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On Spurious Behavior of Super-Stable Implicit Methods

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The objective of this paper is to gain a better understanding of the asymptotic non-linear behavior of super-stable implicit linear multistep methods for constant time steps. Examples of the nonlinear effect caused by grid adaptation and super-stable implicit total variation diminishing (TVD) schemes on the overall performance of the numerical procedure are given. A method to minimize spurious steady-state numerical solutions is discussed.

Keywords: Super-stable, implicit methods, linear multistep methods, TVD schemes, total variation diminishing schemes, grid adaptation, spurious solutions

1. INTRODUCTION

Starting in the late seventies the advances in computer power resulted in attempts to use computational fluid dynamics (CFD) to replace wind tunnel experiments and use numerics to understand dynamical systems. The gap between computation and analysis increased. The nonlinear behavior of commonly used algorithms in CFD was not well understood but at the same time applied CFD increased the intensity of using these algorithms to solve more complex practical problems where the flow physics and configurations under consideration were not understood, and were either too costly for or not amenable to laboratory experiments. CFD was and remains in a stage where computation is ahead of analysis.

In a series of papers by Yee (1991), Yee *et al.* (1991), Yee & Sweby (1991, 1994, 1995), Sweby & Yee (1991, 1994), Lafon & Yee (1991, 1992), and Griffiths *et al.* (1992a,b) some of the steps to help reduce the gap between computation and analysis were carried out. In order to have a basic understanding of the dynamical behavior of numerical methods for **constant time steps**, we take continuum models with known explicit solutions discretize them according to various standard numerical methods commonly used in CFD, and apply techniques from discrete dynamics to analyze the behavior of the resulting systems. Consequently, some of the schemes used for illustration might obviously not be suitable for that particular nonlinear model or spurious dynamics could be avoided easily under that environment.

Our interest here is to compare the nonlinear behavior of these schemes. This paper proceeds in a similar direction, emphasizing the super-stable properties of some of the implicit linear multistep methods (LMMs) (Lambert 1973) commonly used in CFD. For time-accurate computations, the standard practice in ODE solvers is to use local error control for the selection of time step. Practical CFD applications rarely employ this type of variable time step control due to the lack of efficient and practical theory for highly coupled nonlinear time-dependent PDEs. In addition, there still remains the question of spurious dynamics due to spatial discretizations. Moreover, local error controls similar to that used in ODE solvers that were designed for accuracy purpose are neither practical nor appropriate to use in time-marching to steady-state numerical solutions.

The objectives of this paper are to unify our study in Yee & Sweby (1994, 1995) for time discretizations for nonlinear model ordinary differential equations (ODEs) and to exploit the super-stable properties of some LMMs applied to model partial differential equation (PDE) problems with grid adaptation. Note that the ODE study is necessary to isolate the different properties of time-discretizations without the influence of spatial discretizations in PDEs. Section II discusses typical properties of this type of scheme. Particular emphasis will be placed on the phenomena not observed by Estep and Deici (1991), Iserles (1988), Stuart (1994) and references cited therein. Section III illustrates the **role of initial data** in the permissibility of **stabilizing** unstable steady states of the governing equation and the introduction of stable and unstable spurious numerical chaos and other asymptotes by implicit LMMs. Here the type of numerical solutions that are not solutions of the differential equation (DE) but are solutions of the discretized equation is often referred to as spurious numerical solutions. New results on the super-stable implicit LMMs and total variation diminishing (TVD) schemes for a linear and nonlinear model convection-diffusion equation with uniform grid and grid adaptation using the equi-distribution principle will be discussed. Section IV discusses how

to use existing tools in bifurcation theory to minimize the chances of converging to the wrong steady states or asymptotes. This paper is a refinement of a paper in the proceedings of the Conference on Numerical Methods for Euler and Navier-Stokes Equations, Sept. 14–16, 1995, Montreal, Canada.

2. SUPER-STABILITY PROPERTY

Dahlquist *et al.* (1982) first defined super-stability in ODE solvers to mean the region of numerical stability that encloses regions of physical instability of the true solution of the ODE. Dieci & Estep (1991) subsequently gave a broader definition as one in which an ODE solver does not detect that the underlying solution is physically unstable. They observed that super-stability can occur also when the ODE solver is not super-stable in terms of Dahlquist *et al.* They concluded that the key factor which determines the occurrence of super-stability is the iterative solution process for the nonlinear algebraic equations. They indicated that the iterative solution process has its own dynamics, which might be in conflict (as for Newton's method) with the dynamics of the problem. They also indicated that super-stability can arise because of this fact. Their viewpoint is that the numerical scheme and the methods for solving the nonlinear algebraic equations should be considered as a unit. Neglecting this latter aspect and basing step size selection purely on accuracy considerations leads to faulty analysis. They believe that error control strategies for stiff initial value problems ought to be redesigned to take into account stability information of the continuous problem.

In Yee & Sweby (1994, 1995) we exploited the global asymptotic behavior of some of the super-stable implicit LMMs for **constant step sizes**. We concentrated on four of the typical unconditionally stable implicit LMMs. These are backward Euler, trapezoidal rule, midpoint implicit, and three-point backward differentiation (BDF), each with noniterative (linearized implicit), simple, Newton and modified Newton iterative procedures for

solving the resulting nonlinear algebraic equations.

