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The Numerical Study of Blowup with Application to a Nonlinear Schrödinger Equation

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DEDICATED TO PROFESSOR A. R. MITCHELL WHO, AS ON MANY OTHER OCCASIONS, PROVIDED THE INITIAL SPUR

We discuss the use of numerical methods in the study of the solutions of evolution problems which exhibit finite-time unbounded growth. We first examine a naive approach in which the growth rate of the numerical solution is accepted as an approximation of the true growth rate. As we shall demonstrate for a radial nonlinear Schrödinger equation, this approach is inadequate since different discretizations exhibit different growth rates. The spurious behaviour of discretizations in the neighbourhood of the singularity is discussed. A reliable procedure for the estimation of the blowup parameters is considered which eliminates the discrepancies between different numerical methods.

1. INTRODUCTION

In recent years, blowup phenomena have become a major topic in the theory of nonlinear evolution equations (cf. [1, 20, 23] and the many references therein). Since the early work of Fujita [8] on semilinear parabolic equations, the interest in problems which feature blowup has now spread to such diverse fields as fluid dynamics [4], combustion [6], plasma physics [12], and nonlinear optics [16].

One of the dominant themes of blowup theory concerns the behaviour of the solution, say u, or its derivatives near the blowup time $t_{\max}$. It is often conjectured that the growth of u near the singularity can be described by

$$\max_x |u(x, t)| \propto (t_{\max} - t)^{-\alpha},$$

in which case the values of α and $t_{\max}$ are naturally of interest. (Needless to say, one could also envisage more sophisticated functional relationships involving other unknown parameters.) Unfortunately, due to the inadequacy of the mathematical tools available at present, the determination of those parameters must often rely on a mixture of heuristic reasoning and numerical evidence.

Since the convergence properties of any numerical scheme depend on the good behaviour of u and its derivatives, it is clear that the calculation of $t_{\max}$ and α poses some difficulty. As $t_{\max}$ is approached, the discretization of the original problem results in a distortion of the blowup mechanism and, unless care is exercised, the numerical results can be misleading.

This paper has two main objectives: first, to offer a simple general procedure which should ensure that reliable conclusions can be drawn when numerical methods are used in the investigation of blowup phenomena. Second, to provide insight into the behaviour of discretizations near $t_{\max}$. While the method considered here can cater for large classes of problems, we have deemed it best to concentrate on the cubic Schrödinger equation (henceforth, CSE). This is used as a model equation which encapsulates the main features of the issues which will be discussed. In Section 2, the physical origin and mathematical theory of the equation are discussed with particular emphasis on results pertaining to blowup. As we shall see, several conflicting conjectures have been made as to the correct value of α. In Section 3, we describe two different discretizations of the CSE. In Section 4, we carry out a computer experiment which illustrates the pitfalls of a naive approach to the calculation of the blowup parameters. With this approach, different

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discretizations yield different values of α. In Section 5, we consider a simple procedure to obtain reliable results in the presence of a singularity. In Section 6, we discuss the significance of the results in the broader context of ODEs and PDEs featuring finite-time blowup. Finally, Section 7 is devoted to concluding remarks.

2. THE CUBIC SCHRÖDINGER EQUATION

If we assume radial symmetry, the CSE in $(N+1)$-dimensional space–time becomes

$$i\frac{\partial u}{\partial t}+\frac{\partial^2 u}{\partial r^2}+\frac{N-1}{r}\frac{\partial u}{\partial r}+|u|^2 u=0, \tag{2.1}$$

where u is complex-valued, $t \geqslant 0$, $r=(x_1^2+\cdots+x_N^2)^{1/2} \geqslant 0$, and $i^2=-1$.

The case $N=2$ arises in nonlinear optics: u is then the envelope of an electromagnetic wave propagating along the t axis in a three-dimensional optical medium. The cubic term comes about by assuming that the refractive index increases with the square of the intensity of the beam [16]. In the case $N=3$, the equation has been derived in the context of plasma physics: u is then the envelope of a Langmuir wave. The appearance of a cubic term is due to the ponderomotive force [33, 12].

The mathematical theory of the initial-value problem for (2.1) relies to a considerable extent on two invariance properties satisfied by the solution [3, 31]:

$$\int_0^\infty |u(r,t)|^2 r^{N-1}\,dr \equiv P=\text{const} \quad \text{for} \quad t \geqslant 0; \tag{2.2}$$

$$\int_0^\infty \left\{\left|\frac{\partial u}{\partial r}(r,t)\right|-\frac{1}{2}|u(r,t)|^4\right\} r^{N-1}\,dr \equiv E=\text{const} \quad \text{for} \quad t \geqslant 0. \tag{2.3}$$

When $N=1$, the constancy of P and E ensures the boundedness of the solution. When $N>1$ and $E<0$, however, it has been proved [33] that the solution u must cease to exist at some finite value of $t=t_{\max}$. More precisely,

$$\lim_{t \to t_{\max}} \|u(t)\|_{L^\infty(\Omega)}=+\infty. \tag{2.4}$$

Figure 1 illustrates the development of the singularity for a gaussian initial condition of the type

$$u(r,0)=ae^{-(r/l)^2} \tag{2.5}$$

with $N=2$, $a=4$, and $l=1$. As $t \to t_{\max}$, the solution becomes unbounded at the origin.

