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REVISITING A FLAME PROBLEM. REMARKS ON SOME NON-STANDARD FINITE DIFFERENCE SCHEMES

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Abstract. We consider the flame problem, a standard example of a stiff ordinary differential equation, and several non-standard finite difference methods (NSFDMs) recently developed for solving it. We highlight the large errors around the middle of the integration interval between the numerical solutions given by these schemes and the exact solution showing that considering relatively large step-sizes, which was thought to be one of the main advantages of NSFDMs, leads to poor accuracy. Emphasizing mild instability and the rapid transition on a short interval as the sources of these errors we indicate ways of obtaining accurate numerical results and we provide examples of highly accurate numerical solutions obtained with several standard routines for solving initial value problems.

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Key words. Stiff differential equations, Nonstandard finite difference methods, MATLAB ode solvers, Numerical comparisons

1. INTRODUCTION

One standard example of a stiff ordinary differential equation, which has been considered e.g., in [8], [9], [5], [4] or [6] is the following simple model of flame propagation

$$y'(t) = y^2(t) - y^3(t), \quad y(0) = \delta, \quad 0 \le t \le \frac{2}{\delta}. \tag{1}$$

The analytical solution for the initial value problem (1) involves the Lambert W function and is given by

$$y(t) = \frac{1}{W(ae^{a-t}) + 1}, \qquad a = \frac{1}{\delta} - 1. \tag{2}$$

The initial condition $\delta > 0$ is a small perturbation of zero and the solution is sought on an interval inversely proportional to δ. The problem (1) is known to be non-stiff on the interval $[0, 1/\delta]$ and stiff on the region where the solution approaches steady state, i.e., on the subinterval of $[1/\delta, 2/\delta]$ on which $y(t) \approx 1$ (e.g., [8], [9]). The smaller the value of δ, the more exacerbated the stiffness behaviour is. An asymptotic analysis in [7] shows that the exact solution has a rapid transition towards the steady state on an interval of length $O(-\ln \delta)$ around $1/\delta$. Thus, as δ decreases the transition region becomes narrower, relative to the length of the integration interval.

The error between a numerical solution and the exact solution (2) provides an important criteria for comparing different numerical methods applied to the flame problem (1). Using MATLAB's implementation of the Lambert W function we study the accuracy of several numerical methods. In Section 2 we reconsider the numerical simulations in [1], analyzing two non-standard finite difference schemes (NSFDMs) designed to solve this combustion equation. The numerical solutions obtained with these schemes haven't been compared in [1] with the exact solution. Although they behave very similar to the analytical solution, a comparison of the two reveals large errors around $1/\delta$. We underline the poor accuracy on this region of these schemes for relatively large step-sizes, which was considered in [1] to be one of their main advantages. In Section 3 we discuss the sources of these large errors, emphasizing the mild instability of the problem on the interval $[0, 1/\delta]$ and the rapid transition in the middle that imposes a drastic decrease of the step size. We also prove that the exact solution increases from a value α to a value β $(0 < \alpha < \beta < 1)$ in a time that doesn't depend on δ and, hence, the transition region is constant for all integration intervals. We end this section with numerical results showing that standard routines can solve the flame problem with very high accuracy if the step size is properly controlled by taking suitable values for the relative and absolute error tolerances.

2. ACCURACY OF NON-STANDARD FINITE DIFFERENCE SCHEMES

Several non-standard finite difference schemes have been recently devised for solving the flame problem (1), based on discretizations of the first derivative and on different approximations of the nonlinear terms. In [1] the authors consider the following two one-step schemes

