, t)$; thus it is important to have an accurate knowledge of the peak position and value. Again this suggests that tracking the position of the peak is important.

We now describe the formulation of (4.1)–(4.3) as a moving boundary problem. In the following we shall use the variable $s(t)$ determined by the condition

$$u_x(s(t), t) = 0 \tag{5.1}$$

and assume that the point $x = s(t)$ defines a local maximum in $x$ for the function $u(x, t)$. As stated, $s(t)$ is not uniquely defined in general, since the solution $u(x, t)$ of (4.1)–(4.3) may possess several maxima or minima. However, we shall mainly consider classes of initial data for which $s(t)$ *is* uniquely defined. Note that theorem 4.3 shows that any new maxima must form in $(0, s(t))$. By monitoring the solution in this region we can determine numerically when this occurs and, if desired, re-start the numerical method and track the position of the new peak which has formed nearer the boundary $x = 0$.

The function $s(t)$ determines an internal moving boundary for the solution of (4.1)–(4.3) and we consider its determination as part of the problem. The extra condition that we shall use to determine $s(t)$ numerically is that $u(x, t)$ be continuous at $x = s(t)$. Thus we can state the moving boundary problem as follows: find $u(x, t) \in C^{2,1}((0, 1) \times (0, \tau))$ and $s(t) \in C^1(0, \tau)$ satisfying

$$x^q u_t = u_{xx} + f(u), (x, t) \in (0, s(t)) \times (0, \tau), \tag{5.2}$$

$$u(0, t) = 0, u_x(s(t), t) = 0, 0 < t < \tau, \tag{5.3}$$

$$x^q u_t = u_{xx} + f(u), (x, t) \in (s(t), 1) \times (0, \tau), \tag{5.4}$$

$$u_x(s(t), t) = 0, u(1, t) = 0, 0 < t < \tau, \tag{5.5}$$

$$u(x, t) \text{ continuous at } x = s(t), \tag{5.6}$$

together with a suitable initial condition on $u(x, 0)$, which will determine $s(0)$.

We shall use a numerical method for the solution of (5.2)–(5.6) based on a co-ordinate transformation. This idea was introduced for the Stefan problem in Landau (1950); its application to a problem with an internal moving boundary is described in Stuart (1985). The essence of the transformation is this: we introduce a co-ordinate change which maps $0 < x < s(t)$ onto $0 < X < 1$ and which maps $s(t) < x(t) < 1$ onto $1 < X < 2$. The use of a fixed spatial grid in the variable $X$ corresponds to a moving mesh in the variable $x$. Furthermore, we can guarantee as much spatial resolution as we desire between the boundary $x = 0$ and the position of the maximum $x = s(t)$, by use of a suitable number of grid points in $0 < X < 1$. Thus arbitrarily thin boundary layers, which form in the cases when blow-up occurs at the boundary ($s(t) \to 0$), can be resolved.

We introduce the new variable $X$ defined by

$$X = \frac{x}{s(t)}, 0 < x < s(t) \quad \text{and} \quad X = \frac{x+1-2s(t)}{1-s(t)}, s(t) < x < 1. \tag{5.7}$$

We also define $T = t$ and introduce

$$U(X,T) = u(x,t), 0 < X < 1 \quad \text{and} \quad V(X,T) = u(x,t), 1 < X < 2. \tag{5.8}$$

Under (5.7) and (5.8) equations (5.2)–(5.6) give the following problem: find

$$U(X,T) \in C^{2,1}((0,1)\times(0,\tau)), V(X,T) \in C^{2,1}((1,2)\times(0,\tau)) \quad \text{and} \quad s(T) \in C^1(0,\tau)$$

satisfying, for $\dot{s} = \mathrm{d}s/\mathrm{d}T$,

$$X^q s^{2+q} U_T = U_{XX} + X^{q+1} s^{q+1} \dot{s} U_X + s^2 f(U), \quad (X,T) \in (0,1)\times(0,\tau), \tag{5.9}$$

$$U(0,T) = U_X(1,T) = 0, \tag{5.10}$$

$$((1-s)X+2s-1)^q (1-s)^2 V_T = V_{XX} \\ + ((1-s)X+2s-1)^q (2-X)(1-s)\dot{s} V_X + (1-s)^2 f(V), (X,T) \in (1,2)\times(0,\tau), \tag{5.11}$$

$$V_X(1,T) = V(2,T) = 0, \tag{5.12}$$

$$U(1,T) = V(1,T), \tag{5.13}$$

and suitable initial conditions on $U(X,0)$, $V(X,0)$ and $s(0)$.