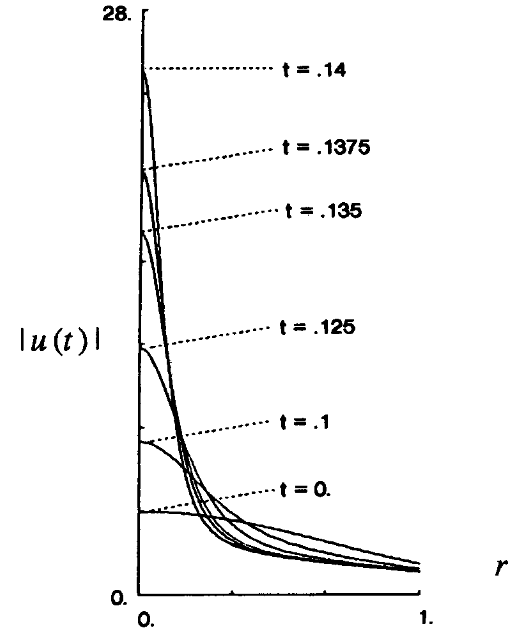

FIG. 1. Example of self-similar blowup in the case $N=2$.

In the case $N=2$, this blowup of the solutions corresponds to a physical phenomenon known as self-focusing. It has indeed been observed in laboratory experiments that laser beams propagating for some distance in optical materials may rapidly become so intense as to damage the material [16]. In the case $N=3$, Eq. (2.4) has a useful interpretation in plasma physics and describes the nonlinear stage of Langmuir turbulence [33]. Thus, while the assumptions upon which the mathematical model (2.1) is based cease to be valid as t approaches $t_{\max}$, the behaviour of the solution u near the singularity is a matter of great practical interest in both plasma physics and nonlinear optics.

Many authors have conjectured that the singular solutions of Eq. (2.1) exhibit a self-similar structure as t approaches $t_{\max}$ [23]; i.e.,

$$\lim_{t \to t_{\max}} |u(r,t)| = \lim_{t \to t_{\max}} \gamma(t)\,\Phi(\gamma(t)\,r), \tag{2.6}$$

where $\gamma(t)$ is singular at $t_{\max}$. It turns out, however, that Eq. (2.1) is consistent with different choices of γ and Φ, so that one needs to determine which particular self-similar structure acts as an attractor for a given class of initial conditions. In this paper, we shall, for the sake of convenience, restrict ourselves to the blowup arising from (2.5).

In the case $N=2$, most authors agree that the function Φ in (2.6) is in fact the envelope of the ground state [23, 31]. However, disagreement has existed regarding the nature of the singularity $\gamma(t)$. In Table I, we have listed some of the conflicting claims which have been made in the past. Note that, in the case $N=2$, each reference appearing in the table

TABLE I

The Nature of the Singularity $\gamma(t)$

	$N=2$	
$(t_{\max}-t)^{1/2}$	$(t_{\max}-t)^{2/3}$	$\left(\frac{\lvert\log(t_{\max}-t)\rvert}{(t_{\max}-t)}\right)^{1/2}$
Kelley [16]	Zakharov and Synakh [35] Sulem *et al.* [26]	Vlasov *et al.* [30] Wood [32] Rypdal and and Rasmussen [23]
	$N=3$	
"weak collapse" $(t_{\max}-t)^{1/2}$		"strong collapse" $(t_{\max}-t)^{3/5}$
McLaughlin et al. [21] Goldman *et al.* [11]		Rypdal and Rasmussen [23] Zakharov *et al.* [34]

includes the results of numerical experiments purporting to verify the conjectured power law. It should be said, however, that, in more recent contributions [17, 18], Sulem and his collaborators have abandonned the power law $(t_{\max}-t)^{-2/3}$. Instead, they present new calculations in support of the conjecture

$$\left(\frac{\log\log(t_{\max}-t)}{t_{\max}-t}\right)^{1/2}.$$

In the case $N=3$, McLaughlin *et al.* [21] have derived a semilinear elliptic equation for Φ. They have carried out calculations with initial conditions of the type (2.5) which support the conjecture (2.6) with $\gamma(t)\approx(t_{\max}-t)^{-1/2}$. This is in agreement with earlier findings by Goldman *et al.* [11]. However, Zakharov *et al.* [34] and Rypdal and Rasmussen [23] present other asymptotic arguments which suggest that another self-similar blowup regime which they call "strong collapse" is possible for suitable initial data. In this regime, the solution grows like $(t_{\max}-t)^{3/5}$. This does not contradict the findings of McLaughlin *et al.*, but it does, however, raise the possibility of two distinct blowup regimes for solutions arising from (2.5), depending on the particular choice of a and l.

The complex situation summarised in Table I indicates that considerable care must be exercised if numerical methods are to provide a reliable tool in the investigation of blowup phenomena. The results of our own calculations will be discussed in the next sections. In the case $N=3$, detailed experiments will confirm the results of McLaughlin *et al.* At the same time, we also show that a careless approach may suggest the "wrong" power law $(t_{\max}-t)^{-3/5}$.

3. TWO FINITE-ELEMENT METHODS FOR THE CSE

The solutions generated by gaussian initial conditions remain exponentially small as $r\to\infty$. Let $\Omega\subset IR^N$ be the ball of radius $R>0$ centered at the origin. If R is sufficiently large, we may, without significant loss of accuracy, replace the initial value problem (2.1), (2.5) by an initial boundary value problem on Ω with homogeneous Dirichlet boundary conditions. We refer to Goldstein [13] for a rigorous analysis of this truncation procedure for a simpler linear elliptic problem.