We believe that some of the phenomena observed in our study were not observed by Dieci & Estep (1991) or by Iserles (1988). Based on our study, we now give a loose definition of an implicit time discretization as having a super-stability property if, within the linearized stability limit for a combination of initial data and time step (fixed) or starting time step (using standard variable time step control based on accuracy requirements), the scheme stabilizes unstable steady states of the governing equations in addition to having the property of Dieci and Estep. The definition includes the procedures in solving the nonlinear algebraic equations. This loose definition fits the behavior that was observed in Yee & Sweby (1994, 1995), while at the same time it fits the framework of dynamics of numerics in time-marching approaches in CFD. This is not a re-definition of Dieci and Estep, but rather a clarification of their definition when asymptotic numerical solutions of the governing equations are desired. In this case, superstable schemes might have the property of a “numerical basin of attraction” of the true steady state that is larger than the underlying “exact basin of attraction”. As can be seen in Yee & Sweby (1994, 1995), the trapezoidal method is more likely to exhibit this property than the other three LMMs. The stabilization of unstable steady states by LMMs was also observed by Embid *et al.* (1984), Salas *et al.* (1986), Burton & Sweby (1995) and Poliashenko (1995).

In our previous study we concentrated on the global asymptotic behavior of iterative implicit methods on four 2×2 systems of nonlinear autonomous ODEs. The bifurcation diagram with numerical basins of attraction shown were rather complex to explain and the property of super-stability was not discussed. Here we attempt to clarify some of the super-stability behavior of implicit LMMs for nonlinear scalar autonomous ODEs and present new results for convection-diffusion model PDEs. The basin of attraction of an asymptote is a set of all initial data asymptotically approaching that asymptote. We use the term

“exact” basin of attraction and “numerical” basin of attraction to mean the basin of attraction of the DE and basin of attraction of the underlying discretized counterpart.

3. NUMERICAL RESULTS

Unlike the linear model equations, there is no equivalent unique nonlinear model equation for hyperbolic and parabolic PDEs for fluid dynamics. A numerical method behaving in a certain way for a particular nonlinear PDE might give a different behavior for a different nonlinear PDE even though the PDEs are of the same type. This phenomena is true not only for time-dependent nonlinear PDEs, but also for nonlinear ODEs as well. In addition, even for simple nonlinear model DEs with known solutions, depending on the numerical methods, the discretized counterparts can be extremely complex. Whenever analytical analysis of the discretized counterparts is not possible, the associated bifurcation phenomena and asymptotic behavior are obtained numerically using supercomputers. Analysis here means analysis of the discretized counterparts by (a) searching for asymptotic solution behavior without resorting to purely numerical computations and (b) using arclength continuation types of methods to trace out the bifurcation diagrams (Keller 1977). This is the case for most of the illustrations throughout this paper. The numerical computations were performed on the NASA Ames CM-5. The methods of detecting numerical asymptotes and numerical basins of attraction are the same as in Yee & Sweby (1994, 1995) and Sweby & Yee (1991).

3.1. Numerical Methods

Time Discretizations

Denoting Δt as the time step, the time discretizations considered, written for a nonlinear system of autonomous ODEs

$$dU/dt = S(U) \quad (3.1)$$

are

(1) Implicit Euler Method

$$U^{n+1} = U^n + \Delta t S^{n+1}, \quad (3.2)$$

(2) Trapezoidal Method

$$U^{n+1} = U^n + \frac{1}{2} \Delta t (S^n + S^{n+1}), \quad (3.3)$$

(3) 3-level Backward Differentiation Formula (BDF)

$$U^{n+1} = U^n + \frac{2}{3} \Delta t S^{n+1} + \frac{1}{3} (U^n - U^{n-1}), \quad (3.4)$$

(4) Semi-Implicit Predictor-Corrector Method

The semi-implicit predictor method is the same as (3.2) but with an added predictor step using the explicit Euler before the implicit step (3.2). The four methods of solving the resulting nonlinear algebraic equations are as follows.

Linearization (a noniterative procedure) is achieved by expanding S^{n+1} as $S^n + J(U^n)(U^{n+1} - U^n)$ where $J(U^n)$ is the Jacobian of S .

Simple Iteration is the process where, given a scheme of the form $U^{n+1} = G(U^n, U^{n+1})$, we perform the iteration

$$U_{(v+1)}^{n+1} = G(U^n, U_{(v)}^{n+1}) \quad (3.5)$$

where $U_0^{n+1} = U^n$ and “(v)” indicates the iteration index. The iteration is continued either until some tolerance between iterates is achieved or a limiting number of iterations has been performed. In all of our computations the tolerance “tol” is set as $\|U_{(v)}^{n+1} - U_{(v-1)}^{n+1}\| \leq \text{tol}$ and the maximum number of iterations is 15. The major drawback with simple iteration is that for guaranteed convergence the iteration must be a contraction, i.e.

$$\|G(U^n, V) - G(U^n, W)\| \leq \alpha \|V - W\|, \quad (3.6)$$

where $\alpha < 1$. Whether or not the iteration is a contraction at the fixed points will influence the stability of that fixed point, overriding the stability of the implicit scheme. Away from the fixed points the influence will be on the basins of attraction. In other words, “implicit method + simple iteration” behaves like explicit methods. As can be seen in Yee & Sweby (1994, 1995) and also the present study, the numerical results illustrate this limitation in terms of basins of attraction as well. One advantage of the “implicit method + simple iteration” over non-LMM explicit methods is that spurious steady states cannot occur. Due to this fact, results using simple iteration will not be presented here. See Yee and Sweby (1994) for examples.

Newton Iteration for the implicit schemes is of the form

$$U_{(v+1)}^{n+1} = U_{(v)}^{n+1} - F'(U^n, U_{(v)}^{n+1})^{-1} F(U^n, U_{(v)}^{n+1}), \quad (3.7)$$

where $U_0^{n+1} = U^n$. The differentiation is with respect to the second argument and the scheme has been written in the form (for two-level schemes) $F(U^n, U^{n+1}) = 0$.