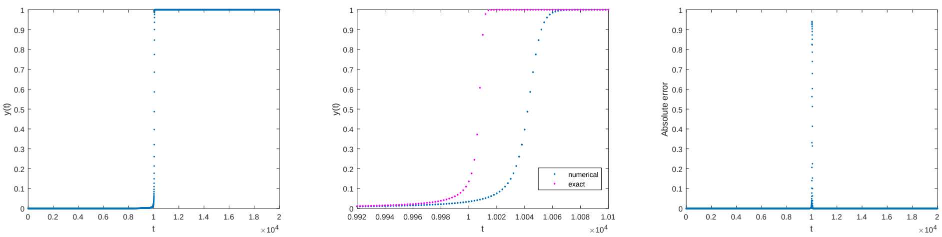
$$y_{k+1} = \frac{(1 + 2\phi(h)y_k)\, y_k}{1 + y_k(1 + y_k)\phi(h)} \tag{3}$$

and

$$y_{k+1} = y_k + \phi(h) \left(ay_k^2 + (1-a)y_k y_{k+1} - by_k^3 - (1-b)y_k^2 y_{k+1} \right), \tag{4}$$

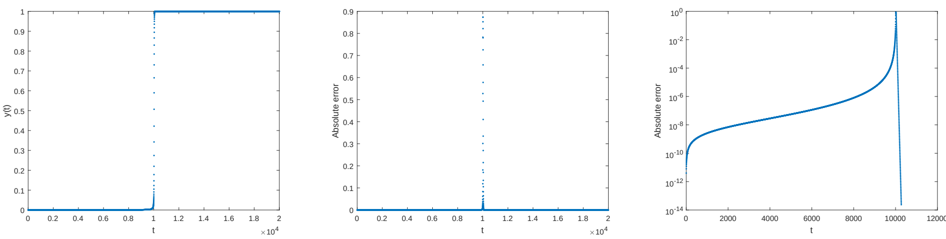
where $\phi(h) = 1 - e^{-h}$ or $\phi(h) = h$, $a \geq 1$ and $b \leq -1/2$.

The numerical simulations in [1] presenting the solutions in Figs. 2.1a and 2.2a suggest that the NSFDMs (3) and (4) provide satisfactory results for a step size $h = 2$, but a comparison with the exact solution shows large errors around $1/\delta$, as it can be seen in Figs. 2.1b and 2.2b. Semilog plots of the absolute errors to the exact solution (Figs. 2.1c and 2.2c) give more insight: the errors accumulate on $[0, 1/\delta]$, then grow fast nearby $1/\delta$, the methods succeeding to solve the problem with high accuracy on the region of stiffness in $[1/\delta, 2/\delta]$. These aspects will be clarified in Section 3.



(A) Numerical solution. (B) Around $1/\delta$. (C) Absolute error.

FIG. 2.1 – Solving (1) with NSFDM (3) for $\delta = 10^{-4}$, $\phi(h) = h$, $h = 2$.



(A) Numerical solution. (B) Absolute error. (C) Semilog of absolute error.

FIG. 2.2 – Solving (1) with NSFDM (4) for $\delta = 10^{-4}$, $a = 1$, $b = -3$, $\phi(h) = h$, $h = 2$.

3. REVISITING THE FLAME PROBLEM

A linear stability analysis in [8] and [9] explains the source of errors obtained in numerical simulations. The scalar Jacobian $J = \frac{\partial F(t,y)}{\partial y} = 2y - 3y^2$ on is positive on $[0, y^{-1}(1/3)) \supset [0, 1/\delta]$ and the problem is unstable. At the same time $J = O(\delta)$ on most of the interval $[0, 1/\delta]$ so the problem is only mildly unstable on an interval of length $O(1/\delta)$. Standard methods for non-stiff problems, like explicit Runge-Kutta, can be employed successfully. On the transition region where the solution rapidly increases to the steady state value 1 any method will need a relatively small step size to handle the sharp change. With control over the step-size, standard non-stiff methods are again feasible. On the interval in $[1/\delta, 2/\delta]$ where $y(t) \approx 1$ we have $J \approx -1$. Stability combined with the long integration interval and a slowly varying solution make the problem stiff. On this interval non-stiff methods have many failed steps and stability concerns regarding the computed solution impose a small step-size. Methods for stiff problems provide satisfactory results.