Let $\Delta_h: 0=r_1<r_2<\cdots<r_{n+1}=R$ be a partition of the interval $[0, R]$. We introduce the finite-dimensional space S_h consisting of all the functions defined on $[0, R]$ which are continuous and piecewise linear with respect to Δ_h. We also introduce the discrete time levels

$$0=t_0<t_1<\cdots<t_m<\cdots$$

and use the notation

$$h=\max_{1\leqslant i\leqslant n}(r_{i+1}-r_i),$$

$$\mathbf{h}=\min_{1\leqslant i\leqslant n}(r_{i+1}-r_i),$$

$$\Delta t=\max_{0\leqslant m}(t_{m+1}-t_m).$$

Let $u_h^m\in S_h$ denote an approximation to $u(t_m)$. We shall consider two different ways of constructing an approximation to u at the next time level. In the first method, due to Delfour *et al.* [5] (DFP for short), $u_h^{m+1}\in S_h$ is defined as the solution of the problem

$$i\int_0^R \frac{u_h^{m+1}-u_h^m}{t_{m+1}-t_m}\phi r^{N-1}\,dr-\int_0^R\frac{d}{dr}u_h^{m+1/2}\frac{d\phi}{dr}r^{N-1}\,dr$$
$$+\int_0^R\frac{|u_h^{m+1}|^2+|u_h^m|^2}{2}u_h^{m+1/2}\phi r^{N-1}\,dr=0 \qquad \text{(DFP)}$$

for all $\phi\in S_h$, where $u_h^{m+1/2}=\frac{1}{2}(u_h^{m+1}+u_h^m)$.

The main feature of the DFP scheme is the existence of discrete invariance properties analogous to (2.2) and (2.3), namely,

$$\int_0^R |u_h^m|^2 r^{N-1}\,dr=\text{const}\quad\text{for all } m, \tag{3.1}$$

$$\int_0^R\left\{\left|\frac{du_h^m}{dr}\right|^2-\frac{1}{2}|u_h^m|^4\right\}r^{N-1}\,dr=\text{const}\quad\text{for all } m. \tag{3.2}$$

The second numerical method which we shall use is due to

Griffiths *et al.* [14] (GMM for short). It consists of defining $u_h^{m+1} \in S_h$ as the solution of the problem

$$i \int_0^R \frac{u_h^{m+1} - u_h^m}{t_{m+1} - t_m} \phi r^{N-1}\, dr - \int_0^R \frac{d}{dr} u_h^{m+1/2} \frac{d\phi}{dr} r^{N-1}\, dr + \int_0^R I_h(F(u_h^{m+1/2}))\, \phi r^{N-1}\, dr = 0, \qquad \text{(GMM)}$$

where $F(z) = |z|^2 z$ and $I_h(\cdot): C(0, R) \to S_h$ denotes the interpolation operator. (The technique which consists of replacing the nonlinear term by its interpolant is known as "product approximation" [28].) Thus, our two numerical methods differ only in their treatment of the nonlinear term. Unlike the DFP scheme, the GMM method does not feature discrete invariance properties. However, the latter leads to a more efficient computer code.

If the partitions Δ_h are refined in such a way that

$$h = O(\mathbf{h}^\theta), \qquad \frac{N}{4} < \theta \leqslant 1, \tag{3.3}$$

then both methods enjoy the rate of convergence [27, 29]

$$\|u_h^m - u(t_m)\|_{L^2(\Omega)} \leqslant C(u, T)(h^2 + \Delta t^2) \tag{3.4}$$

for $t_m \leqslant T < t_{\max}$. This result only holds for $N = 1, 2, 3$. No convergence results are available in higher dimensions. It must be emphasized that the constant C in (3.4) depends on the size of u and its derivatives in the interval $[0, T]$. This constant becomes unbounded as $T \to t_{\max}$.

The calculation of u_h^{m+1} in both the GMM and DFP methods involves the solution of a system of nonlinear algebraic equations. In order to solve this system, we shall use a simple fixed-point iteration procedure. Let $z_0 = u_h^m$. In the case of the DFP scheme, we obtain $z_{k+1} \in S_h$ by solving the linear problem

$$i \int_0^R \frac{z_{k+1} - u_h^m}{t_{m+1} - t_m} \phi r^{N-1}\, dr - \int_0^R \frac{d}{dr} \frac{z_{k+1} + u_h^m}{2} \frac{d\phi}{dr} r^{N-1}\, dr + \int_0^R \frac{|z_k|^2 + |u_h^m|^2}{2} \frac{z_k + u_h^m}{2} \phi r^{N-1}\, dr = 0. \tag{3.5}$$

The sequence $\{z_k\}$ will converge to u_h^{m+1} geometrically provided that $(t_{m+1} - t_m)$ is sufficiently small. (Roughly speaking, $(t_{m+1} - t_m)$ should be small compared to $|u(t_m)|^2$; cf. [27] for details.) In the case of the GMM scheme, we have to solve a linear problem similar to (3.5) with the appropriate modification to the nonlinear term.

4. A FIRST APPROACH TO THE CALCULATION OF THE BLOWUP PARAMETERS

In this section, we describe the results of a calculation of the blowup parameters based on a "naive" approach. As we shall see, the two numerical schemes discussed in the previous section then lead to conflicting results.