We now describe the numerical method that we use for the determination of $U$, $V$ and $s$. First we descretize equations (5.9) and (5.10) for $U(X,T)$ and equations (5.11) and (5.12) for $V(X,T)$ as if $s(T)$ were a known function at the grid points $T = n\,\Delta T$; thus we may use a standard difference approximation to $\dot{s}$. Secondly we employ the condition (5.13) to determine $s(T)$.

### (i) Introduction of discrete variables

Let $\Delta X$ and $\Delta T_n$ denote step-sizes in the $X$ and $T$ directions respectively. We assume that $J\Delta X = 1$, for some integer $J$. We shall fix $\Delta X$ but vary the time-step. Our choice of time-stepping algorithm is motivated by the discussion in §3. Let $U_j^n$, $V_j^n$ and $s^n$ denote our numerical approximations, defined as follows:

$$U_j^n \approx U(j\Delta X, T_n), j = 0, \ldots, J, \tag{5.14}$$

$$V_j^n \approx V(1+j\Delta X, T_n), j = 0, \ldots, J, \tag{5.15}$$

$$s^n \approx s(T_n), \tag{5.16}$$

where

$$T_n = \sum_{j=0}^{n-1} \Delta T_j. \tag{5.17}$$

### (ii) Choice of time-step

The time-step is chosen adaptively in a manner analogous to that used for the ODE case described in §3. Motivated by (3.6) we set, for $\|U_j^n\|_\infty = \sup_j |U_j^n|$,

$$\Delta T_n = hH(\|U_j^n\|_\infty), \tag{5.18}$$

for some suitable rescaling function $H(u)$; guided by theorem 3.2 and result 3.3 we shall choose $H(u)$ carefully, depending on the growth of $f(u)$ at infinity. Note that, for solutions $u(x,t)$ with a single maximum, we have $\|U_j^n\|_\infty = U_J^n$. This is the class of solutions with which we compute.

### (iii) Time-stepping algorithm

Assuming that $s(T)$ is known at the grid points $T = T_N$, we can write down standard finite difference discretizations of equations (5.9)–(5.12). We choose a fully implicit (in time) discretization of all terms involving derivatives, but an explicit evaluation of the nonlinear source terms involving the function $f$. The implicit discretization of the differential operators is chosen because it is the only scheme known to have a maximum principle when applied to the linear heat equation (with unrestricted values of $\Delta T_n/\Delta X^2$) (Richtmyer & Morton 1967), and we consider this a valuable property to preserve; this is especially so since we are interested in solutions with a unique point at which $u_x = 0$. The explicit evaluation of the source terms is chosen since we have shown in §§2 and 3 that implicit evaluation of the source term can lead to multiple solutions in the time-stepping. The second order spatial differential operators are replaced by the standard three point approximation, and the first order spatial differential operators are replaced by centred approximations. We introduce the usual artificial points $U_{J+1}^{n+1}$ and $V_{-1}^{n+1}$ to deal with the zero gradient boundary conditions at $X = 1$.

Observe that $U_0^{n+1} = V_J^{n+1} = 0$, from the boundary conditions. Let $\underline{U} = (U_1^{n+1}, \ldots, U_J^{n+1})^T$ and $\underline{V} = (V_0^{n+1}, \ldots, V_{J-1}^{n+1})^T$. Then, assuming $s^{n+1}$ to be known, we have two systems of $J$ linear, tridiagonal equations, one for $\underline{U}$ and the other for $\underline{V}$. The equations come from the discretization of equations (5.9)–(5.10) and (5.11) and (5.12), respectively. Each system of equations depends nonlinearly on the parameter $s^{n+1}$. Thus the two systems can be written as

$$A(s^{n+1})\,\underline{U} = B(s^{n+1})\,\underline{V} = 0, \tag{5.19}$$

where $A$ and $B$ are tri-diagonal matrices depending nonlinearly on $s^{n+1}$.

### (iv) Determination of $s$

To determine $s^{n+1}$ it is necessary to impose condition (5.13) which requires

$$U_J^{n+1} = V_0^{n+1}. \tag{5.20}$$

Thus each time-step of the numerical method involves solving equations (5.19) and (5.20) for the unknowns $\underline{U}$, $\underline{V}$ and $s^{n+1}$.