We exemplify these remarks in Tables 1 and 2 with more numerical simulations using MATLAB's ode solvers, the explicit Runge-Kutta method of order

solver	RelTol	AbsTol	Max. Err.	Err. Norm	Steps
radau	1.00e-03	1.00e-06	2.34e-02	4.41e-02	4.70e+01
dop853	1.00e-03	1.00e-06	1.36e-03	3.19e-02	1.58e+03
ode45	1.00e-03	1.00e-06	3.37e-02	9.97e-02	1.21e+04
ode113	1.00e-03	1.00e-06	9.84e-01	3.16e+00	6.11e+03
ode15s	1.00e-03	1.00e-06	9.97e-01	4.79e+00	1.08e+02
radau	1.00e-08	1.00e-12	1.37e-07	5.16e-07	1.43e+02
dop853	1.00e-08	1.00e-12	2.75e-06	5.71e-06	1.62e+03
ode45	1.00e-08	1.00e-12	3.22e-07	2.18e-06	1.28e+04
ode113	1.00e-08	1.00e-12	4.30e-05	1.86e-04	6.63e+03
ode15s	1.00e-08	1.00e-12	4.95e-04	3.22e-03	5.63e+02
radau	1.00e-13	1.00e-20	2.24e-11	3.39e-11	1.44e+02
dop853	1.00e-13	1.00e-20	1.29e-11	5.32e-11	7.54e+02
ode45	1.00e-13	1.00e-20	2.59e-11	5.61e-10	2.04e+04
ode113	1.00e-13	1.00e-20	1.08e-09	7.19e-09	6.80e+03
ode15s	1.00e-13	1.00e-20	3.25e-08	5.56e-07	3.72e+03

Table 1 – $\delta = 10^{-4}$

solver	RelTol	AbsTol	Max. Err.	Err. Norm	Steps
radau	1.00e-03	1.00e-06	9.97e-01	4.12e+00	6.40e+01
ode45	1.00e-03	1.00e-06	–	–	1.20e+06
ode113	1.00e-03	1.00e-06	–	–	5.82e+05
ode15s	1.00e-03	1.00e-06	1.00e+00	6.31e+00	1.17e+02
radau	1.00e-08	1.00e-12	2.47e-03	5.02e-03	1.97e+02
ode45	1.00e-08	1.00e-12	–	–	1.21e+06
ode113	1.00e-08	1.00e-12	–	–	6.21e+05
ode15s	1.00e-08	1.00e-12	8.57e-01	7.88e+00	7.47e+02
radau	1.00e-13	1.00e-20	1.36e-09	4.14e-09	2.03e+02
ode45	1.00e-13	1.00e-20	–	–	1.22e+06
ode113	1.00e-13	1.00e-20	–	–	5.18e+05
ode15s	1.00e-13	1.00e-20	3.26e-06	5.56e-05	5.34e+03

Table 2 – $\delta = 10^{-6}$

8 DOP853 from [2] and the implicit Runge-Kutta method of variable order (5, 9, 13) RADAU from [3]. The columns represent the used solver, relative error tolerance, absolute error tolerance, maximum error, error norm and the total number of steps.

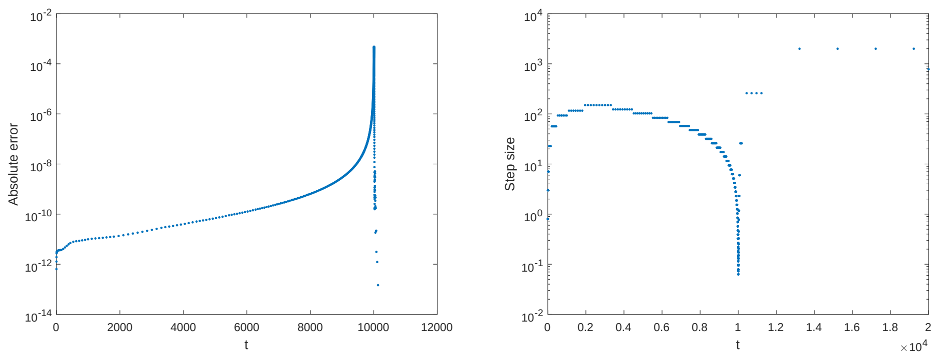
From (2) one can find the inverse y^{-1} of the exact solution and obtain

$$y^{-1}(z) = \ln a + a - \ln\left(\frac{1}{z} - 1\right) - \frac{1}{z} + 1, \qquad \forall z \in (0,1). \tag{5}$$

Using the inverse function we determine the length of the transition interval between two values α and β of the exact solution, with $0 < \alpha < \beta < 1$.