Modified Newton Iteration is the same as (3.7) except it uses a frozen Jacobian $F'(U^n, U^n)$. The same tolerance and maximum number of iterations used for the simple iteration are also used for the Newton and modified Newton iterations. In all of the computations, the starting scheme for the 3-level BDF is the linearized implicit Euler.

We also considered two variable time step control methods. The first one is “implicit Euler + Newton iteration with local truncation error control” (Yee & Sweby 1994)

$$U_0^{n+1} = U^n$$

$$U_{(v+1)}^{n+1} = U_{(v)}^{n+1} + \left[I - \Delta t^n J(U_{(v)}^{n+1}) \right]^{-1} \times \left[U_{(v)}^{n+1} - U^n - \Delta t^n S(U_{(v)}^{n+1}) \right] \quad (3.8a)$$

$v = 1, \dots$

with

$$\Delta t^n = 0.9 \Delta t^{n-1} \{ \text{tol}_1 / \|U^n - U^{n-1} - \Delta t^{n-1} S(U^n)\| \}^{1/2} \quad (3.8b)$$

where the $(n+1)$ th step is rejected if $\|U^n - U^{n-1} - \Delta t^{n-1} S(U^n)\| > 2\text{tol}_1$. In this case, we set $\Delta t^{n-1} = \Delta t^n$. The value “tol₁” is a prescribed tolerance and the norm is an infinity norm. The second one is the popular “ode23” method

$$k_1 = S(U^n)$$

$$k_2 = S(U^n + \Delta t^n k_1)$$

$$k_3 = S(U^n + \Delta t^n (k_1 + k_2)/4)$$

$$U^{n+1} = U^n + \Delta t^n (k_1 + k_2 + 4k_3)/6$$

$$\Delta U^{n+1} = \Delta t^n (k_1 + k_2 - 2k_3)/3 \quad (3.9a)$$

with

$$\Delta t^n = 0.9 \Delta t^{n-1} \sqrt{\frac{\text{tol}_1}{\|\Delta U^n\|}}, \quad (3.9b)$$

where the $(n+1)$ th step is rejected if $\|\Delta U^{n+1}\| > \text{tol}_1 \max\{1, \|U^{n+1}\|\}$. In that case, we set $\Delta t^{n-1} = \Delta t^n$. Again, “tol₁” is a prescribed tolerance and the norms are infinity norms. We also use the straight Newton method to obtain the numerical solutions of $S(U) = 0$, which is the one-step Newton iteration of the implicit Euler method of (3.7).

Spatial Discretizations

The spatial discretizations considered for time-dependent model PDEs are the standard Harten-Yee implicit TVD schemes of equation (3.50) of Yee (1989). We compared the dynamics of all of the five limiters of (3.50) in Yee (1989) for two convection-diffusion scalar PDEs with and without grid adaptations. Since these schemes are well known in CFD literature, readers are referred to Yee (1989) or references cited therein for the exact formula and

background. These types of TVD schemes are high-resolution shock-capturing methods without the spurious oscillations associated with shock and contact discontinuity computations.

3.2. Nonlinear Scalar Autonomous ODE Models

The two scalar first-order autonomous nonlinear ODEs are

$$\frac{du}{dt} = au(1-u) \quad (3.10)$$

$$\frac{du}{dt} = au(1-u)(b-u), \quad 0 < b < 1. \quad (3.11)$$

The fixed points for (3.10) with $a > 0$ are $u = 0$ (unstable) and $u = 1$ (stable), and no additional periodic solutions or asymptotes exist. The basin of attraction for the stable fixed point $u = 1$ is the entire positive half-plane for all values of $a > 0$. The fixed points for (3.11) with $a > 0$ are $u = 0$ (unstable), $u = 1$ (unstable) and $u = b$ (stable) and no additional higher-order periodic solutions or asymptotes exist. The basin of attraction for the stable fixed point $u = b$ is $0 < u < 1$ for all $a > 0$. The fixed points (steady states) u^* of (3.1) are when $S(U^*) = 0$. The fixed points of the discretized counterparts are when $U^{n+1} = U^n$ and the fixed point of period p is when $U^{n+p} = U^n$ but $U^{n+q} \neq U^n$ for $q < p$. These two ODEs were studied in Yee *et al.* (1991), and Yee & Sweby (1992, 1993) for 9 explicit methods.

It is noted that some of the global solution behavior of steady states of the nonlinear discretized equations of (3.1) can be obtained by the pseudo arclength continuation method devised by Keller (1977), a standard numerical method for obtaining bifurcation curves in bifurcation analysis. A major shortcoming of the pseudo arclength continuation method is that for problems with complicated bifurcation patterns, it cannot provide the complete bifurcation diagram without known start up solutions for each of the main bifurcation branches before one can continue the solution along each of

these main branch. For spurious asymptotes it is usually not easy to locate even just one solution on each of these branches.

Selected results in the form of bifurcation diagrams and basins of attraction are shown in Figures 1–7 for the first model and Figures 8–10 for the second model. In Figures 1, 3, 5, 7–10, the left diagrams show the bifurcation diagrams and the right diagrams show the bifurcation diagrams with basins of attraction superimposed on the same plot. However, Figures 2, 4 and 6 show only the bifurcation diagrams with basins of attraction superimposed on the same plot. In all of Figures 1–10 the abscissa is $r = a\Delta t$. These figures show how the true unstable steady states undergo stabilization by the studied implicit LMMs. They also show the relationship of the birth of stable and unstable spurious asymptotes (other than steady states) as a function of initial data and time steps.