Consider the case $N = 3$ in Table I. We use the initial condition

$$u(r, 0) = 6\sqrt{2}\, e^{-r^2} \tag{4.1}$$

and take $R = 5$ for the radius of the sphere Ω. Assuming that the behaviour of u near $t_{\max}$ takes the form

$$|u(0, t)| \propto (t_{\max} - t)^{-\alpha}, \tag{4.2}$$

we would like to estimate α and $t_{\max}$. The problem (2.1), (4.1) has been considered by McLaughlin *et al.* [21] who computed $t_{\max} \approx 0.034302$ and $\alpha \approx \frac{1}{2}$.

As far as the implementation of the numerical method is concerned, we have used uniform grids in space and time. The fixed-point iteration procedure was terminated whenever the difference between two successive iterates z_k and z_{k+1} proved sufficiently small. More precisely, we have used the stopping criterion

$$\|z_{k+1} - z_k\|_{L^2(\Omega)} < 10^{-10}.$$

If this condition could not be met in less than 10 iterations, we would set

$$u_h^{m+1} = z_{10}$$

and proceed to the next time level. Our calculations were carried out on a network of Sun computers 3/50 and 3/60, using double precision arithmetic. We shall write α^h and $t_{\max}^h$ to denote the estimates of α and $t_{\max}$, respectively. We emphasize, however, that those estimates depend on Δt as well as on h. Our "naive" approach to the estimation of $t_{\max}$ and α consists of the following two basic steps:

- Given h and Δt, integrate forward in time until overflow occurs. (This happens whenever the numerical method generates a number in excess of 10^{308}). Let $t_{\max}^h$ be the last time level prior to overflow.
- Having estimated $t_{\max}$, calculate α^h by a linear least-square fit of the curve

$$\log |u_h^m(0)| \text{ vs } \log(t_{\max}^h - t_m).$$

In doing so, one should avoid using the results from the last few computed steps, as these will be very inaccurate. Naturally, this procedure should be repeated with decreasing values of h and Δt.

TABLE II

Computed Estimates of $t_{\max}$

	$h=0.002$		$h=0.001$	
Δt	DFP	GMM	DFP	GMM
10^{-3}	0.034	0.035	0.034	0.035
10^{-4}	0.0343	0.0343	0.0343	0.0343
10^{-5}	0.03430	0.03431	0.03430	0.03431

In accordance with this program, our first task was to estimate $t_{\max}$. The result of this calculation, for different values of h and Δt, is given in Table II. The good agreement between the two numerical methods is encouraging and it seems that the computed values of $t^h_{\max}$ are converging to a limit which is close to McLaughlin *et al.*'s $t_{\max}=0.034302$. Using the discrete solution corresponding to $h=10^{-3}$ and $\Delta t=10^{-5}$, we have then sought to estimate the local value of the exponent α in Eq. (4.2) on different sections $[t_a, t_b]$ of the time interval. The results are displayed in Table III.

Once again, we observe that our two numerical schemes are in good agreement in the early stage of the blowup. Near $t_{\max}$, however, they produce conflicting evidence: the DFP method yields a "weak collapse" which supports the claim of McLaughlin *et al.* [21]. In contrast, the numerical solution obtained by the GMM scheme exhibits a growth rate consistent with the "strong collapse" discussed by Rypdal and Rasmussen [23] and Zakharov *et al.* [34].

This discrepancy stems for the fact that, for h and Δt fixed as $t\to t_{\max}$, the behaviour of the numerical methods does not reproduce the true behaviour, no matter how small h and Δt are; cf. the discussion in Section 6. Recently, Berger and Kohn [1] and LeMesurier *et al.* [19] have proposed rescaling algorithms which reduce *both* the spatial and temporal grids in accordance with the current size of the solution. The underlying aim is to achieve uniform accuracy as t approaches $t_{\max}$. Such procedures appear to be useful, although it is fair to say that they owe more to heuristic considerations regarding the structure of the solution of the PDE, than to actual facts obtained from a numerical analysis. (Cf., however, the interesting result of Nakagawa [22]). An alternative approach will be considered in the next section.

TABLE III

Local Estimates of the Exponent α

Fit between		α^h	
t_a	t_b	DFP	GMM
0.01000	0.02000	0.31	0.31
0.02000	0.03000	0.46	0.46
0.03000	0.03428	0.53	0.54
0.03200	0.03428	0.53	0.55
0.03400	0.03428	0.52	0.58
0.03410	0.03428	0.52	0.59
0.03420	0.03428	0.52	0.62

5. A RELIABLE PROCEDURE FOR THE CALCULATION OF THE BLOWUP PARAMETERS

The procedure which we shall discuss in this section is based on the simple observation that it is not necessary to compute all the way up to $t_{\max}$ in order to obtain estimates of the blowup parameters. For example, take M "large," then calculate and sample the discrete solution in the range

$$\frac{M}{2}\leqslant \|u_h^m\|_{L^\infty(\Omega)}\leqslant M;$$

α^h and $t^h_{\max}$ can then be obtained via a nonlinear least-square fit. More precisely, if the discrete solution is sampled at the time levels t_{m_i}, $i=1, ..., N_s$, then it suffices to minimise

$$\sum_{i=1}^{N_s}\left[\log\|u_h^{m_i}\|_{L^\infty(\Omega)}-\log C^h-\alpha^h\log(t^h_{\max}-t_{m_i})\right]^2$$

with respect to $\log C^h$ (where C^h is an estimate of the underlying proportionality constant in (4.2)), α^h, and $t^h_{\max}$ to obtain estimates of the blowup parameters. Note that those estimates now depend not only on h and Δt, but also on M. Since our numerical methods are convergent in compact intervals contained in $[0, t_{\max}[$, it follows that α^h and $t^h_{\max}$ should also convergence in the following sense: given $\varepsilon>0$, there exists M_ε such that for all $M\geqslant M_\varepsilon$, we can find $h_{M,\varepsilon}$ and $\Delta t_{M,\varepsilon}$ which have the property that

$$|\alpha-\alpha^h|+|t_{\max}-t^h_{\max}|<\varepsilon$$

for all $h<h_{M,\varepsilon}$ and $\Delta t<\Delta t_{M,\varepsilon}$.