The fact that equations (5.19) are linear in $\underline{U}$ and $\underline{V}$ suggests that we employ an iterative procedure to solve (5.19) and (5.20) for $s^{n+1}$. Newton iteration is the obvious choice for such a scheme since the value of $s$ at the previous time-step, $s^n$ provides a good initial guess; however, we wish to minimize the number of matrix inversions, and so we choose secant iteration as being a reasonable compromize between rate of convergence and ease of implementation. We have found this iteration scheme to be very satisfactory in practice, subject to a careful choice of the two starting values for the iteration, which we now discuss.

### (v) Starting values for the secant iteration

The secant iteration to determine $s^{n+1}$ requires two starting values. We take these to be the value of $s^n$ from the previous time-step, and an estimate of $s^{n+1}$ calculated from an approximation of the rate of change of $s$ with respect to $t$. Specifically, we choose the initial approximations

$$s^n \quad \text{and} \quad s^n + \frac{\Delta T_n}{\Delta T_{n-1}}(s^n - s^{n-1}).$$

This completes the description of the numerical method. □

We now present results from the numerical solution of (4.1) and (4.3) using the method described above. In all the examples the discretization parameters are set at $\Delta X = 0.01$ and $h = 0.0004$.

**Example 5.1** In this example we take $f(u) = 15u^2$ and $u_0(x) = 4x(1-x)$. The re-scaling function $H(u)$ in (5.18) is chosen so that $H(u) \propto u/f(u)$; see result 3.3. By theorem 4.1 the solutions blows up in finite time. Furthermore, by theorem 4.2(ii), the peak value of $u(x, t)$ tends to $x = 0$ as the blow-up time is approached. The numerical method handles this successfully. Figure 5 shows a graph of the position of the peak, $s(t)$, against $t$. Notice that the peak is tracked into the origin. Figure 6 shows the value of $1/u(s(t), t)$ against time and establishes that blow-up occurs for $t \approx 0{\cdot}06$. Figure 7 shows successive profiles of the solution $u(x, t)$ against $x$ at intervals of 50 time-steps; the solutions have been scaled to have maximum values of unity. Notice how the peak moves towards the boundary $x = 0$ as time progresses.

**Example 5.2** In this example we take $f(u) = 4e^u$ and $u_0(x) = 4x(1-x)$. The re-scaling function $H(u)$ in (5.18) is chosen so that $H(u) \propto 1/f(u)$; see result 3.3. By theorem 4.1 the solution blows up in finite time. However, since $e^u \gg u^p$ for large $u$ for any $p > 0$, we suspect that blow-up does not occur at the boundary $x = 0$. (See theorem 4.2(ii).) This is borne out

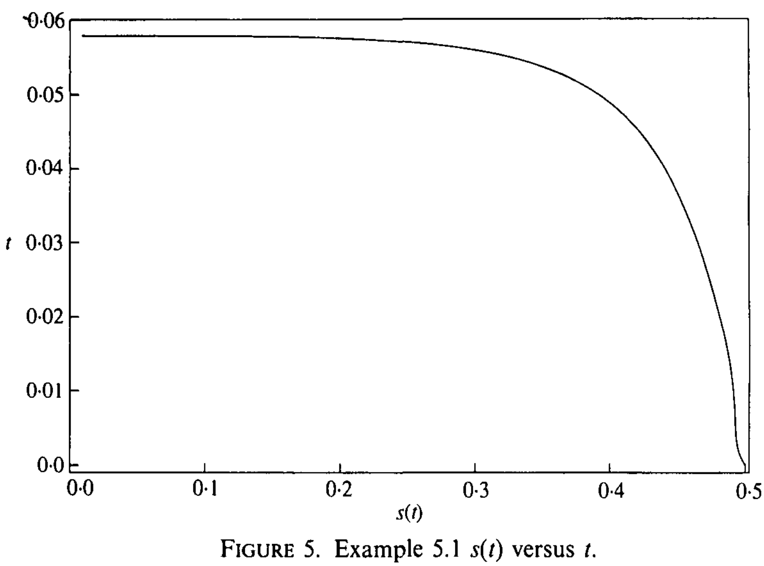


FIGURE 5. Example 5.1 $s(t)$ versus $t$.