Note that the preselected regions of Δt and the initial data were determined by examining a wide range of Δt and initial data. In most cases, we

examined Δt from close to zero up to one million. What is shown in these figures represents some of the Δt and initial data ranges that are most interesting. Due to this fact, the Δt and initial data ranges shown are different from one method to another for the same model problem. The streaks on some of the plots are either due to the non-settling of the solutions within the prescribed number of iterations or the existence of small isolated spurious asymptotes. No further attempts were made to refine their detailed behavior since our purpose was to show how, in general, the different numerical methods behave in the context of nonlinear dynamics.

To obtain a bifurcation diagram with numerical basins of attraction superimposed using the CM-5, the preselected domain of initial data and the preselected range of the Δt parameter are divided into 512 equal increments. For the bifurcation part of the computations, the discretized equations are, in general, preiterated 3,000 steps for each initial datum and Δt before the next 1,000 itera-

FIGURE 1 (See Color Plate I).

FIGURE 2 (See Color Plate II).

FIGURE 3 (See Color Plate III).

FIGURE 4 (See Color Plate IV).

FIGURE 5 (See Color Plate V).

FIGURE 6 (See Color Plate VI).

tions (more or less depending on the problem and scheme) are plotted. The preiterations are necessary in order for the trajectories to settle to their asymptotic value. The high number of iterations are plotted (overlaid on the same plot) to detect periodic orbits or invariant sets. The bifurcation curves appear on the figures as white curves, white dots and dense white dots. While computing the bifurcation diagrams it is possible to overlay basins of attraction for each value of Δt used. For the numerical basins of attraction part of the computations, with each value of Δt used, we keep track of where each initial datum asymptotically approaches, and color code each basin (appearing as a multi-color vertical line) according to the individual asymptotes. Black regions denote basins of divergent solutions. While efforts were made to match color coding of adjacent multi-color vertical lines on the bifurcation diagram, it was not always practical or possible. Care

must therefore be taken when interpreting these overlays.

In other words, the color coding of the basin of attraction associated with a particular asymptote might vary from one vertical line to the next vertical line (i.e., from one Δt to the next). This is the case for Figures 1, 2, 5, 9 and 10. For example in Figure 1 the basin of attraction (as a function of Δt) for the steady state $u = 1$ is the red region before the appearance of the light blue strip. After the appearance of the blue strip, it is the region above the envelope that separates the green and red regions. When in doubt, use the bifurcation diagram as a guide and identify the r value where the sudden birth of stable spurious asymptotes occurred. Incidentally, this envelope and the critical value r which undergoes stabilization of the fixed point $u = 0$ can be obtained analytically. See Arriola (1993) for the analytical form of the envelope.

FIGURE 7 (See Color Plate VII).

Intuitively, in the presence of spurious asymptotes the basins of attraction of the true stable steady states can be separated by the numerical basins of attraction of the stable and unstable spurious asymptotes (allowable initial data for the numerical asymptotes). Take as an example the ODE (3.10) where the entire domain u is divided into two basins of attraction for the ODE independent of any real a . If one numerically integrates the ODE, depending on the scheme and Δt , extra stable and unstable fixed points of any order can be introduced by the scheme. See Yee *et al.* (1991), Yee & Sweby (1994), Lafon & Yee (1991, 1992) and Yee & Sweby (1995), for examples. See Section III of Yee & Sweby (1996) for an overview of the subject. The exact basins of attraction of the DEs can undergo drastic changes due to the nu-

merical method. That is, the allowable initial data of the numerical method associated with a particular asymptote of the DE can experience enlargement or contraction, and can become null or consist of a union of disjoint regions. These regions can be fractal like.

The bifurcation diagram alone cannot distinguish the types of bifurcation and the periodicity of the spurious fixed points of any order. See the left diagrams of Figures 1, 3, 5 and 7–10. With the numerical basins of attraction and their respective bifurcation diagrams superimposed on the same plot, the type of bifurcation and which initial data asymptotes to which stable asymptote become apparent. See the right diagrams of Figures 1, 3, 5 and 7–10. In an idealized situation it is best if we also know the critical value of Δt for the onset of

FIGURE 8 (See Color Plate VIII).

FIGURE 9 (See Color Plate IX).

FIGURE 10 (See Color Plate X).

unstable spurious asymptotes. However, with the current method of detecting the bifurcation curve only the stable ones are detected. For example, a steady bifurcation would break the domain immediately before the bifurcation point into two different color domains immediately after the bifurcation point. For unconditionally stable LMMs, the scheme should not experience any steady bifurcation from the stable branch ($u = 1$) because unconditionally stable LMMs **preserve** the stability of the stable steady states. This rule does not apply to **unstable** steady states using super-stable LMMs. Before stabilization of the unstable steady state, super-stable LMMs typically undergo “inverted period doubling bifurcations” or the “inverted logistic-map-type bifurcations” (or crisis in terms of Grebogi *et al.* 1983). See Figure 1 for $0.2 < u'' < -1$ for an example. For the ODE (3.11), all of the implicit methods experience at least two inverted logistic-map-type bifurcations. See

Figures 8–10. From these figures, we can observe that all of the studied implicit methods can introduce stable spurious chaos since a logistic-map-type of spurious bifurcations occur.

Unless otherwise stated, the basin of attraction in the following refers to the “numerical” basin of attraction. The procedures or other methods for solving the algebraic equation from here on exclude simple iterations.

Figures 1, 2, 5, 7–10 show the situation where the three LMMs and the semi-implicit method stabilize the unstable steady states of the ODEs (white line on $u = 0$). It appears that the onset of stabilization of the unstable steady states arises in two ways. One way is the birth of stable spurious asymptotes or stable spurious chaos in the form of an inverted logistic map. The second way is the birth of unstable spurious asymptotes (fixed points other than period one) leading to the onset of stabilization of unstable steady states. Although the two ways of

stabilization of the unstable steady states are similar, their corresponding basins of attraction are very different. See Figures 1, 5 and 7–10.