In our opinion, this procedure has the merit of making a distinction between two separate aims: the first aim being to estimate the blowup parameters in a reliable way; the second aim being to design spatial and temporal grids which will afford an economical computation. For each value of M, we have the freedom of choosing and adapting the grids according to error-control requirements, and there is no need to build in any a priori information on the nature of the singularity.

It is not the purpose of this paper to discuss mesh adaption, and we have therefore opted for the simplest refinement strategy consistent with the convergence properties of our two discretisations. As far as the spatial grid is concerned, it is natural to select a mesh which is fine near

$r=0$ and then gradually coarsens as $r \to R$. For example, let h and $\mathbf{h}$ be given parameters and define

$$r_{i+1}=r_i+\mathbf{h}\left(1-\frac{i-1}{n-1}\right)+h\frac{i-1}{n-1}, \qquad i=1, ..., n \tag{5.1}$$

We require $r_{n+1} \approx R$. Take $n=[2R/(h+\mathbf{h})]$. The recursion (5.1) then defines a partition of the interval $[0, R_h]$, where $R_h=\frac{1}{2}(h+\mathbf{h})n$. Note that $R_h=R+O(h)$.

In the numerical experiment which we shall describe below, we have used $\mathbf{h}=h^{3/2}$ in the case $N=2$ and $\mathbf{h}=h^{5/4}$ in the case $N=3$. This choice is permitted by condition (3.3) and allows the ratio $h/\mathbf{h}$ to increase without bound as $h \to 0$.

Regarding the choice of time step, we have opted for a simple (and common) error control strategy (cf. [9]). Observe that both the GMM and DFP schemes are second-order accurate time-discretisations of appropriate systems of ODEs. In order to estimate the error for a given step (say Δt), it suffices to carry out two calculations from the previous time level: one with a full step of length Δt and one by taking two steps of length $\Delta t/2$. From those two calculations, it is simple to obtain an estimate of the local error. If this error exceeds a given tolerance TOL or if the fixed-point iterative procedure fails to converge, then the calculation should be carried out with a reduced time step. Otherwise, the calculation is deemed acceptable and we can proceed to the next time level.

In summary, we have the following algorithm for the calculation of the blowup parameters:

- For M, h, and TOL given, calculate u_h^m in the range

$$\frac{M}{2} \leqslant \|u_h^m\|_{L^\infty(\Omega)} \leqslant M.$$

- Obtain α^h and $t_{\max}^h$ by a nonlinear least-square fit.
- Reduce h and TOL until α^h and $t_{\max}^h$ converge.
- Increase M and repeat the above steps.

In order to illustrate the effectiveness of this procedure, we return to the example discussed in Section 4; i.e., we consider the cubic Schrödinger equation in the case $N=3$ with the initial condition (4.1).

In Tables IV to VI, estimates of the blowup parameters computed by the GMM and DFP schemes are displayed. For each value of h, TOL and M, there are three entries: the top, middle, and bottom entries correspond respectively to $\log C^h$, α^h, and $t_{\max}^h$.

TABLE IV

$N=3$, $u(x,0)=6\sqrt{2}\,e^{-r^2}$, $M=100$

	GMM		DFP	
h \ TOL	10^{-10}	10^{-12}	10^{-10}	10^{-12}
0.01	−0.019270447	−0.019132797	−0.017110775	−0.018221558
	0.53571370	0.53567437	0.53532158	0.53546687
	0.034306245	0.034303449	0.034295642	0.034299875
0.005	−0.013431050	−0.013626867	−0.012178652	−0.013273416
	0.53480179	0.53481071	0.53458869	0.53473497
	0.034308516	0.034305733	0.034299620	0.034303900
0.0025	−0.012550037	−0.012785942	−0.011544996	−0.011241855
	0.53466680	0.53468150	0.53449873	0.53444771
	0.034309107	0.034306327	0.034300549	0.034304732
0.00125	−0.012447952	−0.012647548	−0.011456959	−0.012046088
	0.53465159	0.53466092	0.53448690	0.53456033
	0.034309249	0.034306465	0.034300751	0.034304985

TABLE V

$N=3$, $u(x,0)=6\sqrt{2}\,e^{-r^2}$, $M=200$

	GMM		DFP	
h \ TOL	10^{-10}	10^{-12}	10^{-10}	10^{-12}
0.01	0.025269411	0.022687745	0.020852332	0.022247586
	0.52986332	0.53016879	0.53030770	0.53011999
	0.034304188	0.034301500	0.34293817	0.034297934
0.005	0.058120525	0.057017115	0.056760725	0.055795459
	0.52545817	0.52558128	0.52559532	0.52569607
	0.034305357	0.034302615	0.034296605	0.034300806
0.0025	0.063651301	0.062445358	0.061639751	0.064939091
	0.52472238	0.52485770	0.52495593	0.52454372
	0.034305758	0.034303018	0.034297357	0.034301508
0.00125	0.067140219	0.063122425	0.062421315	0.062168475
	0.52428620	0.52476571	0.52485429	0.52486591
	0.034305804	0.034303129	0.034297532	0.034301713