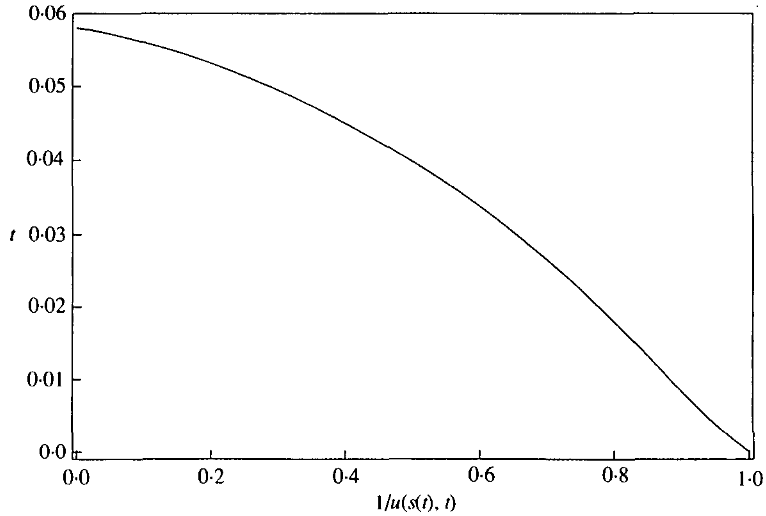


FIGURE 6. Example 5.1 $1/u(s(t), t)$ versus $t$.

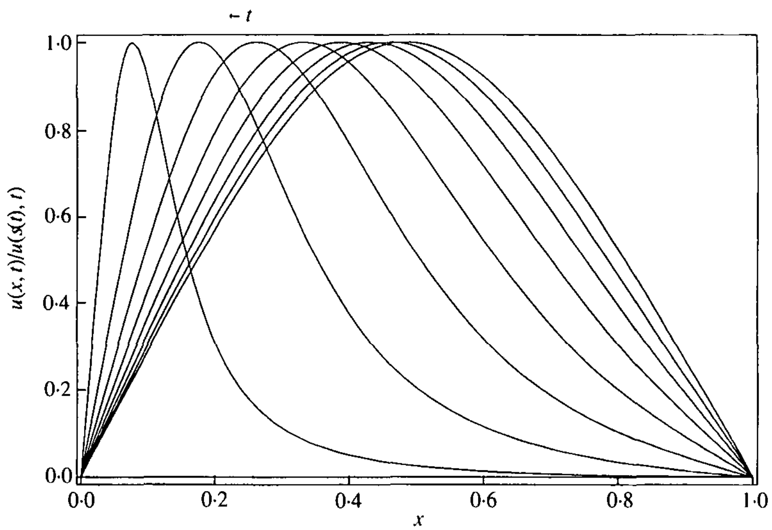


FIGURE 7. Example 5.1 $u(x, t)/u(s(t), t)$ versus $x$.

by the numerical evidence. In figure 8 we plot the peak value $u(s(t), t)$ against $s(t)$ and it is clear that the limiting value of $s(t)$ as blow-up is approached ($u(s(t), t) \to \infty$) is bounded away from $x = 0$.

**Example 5.3** In this example we take $f(u) = 25u^{\frac{3}{2}}$ and $u_0(x) = 4x(1-x)$. The rescaling function $H(u)$ in (5.18) is chosen so that $H(u) \propto u/f(u)$. As in example 5.1, the solution blows up at the boundary. Figure 9 shows the profile of $u(x, t)$ against $x$, close to the blow-up time.

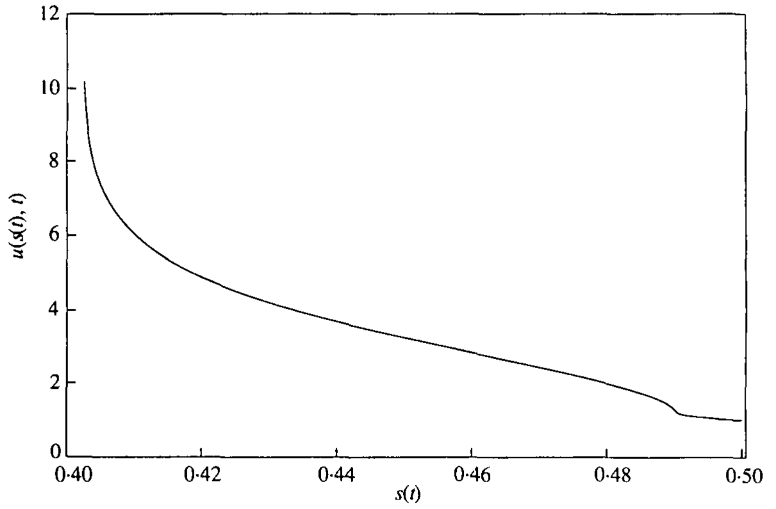


FIGURE 8. Example 5.2 $u(s(t), t)$ versus $s(t)$.