The critical value of Δt_c for the onset of stabilization is not very large (left end value of r on $u = 1$ for (3.10) and $u = b$ for (3.11)). It is problem dependent, method dependent and also procedure dependent (the various ways of solving the nonlinear algebraic equations). In most cases, the value of the Δt_c is comparable to or smaller than the equivalent of the stability limit of standard explicit Runge-Kutta methods. It is not uncommon for the underlying basins of attraction (associated with the stable steady state $u = 1$ for (3.10) and $u = b$ for (3.11)) to be larger than the exact basin of attraction for $\Delta t < \Delta t_c$. Note that the exact basin for (3.10) is $u > 0$ and for (3.11) is $0 < u < 1$.

Among the three procedures, the linearized non-iterative forms have a higher tendency to stabilize unstable steady states. See Figures 1, 5, 7–10. Here the word “procedure” excludes the simple iteration method. Among the three LMMs, the trapezoidal method is the least likely to stabilize unstable steady states, but the corresponding basins of attraction can be very small and more fragmented than for the other two LMMs. Also, the Δt_c for stabilization is bigger than for the other two LMMs. For a particular LMM not all three procedures for solving the nonlinear algebraic equation necessarily stabilize the unstable steady states (see Figs. 5 and 6). But, if they do, the pattern or the method for the onset of the stabilization does not have to be the same (see Figs. 1 and 2) but the value of Δt_c is the same for all of studied models and methods.

For the case of the semi-implicit predictor method, the onset of the stabilization can be accompanied by the birth of other spurious asymptotes (other than steady state). See Figure 7 for $r \geq 2$. It is fascinating to see how complicated the basins of attraction are which compose the many disjoint and fractal like regions. Similar behavior is also observed for the “implicit Euler + modified Newton” but less pronounced as the semi-implicit predictor method. See Figures 2 and 7.

Compared with the other three LMMs, and independent of the method of solving the nonlinear algebraic equation, the semi-implicit method exhibits the smallest basin of attraction (compared with the exact basin of attraction of the stable steady state) and is more fragmented for $\Delta t < \Delta t_c$. Aside from the efficiency issue, the implication is that a higher order accuracy scheme might not be as desirable for the time-marching approach.

Since straight Newton is just a one step “implicit Euler + Newton”, its basins of attraction (for Δt larger than explicit Runge-Kutta) are almost the same even with more than one step iterations. Studies indicated that, contrary to popular belief, the initial data using the straight Newton method may not have to be close to the exact solution for convergence. Straight Newton exhibits stable and unstable spurious asymptotes. Initial data can be reasonably removed from the asymptotic values and still be in the basin of attraction. However, the basins can be fragmented even though the corresponding exact basins of attraction are single closed domains. The cause of non-convergence may just as readily be due to the fact that the numerical basins of attraction are fragmented. If one uses a time step slightly bigger than the stability limit of standard explicit methods for the three LMMs, straight Newton can have similar or better performance. In fact, using a large Δt with the linearized implicit Euler method or the implicit Euler + Newton procedure has the same chance of obtaining the correct steady state as the straight Newton method if the initial data are not known or arbitrary initial data is taken.

A consequence of all of the observed behavior is that the flow pattern can change topology as the discretized parameter is varied. Thus, even though LMMs preserve the same number (but not the same types or stability) of fixed points as the underlying DEs, the numerical basins of attraction of LMMs do not coincide with the exact basins of attraction of the DEs even for small Δt . Some of the dynamics of the LMMs observed in our study can be used to explain the root of why one cannot achieve the theoretical linearized stability limit of

the typical implicit LMMs in practice when solving strongly nonlinear DEs (e.g., in CFD).

3.3. Does Error Control Suppress Spuriousity?

The previous sections discussed mainly the spurious behavior of long time integrations of initial value problems of nonlinear ODE solvers for constant step sizes. The use of adaptive step size based on local error control for implicit methods was studied by Dieci & Estep (1991). Dieci and Estep concluded that for superstable LMMs with local step size error control and depending on the method of solving the resulting nonlinear algebraic equations, spurious behavior can occur. Our study on the two variable step size control methods discussed in the previous section indicated that one shortcoming is that the size of Δt needed to avoid spurious dynamics is impractical (too small) to use, especially for the ode23 method. Theoretical studies on the adaptive explicit Runge-Kutta method for long time integration have been gaining more attention recently. Recent work by Stuart (1994, 1995), Humphries (1992), Higham and Stuart (1995) and Aves *et al.* (1995) showed that local error control offers benefits for long-term computations with certain problems and methods. Aves *et al.* addressed the heart of the question of whether local error control confers global properties of steady states of the IVP of autonomous ODEs using adaptive Runge-Kutta type methods.

Aves *et al.*'s work is concerned with long term behavior and global quantities of general explicit Runge-Kutta methods with step size control for autonomous ODEs. They believed that the limit $t_n \rightarrow \infty$ is more relevant than the limit of the variable step sizes $h_n \rightarrow 0$. They studied spurious fixed points that persist for arbitrarily small error tolerances τ . This type of adaptive Runge-Kutta method usually consists of a primary and secondary Runge-Kutta methods of different order. Their main result is positive. When standard local error control is used, the chances of encountering spuriousity is extremely small. For general systems of ODEs, the constraints imposed by the error control criterion make spuriousity extremely unlikely.

ly. For scalar problems, however, the mechanism by which the algorithm succeeds is indirect – spurious fixed points are not removed, but those that exist are forced by the step size selection mechanism to be locally repelling (with the relevant eigenvalues behaving like $O(1/\tau)$).