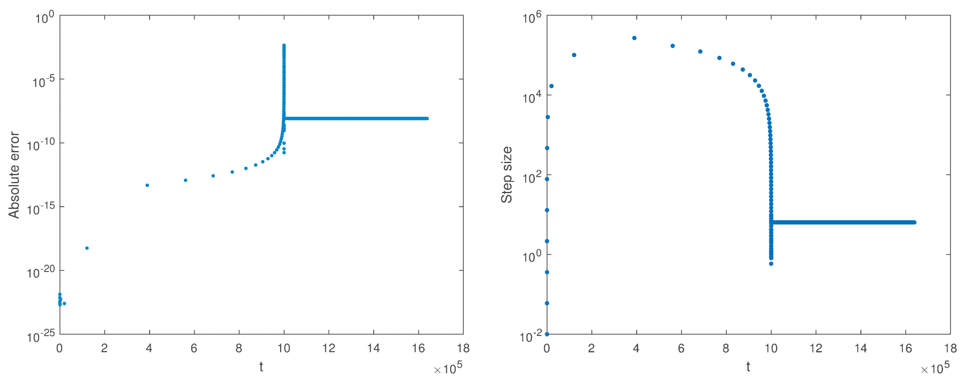
$$|y^{-1}(\alpha) - y^{-1}(\beta)| = \left| \ln \frac{\alpha(1-\beta)}{\beta(1-\alpha)} + \frac{\alpha - \beta}{\alpha\beta} \right|. \tag{6}$$

Hence the length of the transition interval between two fixed values of the exact solution doesn't depend on δ. As δ decreases, the increase of errors is caused only by the more accentuated instability on the first half of the integration interval (due to its increasing length) that leads to error accumulation and not by the transition region, which is constant, as we have proved above.



(A) Absolute error semilog. (B) Step sizes semilog.

FIG. 3.3 – ode15s (BDF) for $\delta = 10^{-4}$, RelTol= 10^{-8}, AbsTol= 10^{-12}.



(A) Absolute error semilog. (B) Step sizes semilog.

FIG. 3.4 – dop853 for $\delta = 10^{-4}$, RelTol= 10^{-8}, AbsTol= 10^{-12}.

REFERENCES

[1] S. Abelman and K. C. Patidar, *Comparison of some recent numerical methods for initial-value problems for stiff ordinary differential equations*, Comput. Math. Appl., 55 (2008), pp. 733–744.
[2] E. Hairer, S. P. Nørsett, and G. Wanner, *Solving Ordinary Differential Equations I, Nonstiff Problems*, Springer-Verlag, Berlin, 2nd ed., 2009.
[3] E. Hairer and G. Wanner, *Solving Ordinary Differential Equations II, Stiff and Differential Algebraic Problems*, Springer-Verlag, Berlin, 2nd ed., 2010.
[4] C. Moler, *Stiff differential equations*, 2003.
[5] ———, *Numerical Computing with MATLAB*, SIAM, Philadelphia, 2008.
[6] ———, *Ordinary differential equations, stiffness*, June 2014.
[7] R. E. O'Malley, *Singular Perturbation Methods for Ordinary Differential Equations*, Springer-Verlag, New-York, 1991.
[8] L. F. Shampine, I. Gladwell, and S. Thompson, *Solving ODEs with MATLAB*, Cambridge University Press, 2003.
[9] L. F. Shampine and S. Thompson, *Stiff systems*, Scholarpedia, 2 (2007), p. 2855.

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