TABLE VI

$N=3$, $u(x,0)=6\sqrt{2}\,e^{-r^2}$, $M=400$

	GMM		DFP	
h \ TOL	10^{-10}	10^{-12}	10^{-10}	10^{-12}
0.01	−0.0089738938	−0.0089480197	−0.078869320	−0.075702874
	0.53356678	0.53357043	0.54110480	0.54077583
	0.034304430	0.034301704	0.034294543	0.034298679
0.005	0.11368666	0.11428648	0.11481839	0.11362816
	0.51918448	0.51912796	0.51904806	0.51915906
	0.034304714	0.034301967	0.034295948	0.034300134
0.0025	0.14098567	0.14360978	0.14438745	0.14444877
	0.51604887	0.51578260	0.51569548	0.51567775
	0.034304913	0.034302156	0.034296478	0.034300688
0.00125	0.14941938	0.14892463	0.14840193	0.14491961
	0.51512993	0.51518122	0.51523484	0.51557946
	0.034304970	0.034302225	0.034296621	0.034300803

There are two points worthy of notice: First, for each value of M, both methods produce estimates which agree closely as h and TOL are reduced. As one would expect, larger values of M require smaller values of h and TOL in order to eliminate the discrepancy between the two numerical methods ($M=400$ was the largest value which could be attempted in the computer environment used in this project). Second, with h and TOL reduced according to M, the estimates appear to converge to a limit as M increases. Both methods suggest that α is close to $\frac{1}{2}$ and that $t_{\max}$ is close to 0.03430. This supports the conjecture of McLaughlin *et al.* [21] (cf. Table I).

To conclude this section, let us mention that we have also carried out calculations in the case $N=2$. In this case also, both discretisations agree closely. The results indicate that the conjecture of Zakharov and Synakh [35] and Sulem *et al.* [26] should be discarded. The blowup rates predicted by Kelley [16], Vlasov *et al.* [30], LeMesurier *et al.* [18, 19], and Landman *et al.* [17] (cf. the discussion pertaining to Table I) are all plausible. Since they only differ in a logarithmic factor, it has not been possible to decide between them numerically.

6. DISCUSSION

So far, our attention has been centered exclusively on the radial CSE. However, it is clear that both the "naive" approach of Section 4 and the procedure of Section 5 can be used for any ODE or PDE featuring finite-time blowup. The purpose of this section is first to broaden the scope of our discussion and, second, to gain further insight into the behaviour of discretisations near a singularity.

As indicated earlier, the failure of the "naive" approach presented in Section 4 reflects the obvious fact that discretisations on fixed meshes cannot maintain a uniform level of accuracy over the whole of $[0, t_{\max}[$, however small h and Δt are. In the ODE case, Sanz-Serna and Verwer [24] have presented a detailed study of the Euler rule for the simple model problem

$$\frac{dy}{dt}=y^2, \qquad y(0)=1 \tag{6.1}$$

which admits the solution

$$y(t)=(t_{\max}-t)^{-1}, \qquad t_{\max}=1.$$

They show that the time $t^{\tau}_{\max}$ by which the numerical solution overflows differs by $O(\tau)$ from $t_{\max}$. However, the behaviour of the numerical solution prior to $t_{\max}$ is quite different from the true behaviour. In fact, at the grid point $t_{\max}-\tau$, the relative error in the numerical solution tends to 1. This demonstrates that the approach of Section 4 is doomed to fail even for the simple problem (6.1). By contrast, the procedure which we advocate yields convergent estimates of the blowup parameters. Further relevant material on the behaviour of the θ method for a related problem can be found in [25].

In the PDE case, it is perhaps illusory to hope for such a sharp analysis near $t_{\max}$. Nevertheless, some insight into the behaviour of discretisations can be gained via the method of modified equations [15]. Loosely speaking, one expects that the discrete solution is in fact closer to the solution of a modified equation with added terms which might either oppose blowup or at least change the nature of the singularity. It is this phenomenon which is presumably responsible for the conflicting claims, based on the results obtained by *different* numerical methods which have been made in the literature.

To illustrate this, let us consider the one-dimensional nonlinear Schrödinger equation

$$i\frac{\partial u}{\partial t}+\frac{\partial^2 u}{\partial x^2}+f(u)=0, \tag{6.2}$$

where now the nonlinearity is of the form $f(u)=|u|^p u$, $p\geqslant 4$. Given a regular initial condition, the solution of Eq. (6.2) exists up to some time $t_{\max}>0$ [3] and satisfies the invariance properties

$$P=\int_{IR}|u(x,t)|^2\,dx=\text{const} \quad \text{for} \quad t\geqslant 0, \tag{6.3}$$

$$\begin{aligned} E&=\int_{IR}\left\{\left|\frac{\partial u}{\partial x}(x,t)\right|^2-\frac{2}{p+2}|u(x,t)|^{p+2}\right\}dx \\ &=\text{const} \quad \text{for} \quad t\geqslant 0, \end{aligned} \tag{6.4}$$

which are the obvious analogs of (2.2) and (2.3). Generalising the result of Zakharov to the case where $p\neq 3$ and $N\neq 2$, 3, Glassey [11] showed that $E<0$ implies $t_{\max}<\infty$. The solution then becomes unbounded. Thus, Eq. (6.2) exhibits features analogous to the higher-dimensional radial CSE.