Griffiths is currently working on the application to hyperbolic PDEs. Preliminary results (private communication with David Griffiths (1996)) showed that it is by no means clear at the moment whether stable spurious solutions may be eliminated. The difference is that, unlike physical problems governed by nonlinear ODEs, nonlinear PDEs may have wave-like solutions rather than fixed points due to the spatial derivatives.

3.4. Convection-Diffusion Model PDEs

Consider a model convection-diffusion equation of the form

$$u_t + f(u)_x = \epsilon u_{xx} \quad (3.12)$$

with the linear case, $f(u) = u$ and the nonlinear case, $f(u) = u^2/2$ (the Burgers equation) respectively. The boundary conditions for the linear case are $u(0, t) = 0$ and $u(1, t) = 1$ and for the nonlinear case, $u(0, t) = 1$ and $u(1, t) = -1$. These boundary conditions result in steady-state solutions of a boundary layer at $x = 1$ and a viscous shock at $x = 1/2$, respectively. In both cases the steepness of the feature is governed by the diffusion coefficient parameter ϵ . Besides its steepness feature, one of the main reasons for considering the linear convection-diffusion equation is to show that grid adaptation alone and/or nonlinear schemes such as TVD schemes can introduce unwanted dynamics to the overall solution procedure. The authors realize that model (3.12) is not the best model to illustrate the dynamics of the studied schemes since the model is not stable under perturbations. However, it serves to show what type of spurious numerics would occur under such an environment.

One common criterion used for grid adaptation is the equidistribution of a positive definite weight

function $w(x, t)$, often taken to be some monitor of the numerical solution $u(x, t)$ of the underlying PDE. A grid $x_0 < x_1(t) < \dots < x_{J-1}(t) < x_J$, where x_0 and x_J are fixed, equidistributes $w(x, t)$ (at time t) if

$$\int_{x_{j-1}}^{x_j} w(x, t) dx = \int_{x_j}^{x_{j+1}} w(x, t) dx = \frac{1}{J} \int_{x_0}^{x_J} w(x, t) dx, \quad (3.13)$$

for $j = 1, \dots, J$. A one-parameter family of weight functions

$$w(x, t) = \sqrt{1 - \alpha + \alpha u_x^2(x, t)}, \quad \alpha \in [0, 1] \quad (3.14)$$

can be chosen where $\alpha = 1/2$ corresponds to equidistribution in the arc-length and $\alpha = 0$ yields a uniform grid. Approximating $w(x, t)$ to be constant in each interval (x_{j-1}, x_j) yields

$$\begin{aligned} & (\sqrt{1 - \alpha + \alpha u_x^2})_{j-1/2} (x_j - x_{j-1}) \\ &= (\sqrt{1 - \alpha + \alpha u_x^2})_{j+1/2} (x_{j+1} - x_j). \end{aligned} \quad (3.15)$$

Given a numerical solution of the PDE we can approximate the derivatives by

$$u_x|_{j-1/2} \approx \frac{u_j - u_{j-1}}{x_j - x_{j-1}} \quad (3.16)$$

Equation (3.15) is nonlinear in $\{x_j\}$ we use (3.16). However, (3.15) is linear in $\{x_j\}$ if $\{x_j\}$ in (3.16) uses the existing grid. In this case we can solve the tridiagonal system (3.15) for a new set of $\{x_j\}$ to obtain an updated grid.

Given a set of initial data and an initial grid, the procedure is to numerically solve the PDE and (3.15) in a time-lagged manner. We use nodal placement and the l_2 norm of the solution to illustrate our results. We use the previous time step value for x_j in (3.16) to achieve a linear tridiagonal system for the updated grid in (3.15). Our preliminary study shows that the solution procedure of Ren and Russell (1992), and Budd *et al.* (1995a) in solving the coupled PDE and (3.15) are less stable than the present linearized form. See also Neil

(1994) for a similar study and conclusion. The regridding strategy adopted was to regrid after every time step of the PDE method, either interpolating updated solution values from the old grid or performing no adjustment at all due to grid movement. This latter approach in effect presents the PDE method with new initial data to the problem at each step. All of the computations were performed on a CM-5 connection machine at NASA Ames. Before presenting the current results, we first give a short summary of our previous work (Sweby & Yee 1994).

The dynamics of the above one-parameter family of mesh equidistribution schemes coupled with three-point central and second-order upwind spatial discretizations of the above linear and non-linear convection-diffusion model equations were studied numerically by Sweby & Yee (1994) using the above numerical procedure. In a parallel study, Budd *et al.* (1995b) made use of the AUTO computer bifurcation package (Doedel 1986) to obtain bifurcation diagrams for similar grid adaptation methods for the steady part of the above PDEs with a different form than (3.15). However, the dependence on known solutions of the discretized PDEs and grid equations as starting values limits its usage. In Sweby & Yee (1994) we utilize the power of the highly parallel Connection Machine CM-5 to undertake a purely numerical investigation into the dynamics of the time-marching adaptive procedure. To examine the effect of grid adaptation alone compared with the time-dependent approach to the steady states with regridding, we also solve the regridding equations (3.15) and (3.16) iteratively using the analytic solutions of the PDE (3.12), starting from a uniform grid. We used a quadrature based equidistribution applied to (3.13), namely the trapezium rule with a large number of subdivisions, to obtain the "exact" placements of the grid nodes for the analytical steady-state solution. It was shown that nonlinearity due to grid adaptation alone can introduce unwanted dynamics. In addition, when time-marched to the steady state, the grid adaptation not only influences the stability and convergence rate of the overall scheme, but can also in-

introduce spurious dynamics into the numerical solution procedure.