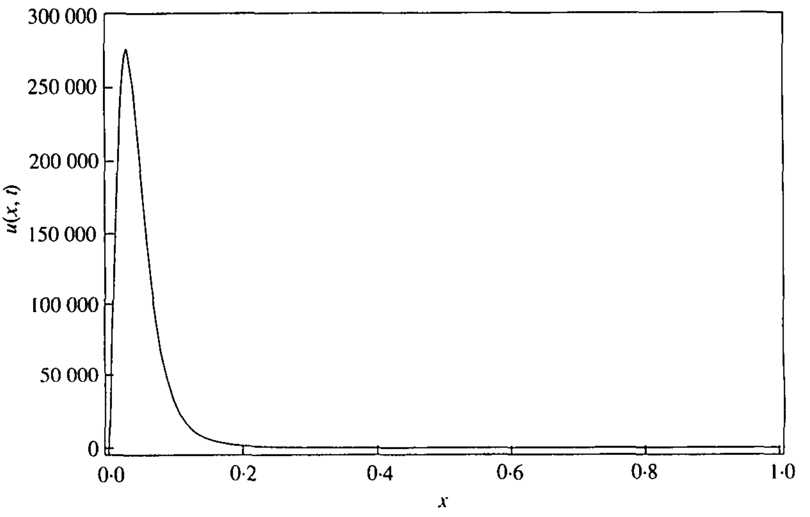


FIGURE 9. Example 5.3 $u(x, t)$ versus $x$.

## 6 Conclusions

In this paper we have examined the asymptotics of numerical methods for initial value problems which develop singularities in finite time. We have analyzed the problem for a scalar ODE in detail and applied the ideas to a specific PDE arising from the study of a fluid with temperature-dependent viscosity.

First we examined fixed-step methods for the scalar ODE and showed that both explicit and implicit methods are wholly inadequate in reproducing the asymptotics of the differential equation: explicit methods have a solution which exists for all values of discrete time, thus missing the blow-up completely; implicit methods have multiple solutions in discrete time and the numerical solution ceases to exist not by blow-up, but by the coalescing of the true trajectory with a spurious trajectory at a particular value of discrete time. Figure 4 gives a summary of these results; the details are given in §2.

Secondly we examined variable-step methods for the scalar ODE. The time-stepping strategies we examined are based on a re-scaling of the time variable in the underlying differential equation, and contact was made with a recent 'modified equations' analysis of the dynamics of multi-step methods. We established criteria on the time re-scaling function under which the numerical solution exists and approaches infinity as the blow-up time is approached; see theorem 3.2 and 3.1. We also established that the discrete blow-up time converges to the true blow-up time, as the discretization parameter tends to zero, in a number of representative cases; see result 3.4. However, it was shown that the problem of multiplicity of solutions in discrete time is *not avoided* by using variable time-stepping strategies; see theorem 3.5. Thus extreme care is required in the choice of algebraic solver if implicit methods are used to solve initial value problems which exhibit finite time singularities. Although the analysis in §3 applies only to scalar ODEs, we believe that theorem 3.2 is useful in guiding the choice of time-stepping strategies for PDEs whch develop singularities in finite time.

Finally we applied our ideas to a PDE. We described a peak-tracking strategy and based the adaptive time-stepping on this peak value. The problem chosen is particularly delicate since an arbitrarily thin and high boundary layer can develop between a boundary at which $u = 0$ and the peak value of the solution, as the blow-up time is approached. The numerical method was shown to cope with this difficulty successfully, and the adaptive time-stepping, based on the analysis of §3, enabled us to solve the problem accurately close to the blow-up time. We believe that the idea of peak-tracking is useful for the computation of many PDEs whose solutions blow up in finite time and the co-ordinate transformation approach used here is easily adapted to other problems.

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