Suppose now that we discretise the spatial variable by means of a Galerkin method with piecewise linear elements and product approximation for the nonlinear term. On a uniform spatial grid, the nodal values $U_j=U(x_j,t)$ of the discrete solution satisfy the differential equation

$$\begin{aligned} &\frac{i}{6}(\dot{U}_{j-1}+4\dot{U}_j+\dot{U}_{j+1})+\frac{1}{h^2}(U_{j-1}-2U_j+U_{j+1}) \\ &\qquad +\frac{1}{6}(f(U_{j-1})+4f(U_j)+f(U_{j+1}))=0, \end{aligned} \tag{6.5}$$

where the dot indicates differentiation with respect to time and h denotes the spatial gridsize. The consistency of this spatial discretisation can be determined by Taylor-expanding the solution u of Eq. (6.2) about x_j. We find that (we write $u(x_j)$ instead of $u(x_j, t)$)

$$\begin{aligned}
&\frac{i}{6}\left(\frac{\partial u}{\partial t}(x_{j-1})+4\frac{\partial u}{\partial t}(x_j)+\frac{\partial u}{\partial t}(x_{j+1})\right)\\
&\quad+\frac{1}{h^2}(u(x_{j-1})-2u(x_j)+u(x_{j+1}))\\
&\quad+\frac{1}{6}(f(u(x_{j-1}))+4f(u(x_j))+f(u(x_{j+1})))\\
&=i\frac{\partial u}{\partial t}(x_j)+\frac{\partial^2 u}{\partial x^2}(x_j)+f(u(x_j))\\
&\quad+h^2\frac{\partial^2}{\partial x^2}\left(\frac{i}{6}\frac{\partial u}{\partial t}(x_j)+\frac{1}{12}\frac{\partial^2 u}{\partial x^2}(x_j)\right.\\
&\quad\left.+\frac{1}{6}f(u(x_j))\right)+O(h^4)\\
&=i\frac{\partial u}{\partial t}(x_j)+\frac{\partial^2 u}{\partial x^2}(x_j)+f(u(x_j))-\frac{h^2}{12}\frac{\partial^4 u}{\partial x^4}(x_j)\\
&\quad+\frac{h^2}{6}\frac{\partial^2}{\partial x^2}\left(i\frac{\partial u}{\partial t}(x_j)+\frac{\partial^2 u}{\partial x^2}(x_j)+f(u(x_j))\right.\\
&\quad\left.-\frac{h^2}{12}\frac{\partial^4 u}{\partial x^4}(x_j)\right)+O(h^4).
\end{aligned}$$

This expansion shows that the scheme (6.5) is, on the one hand, consistent to second order with Eq. (6.2) and, on the other hand, consistent to fourth order with the *modified equation*

$$i\frac{\partial u_h}{\partial t}+\frac{\partial^2 u_h}{\partial x^2}+f(u_h)-\frac{h^2}{12}\frac{\partial^4 u_h}{\partial x^4}=0. \tag{6.6}$$

Consequently, the discrete solution defined by Eq. (6.5), although it was designed to approximate u, might well be closer to u_h. One should immediately add, however, that this statement is not necessarily correct since, as the notation emphasizes, u_h obviously depends on h (cf. [15]). A discussion of Eq. (6.6) is nonetheless enlightening.

We proceed to show that the added dispersion term in Eq. (6.6), which may be thought of as a distortion inherent in the numerical method, opposes blowup if $p<8$. Let us suppose that u_h and its first spatial derivative vanish at the boundary of Ω. If we multiply Eq. (6.6) by $\bar{u}_h$, integrate over Ω, use integration by parts to deal with the spatial derivatives, and retain the imaginary part, we find

$$P \equiv \int_\Omega |u_h(x,t)|^2\,dx=\text{const.} \tag{6.7}$$

If we then multiply the equation by $\partial\bar{u}_h/\partial t$ and take the real part after integration, we obtain

$$\begin{aligned}
E_h \equiv \int_\Omega \left|\frac{\partial u_h}{\partial x}(x,t)\right|^2 dx-\frac{2}{p+2}\int_\Omega |u_h(x,t)|^{p+2}\,dx\\
+\frac{h^2}{6}\int_\Omega \left|\frac{\partial^2 u_h}{\partial x^2}(x,t)\right|^2 dx=\text{const.}
\end{aligned} \tag{6.8}$$

The solution of Eq. (6.6) therefore satisfies two invariance properties closely related to (6.3) and (6.4). However, the additional term in (6.8) ensures the boundedness of u_h if $p<8$. Indeed, the Sobolev–Gagliardo–Nirenberg inequality [7] and (6.8) imply

$$\begin{aligned}
&\frac{h^2}{6}\int_\Omega \left|\frac{\partial^2 u_h}{\partial x^2}(x,t)\right|^2 dx\\
&\quad\leqslant |E_h|+\frac{2}{p+2}\int_\Omega |u_h(x,t)|^{p+2}\,dx\\
&\quad\leqslant |E_h|+\frac{2}{p+2}C_1P^{(p+4)/8}\left(\int_\Omega\left|\frac{\partial u_h}{\partial x}(x,t)\right|^2 dx\right)^{p/4}.
\end{aligned}$$