Numerical experiments in Sweby & Yee (1994) indicate that there is no major difference in the quality of the results with either an odd or an even number of nodes. We divided a chosen parameter space (e.g., ϵ) into 512 equal intervals, with the rest of parameters (α , Δt , initial data) fixed. For each chosen parameter value, we iterated the discretized PDE and the grid function, in general, 4,000 steps (8,000 steps for explicit methods) to allow the solution to settle to an asymptotic state. Then we performed a series of time step/regridding stages, during which we investigated the dynamics by producing an overlaid plot of the l_2 norms of the numerical solution and the grid distribution at each step. This resulted in a bifurcation type diagram or the grid displacement diagram as a function of the physical or discretized parameters. We also performed numerical studies by preiterating the discretized PDEs to the steady state before solving the discretized PDE and the grid function stages. We found in most cases the solution process is less stable and more likely to get trapped in a spurious mode than in the aforementioned process. The present study (using different types of spatial discretizations) confirms this fact as well.

For the present study, the same model PDEs and time discretizations are studied but the spatial discretization uses the TVD schemes as stated in Section II. As in Sweby & Yee (1994), we have experimented with various explicit methods, such as forward Euler, second and fourth order Runge-Kutta, as well as the linearized implicit (backward) Euler method. As expected, the stable time step required for the explicit methods was orders of magnitude lower than that for the implicit method, so we concentrated on this latter method of solution in this paper. For the grid adaptation study, we also take into consideration the grid density, even and odd dependence, and whether or not there is interpolation after each regridding. The grid density studies consists of 4, 5, 6, 9, 10, 19, 20, 49 and 50 grid points. Again, there is no apparent sign of even or odd grid dependence. The

resolution and stability of TVD schemes are also grid independent. However, the central difference scheme experienced instability more often for coarser grids, and the second-order upwind is slightly more stable, with better resolution than the central scheme.

For the TVD schemes, comparison of the dynamical behavior of the five limiters of (3.50) of Yee (1989) was performed. Due to the simplicity of the PDEs, their dynamical behavior is similar, although there were slight differences in the stability and resolution.

Selected results comparing the linear and nonlinear problems with and without interpolation after each regridding using the "minmod" limiter are shown in Figures 11–14. The same spatially first-order conservative linearized implicit operator for implicit TVD schemes developed in Yee (1986) is used here. See Yee (1986) or Section 3.10.2 of Yee (1989) for the formula. Here we focus on only a few of those obtained using $\alpha = 1/2$. All of the initial values start with a uniform grid and linear interpolation between boundaries. Due to the large number of the discretized parameters that are involved, the dependence of the numerics on initial data is not addressed in this particular study. For each chosen parameter value, we iterate the discretized PDE and the grid function 6,000–18,000 steps (depending on the methods and the convergence monitor) to allow the solution to settle to an asymptotic state. Then, we perform a series of time step/regridding stages, during which we investigate the dynamics by producing an overlaid plot of the l_2 norms or grid distributions at each step. This results in a bifurcation type diagram. Due to a space limitation, only grid distributions as a function of the time step or the diffusion coefficient are shown here. Unless we state otherwise the nodal position plots show the final 512 nodal positions for each node overlaid on the same plot.

3.4.1. Uniform Grid

For both convection-diffusion problems, the behavior of the TVD schemes compared with the

FIGURE 11 (See Color Plate XI).

two classical shock-capturing methods for a uniform grid coincide with past numerical experiments on these schemes. The only difference in our current study is that we map out the behavior of these schemes for a full continuous spectrum of the ϵ and Δt parameters. As expected, the TVD scheme remained stable and approached the correct solution for a much wider range of ϵ (including $\epsilon = 0$) and Δt values than the classical shock-capturing counterpart.

3.4.2. Adaptive Grid

We consider separately the cases “with” and “without” interpolations. The term “scheme” from here on means the over all adaptive scheme procedure. Although the adaptive TVD schemes are compared with the adaptive classical shock-capturing methods, figures shown are only the TVD results.

(a) *No Interpolation*: For the linear problem, the behavior of the adaptive TVD schemes is similar to that of the classical shock-capturing methods. As opposed to the uniform grid case, the adaptive TVD schemes without interpolations behave rather poorly in terms of stability and allowable ϵ values. See Figures 11 and 12. The solutions refuse to settle down for larger Δt and/or smaller ϵ . For the nonlinear problem, the behavior of the adaptive TVD schemes is similar to that of the uniform grid case. The range of allowable ϵ and Δt in terms of stability and convergence rate and settling of the grid distribution are far better than in the linear problem. It appears that for problems with shocks, adaptive TVD schemes prefer no interpolation after each regridding. See Figures 13 and 14. Note that the grid distribution for $\Delta t = 1$ is the same as $\Delta t = 0.1$ for the case with or without interpolations in Figure 14. Studies using 5, 6 and 20

FIGURE 12 (See Color Plate XII).

grids and the grid distribution vs. time steps confirm the above as well. We did not save these plots using the same Δt before the CM-5 was removed from NASA Ames.

(b) *With Interpolations:* For the linear problem, as expected, both adaptive TVD schemes and adaptive classical schemes behave in a similar manner in terms of stability and convergence. Adaptive TVD schemes are less stable and have a smaller allowable range of ϵ than the uniform grid case. Overall, adaptive TVD schemes behave far better than their counterparts without interpolation for the linear problem as can be seen in Figures 11 and 12. For the nonlinear problem, the adaptive TVD schemes with interpolations behave like the classical shock-capturing method. They experience non-convergence of the solution, and the grid distribution cannot settle down for a certain range of Δt . This can be seen in Figures 13 and 14.

It is surprising to see the opposite behavior of the adaptive implicit TVD schemes for the two model PDEs with and without interpolation combinations, especially when the same physical parameters, discretized parameters and initial data were used.

4. A METHOD TO MINIMIZE SPURIOUS DYNAMICS

Due to the spurious dynamics introduced by the numerics, one usually will not be able to map out the complete numerical basins of attraction and bifurcation diagrams for the entire problem in practical situations. Only in isolated situations with a particular physical problem and numerical method combination such as the one studied in Lafon & Yee (1991, 1992) are continuation methods

FIGURE 13 (See Color Plate XIII).

(Kellev, 1977) able to locate all of the essential spurious branches of the bifurcation curves.

On the other hand, continuation methods are widely used in dynamical systems when one wants to understand certain properties of key branches of the bifurcation curve, especially if one knows (or can ascertain by other means) a starting solution on that particular branch. For example, in the Taylor-Couette flow problem, extensive use is made of continuation methods to map out the critical Reynolds number when the flow behavior undergoes drastic changes in flow patterns, since in this case we know how the flow behaves for the low Reynolds number case. Another example is in Bailey and Beam (1991) who used it to study the hysteresis behavior of the flow of an airfoil in terms of angles of attack for the steady PDEs. In this case, the flow behavior is readily obtained for

low angles of attack (before hysteresis). Most of the use of the continuation method so far is focused on elliptic PDEs or steady PDEs. These studies seldom address the possibilities of spurious dynamics due to the numerics, especially for IBVPs using time-marching approaches. It is remarked that a shortcoming in association with solving the steady PDEs is that a small radius of convergence or nonconvergence of the numerical solution is often encountered even with the aid of multigrid, preconditioners, and/or relaxation methods, especially when the PDEs are of the mixed type (e.g., the steady inviscid supersonic flow over a blunt body). In addition, the solutions obtained do not distinguish whether the steady states are stable or not.

Besides the study in Lafon & Yee (1991, 1992), here we propose a further step of applying this

FIGURE 14 (See Color Plate XIV).

technique to the discretized counterparts of the time-dependent PDEs in order to minimize spurious asymptotes due to unknown initial data. The idea relies on the knowledge of a known or a reliable numerical solution on the correct (non-spurious) branch of the bifurcation curve as a function of the physical parameter of interest. The logic is that if one starts on the correct branch, one avoids getting trapped on any of the spurious branches. Also the issue of unknown initial data related to time-marching approaches is avoided or can be minimized. Details of the approach and numerical examples will be reported in a forthcoming paper. Here we will give a short narrative summary of the procedure.

In many fluid problems the solution behavior is well known for certain values of the physical parameters, but unknown for other values. For these other values of the parameters, the problem might

become very stiff and/or strongly nonlinear, making the available numerical schemes (or the scheme in use) intractable. In this situation, continuation methods in bifurcation theory can become very useful. If possible, one should start with the physical parameter of a known or reliable steady state (e.g., flow behavior is usually known for low angles of attack but not for high angles of attack). One can then use a continuation method such as the pseudo arclength continuation method of Keller (1977) (or the recent development in this area) to solve for the bifurcation curve as a function of the physical parameter. The equations used are the discretized counterpart of the steady PDEs or the time-dependent PDEs. If time-marching approaches are used, a reliable steady-state numerical solution (as a starting value on the correct branch of the bifurcation curve for a particular

value of the physical parameter) is assumed. This starting steady-state numerical solution is assumed to have the proper time step and initial data combination and to have the grid spacing fine enough to resolve the flow feature. The continuation method will produce a continuous spectrum of the numerical solutions as the underlying physical parameter is varied until it arrives at a critical value p_c such that it either experiences a bifurcation point or fails to converge. Since we started on the correct branch of the bifurcation curve, the solution obtained before that p_c should be more reliable than if one starts with the physical parameter in question and tries to stretch the limitation of the scheme. From the dynamical behavior of unconditionally stable implicit LMMs, spurious steady states are completely avoided if this type of schemes is used. Note that by starting at a reliable solution on the correct branch of the bifurcation curve, the dependence of the numerical solution on the initial data associated with time-marching methods can be avoided.

Finally, when one is not sure of the numerical solution, the continuation method can be used to double check the numerical solution. This approach can even reveal the true limitations of the existing scheme. In other words, the approach can reveal the critical physical parameter for which the numerical method breaks down. On the other hand, if one wants to find out the largest possible time step that one can use for a particular problem and physical parameter, one can also use continuation methods to trace out the bifurcation curve as a function of the time step. In this case, one can start with a small time step with the correct steady state and observe the critical time step as it undergoes instability or bifurcation.

5. CONCLUDING REMARKS

We have studied some of the super-stable properties of four LMMs using dynamical system approaches and the complex interplay of super-stable schemes with nonlinear spatial schemes (e.g., TVD

schemes) for flows containing shock waves and steep gradients. We have shown the danger of schemes having the super-stability property in simulating complex flow patterns that were previously not understood and/or that are too costly for or not amenable to laboratory experiments.

The present study reveals some of the causes of phenomena observed in practice and illustrates the importance of the knowledge of global nonlinear behavior of numerical schemes. Since standard procedures such as using physical guidelines, grid refinement, halving of the time step, and using more than one scheme to assure the quality, reliability and the integrity of the numerical solution for stiff and strongly nonlinear problems are not foolproof, the dynamical systems approach can be a viable complement. Due to the possible stabilization of an unstable steady state by a super-stable scheme, an implication is that the numerics might predict, e.g., an unphysical reattachment flow. Another important implication is the danger of relying on numerical experimentation for the onset of laminar instability and for the prediction of transition to turbulence or chaotic flows. This stems from the fact that numerics can introduce and suppress chaos; numerics can also introduce chaotic transients and spurious steady states or can stabilize unstable steady states. Examples of spurious behavior observed in CFD computations are reported in Yee & Sweby (1996a,b) and Yee *et al.* (1997).

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