Using now another Sobolev inequality [2, p. 195] which states that

$$\begin{aligned}
\int_\Omega \left|\frac{\partial u_h}{\partial x}(x,t)\right|^2 dx \leqslant C_2\left(\int_\Omega\left|\frac{\partial^2 u_h}{\partial x^2}(x,t)\right|^2 dx\right)^{1/2}\\
\times\left(\int_\Omega |u_h(x,t)|^2\,dx\right)^{1/2}
\end{aligned}$$

there follows

$$\begin{aligned}
\frac{h^2}{6}\int_\Omega \left|\frac{\partial^2 u_h}{\partial x^2}(x,t)\right|^2 dx \leqslant |E_h|+\frac{2}{p+2}C_1C_2^{p/4}P^{p/4+1/2}\\
\times\left(\int_\Omega\left|\frac{\partial^2 u_h}{\partial x^2}(x,t)\right|^2 dx\right)^{p/8}.
\end{aligned}$$

Hence, if $p<8$, we have

$$\int_\Omega \left|\frac{\partial^2 u_h}{\partial x^2}(x,t)\right|^2 dx \leqslant C_h$$

which implies the boundedness of u_h.

This suggests that the discrete solution U defined by Eq. (6.5) will also remain bounded if $p<8$, even if the solution u of Eq. (6.2) does not. This prediction has been

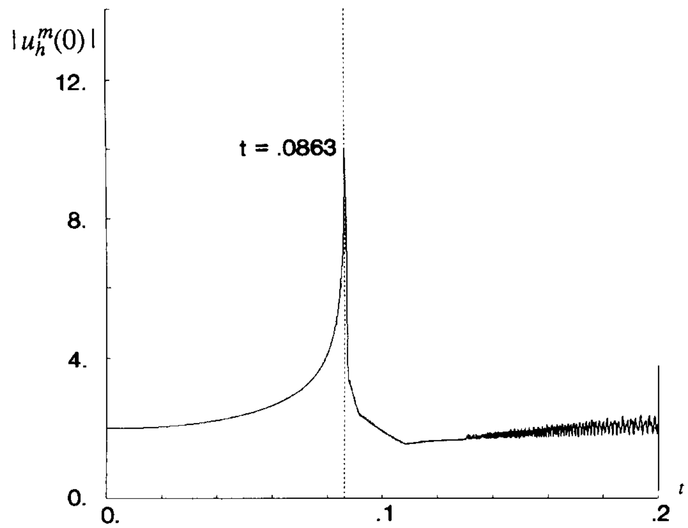

FIG. 2. Evolution of the amplitude of the discrete solution obtained with the GMM scheme for Eq. (6.2) and the initial condition $u(r, 0) = 2e^{-x^2}$; $p=4$, $h=\frac{1}{50}$, and $\Delta t = 10^{-4}$.

confirmed numerically (cf. Fig. 2) in an experiment with Eq. (6.2), $p=4$, and the initial condition

$$u(x, 0) = 2e^{-x^2}.$$

For this initial condition, $E<0$ and Glassey's theorem predicts blowup. We have used the GMM scheme with piecewise linear elements, $h=0.02$, $R=5$, and $\Delta t=10^{-4}$. This time step is so small that the spatial error dominates. We are in effect computing the discrete solution U of Eq. (6.5) and overflow does not take place. If we use $\Delta t = 10^{-3}$, then overflow occurs at $t=0.087$. (Incidentally, we note that, for this example, the discretization in space has a saturating effect on the solution [19, 35] and it could perhaps be argued that, on physical grounds, the discretisation (6.6) is a more realistic model than Eq. (6.2)!)

It is more difficult to derive modified equations in the radial case, owing to the presence of the curvature term. However, an obvious example of numerical distortion arises as a result of discrete invariance properties. Given that the L^2 norm of the discrete solution defined by the DFP method remains the same for all time levels and given that S_h is finite-dimensional, it follows either that the DFP scheme is unsolvable for $t_{m+1} \geqslant t_{\max}$ or else that u_h^m remains bounded for h fixed. The former eventuality is excluded for small enough Δt [27]. This shows that discrete invariance properties are no safeguard against spurious behaviour near $t_{\max}$.

These simple examples help to explain why the naive approach presented in the previous section fails to reveal the nature of the singularity.

7. CONCLUDING REMARKS

In this paper, we have discussed the use of numerical methods in the investigation of blowup phenomena. The spurious behaviour of discretisations as $t \to t_{\max}$ as been illustrated for a nonlinear Schrödinger equation and we have examined a simple procedure to obtain reliable results in the presence of a singularity:

Given spatial and temporal grids and given a "large" number M, calculate the discrete solution in the range

$$\frac{M}{2} \leqslant \|u_h^m\|_{L^\infty(\Omega)} \leqslant M.$$

- Obtain estimates of the blowup parameters by a nonlinear least-square fit.
- Refine the grids until those estimates "converge."
- Repeat the above steps with increasing values of M.

This procedure should yield correct results because it relies on the convergence properties of the numerical method in compact time intervals which exclude $t_{\max}$. Naturally, it may well be that for individual equations more powerful algorithms can be designed by exploiting the peculiarities of the problem. However, if the basic approach advocated here is combined with an adaptive strategy based on error control, then the resulting code should prove both efficient and reliable.

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