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Stability of the leapfrog/midpoint method

L.F. Shampine

Mathematics Department, Southern Methodist University, 208 Clements Hall, 3200 Dyer Street, P.O. Box 750156, Dallas, TX 75275, United States

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ABSTRACT

The leapfrog method is popular because of its good stability when solving partial differential equations with oscillatory solutions. "It has the disadvantage that the solution at odd time steps tends to drift farther and farther from the solution for even time steps, so it is common to stop the integration every twenty time steps or so and reinitialize with the first order forward Euler method ...". We prove that restarting in this way results in a method that is *not* stable. We further show that if the step size is not too big, perturbations grow so slowly that the computations are stable enough for practical purposes. The leapfrog method is not dissipative, but we show that restarting results in a method with a useful amount of dissipation. We also show that Gragg's smoothing scheme improves the stability of the method.

1. Introduction

The leapfrog method is widely used to solve numerically initial-boundary value problems for partial differential equations (PDEs). It is attractive because it is simple, second-order, and has a short memory, but most of all because it has very good stability when computing oscillatory solutions. Some numerical methods for PDEs are commonly studied by viewing them as arising from the method of lines (semi-discretization). In this approach the PDEs are first approximated by a system of ordinary differential equations (ODEs) in time obtained by discretizing the spatial variables and boundary conditions. If the method for solving the PDEs can be viewed as a method for solving the resulting ODEs, the standard absolute stability theory for numerical solution of ODEs can be applied. This approach is especially popular when the spatial discretization is pseudospectral, c.f. [1–3]. In this view of the computations, the leapfrog method for PDEs amounts to solving an initial value problem for a system of ODEs with the midpoint method. Specifically, a first-order system of equations

$$y' = f(t, y) \tag{1}$$

is solved on an interval $[t_0, t_f]$ with initial value $y_0 = y(t_0)$. With $t_n = t_0 + nh$ and $y_n \approx y(t_n)$, the midpoint method is

$$y_{n+1} = y_{n-1} + 2hf(t_n, y_n). \tag{2}$$

A simple and convenient way to start the midpoint method is to use the forward Euler method

$$y_1 = y_0 + hf(t_0, y_0). \tag{3}$$

In this article we analyze a standard way of dealing with a practical difficulty in using the leapfrog method: "It has the disadvantage that the solution at odd time steps tends to drift farther and farther from the solution for even time steps, so it is common to stop the integration every twenty time steps or so and reinitialize with the first order forward Euler method ..." [1, p. 174]. We prove that for all N, restarting after N steps results in a method that is *not* stable in precisely the circumstances for which the leapfrog method is attractive because of its stability! In light of this disconcerting result,

E-mail address: shampine@smu.edu

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we must ask why the computations do not "blow up". That can happen, but we show that if the step size is not too big, perturbations grow so slowly that the computations are stable enough for practical purposes. Because the leapfrog method has no dissipation, many authors, e.g. [3, p. 65], suggest adding some artificial dissipation. We show that restarting already provides a useful amount of dissipation.

Gragg [4] proved that if the midpoint method is started with (3), the error has an asymptotic expansion in powers of h^2. For this reason he suggested using the midpoint method with restart after N steps as the basis of an extrapolation method for solving (1). To improve the stability properties of the method, he proposed a smoothing scheme based on a weighted average. As it turns out, smoothing is not helpful when extrapolating, but we show that it does help in the present context. Indeed, because smoothing is easy enough to implement and our results show it to be worthwhile, we favor using it when restarting to improve the qualitative behavior of the midpoint method.

2. Stability of the midpoint method

The theory of absolute stability studies the propagation of perturbations to the numerical solution of a system of ODEs. As is typical when investigating stability, a given system of equations (1) is linearized and approximations are made to reduce the task to studying the propagation of perturbations to numerical solutions of the test equation

$$y' = \lambda y. \tag{4}$$

In this λ arises as an eigenvalue of a local Jacobian of the function $f(t,y)$, so it may be complex. One of the simplifications made to get insight is to use a constant step size $h > 0$. Because the test equation is linear and homogeneous, stability amounts to computed solutions having the same behavior as solutions of the ODE itself. We assume that the eigenvalues all satisfy $Re(\lambda) \leqslant 0$ because we are most concerned about the stability of numerical methods for computing solutions that are themselves stable. Many methods have unsatisfactory behavior for λ on the imaginary axis. The midpoint method is quite attractive then because it produces a bounded solution, which is to say that it is stable, for $h\lambda \in [-i, i]$. Unfortunately, it is not stable for any $h\lambda$ with $Re(\lambda) < 0$.

For the test equation the midpoint method becomes

$$y_{n+1} = y_{n-1} + 2zy_n,$$

where it is convenient to introduce $z = h\lambda$. An equation of this kind has a solution of the form $y_n = \xi^n$ provided that ξ is a root of the characteristic equation $\xi^2 = 1 + 2z\xi$, namely

$$\xi_1 = z + \sqrt{1+z^2}, \qquad \xi_2 = z - \sqrt{1+z^2}. \tag{5}$$

The two roots lead to two linearly independent solutions, so in general y_n has the form

$$y_n = \alpha\xi_1^n + \beta\xi_2^n \tag{6}$$

with constants α,β that are determined by the initial values y_0, y_1. The absolute stability region of the method is the region S in $Re(z) \leqslant 0$ such that if $z \in S$, then $|y_n|$ is bounded for all n. For linear multistep methods like the midpoint method, this is equivalent to the region in the left-half complex plane where the characteristic roots have magnitude no greater than 1. All we need right now is the observation that if the eigenvalue is pure imaginary, $\lambda = \omega i$, and $(h\omega)^2 \leqslant 1$, then both roots satisfy $|\xi|^2 = (h\omega)^2 + [1 - (h\omega)^2] \equiv 1$. This says that the method is stable for z in the interval $[-i, +i]$.

Gragg [4] proposed starting the explicit midpoint method with the forward Euler method because it is a simple way to obtain a method with an error that can be expanded in powers of h^2. The idea of extrapolation is to integrate repeatedly to a fixed point t with various step sizes h. The results are then combined, *extrapolated*, so as to remove successive terms in the error expansion. Some notation will make it easier to discuss the asymptotic behavior of the error. If $t = t_0 + nh$, let $\eta(t; h) = y_n$. If the function $f(t,y)$ in (1) is sufficiently smooth, then

$$\eta(t;h) = y(t) + \sum_{k=1}^{M} h^{2k}[u_k(t) + (-1)^{(t-t_0)/h} v_k(t)] + O(h^{2M+2}). \tag{7}$$

The leading terms satisfy differential equations of the form

$$u_1'(t) = f_y(t, y(t))u_1(t) + \text{function of } t, \quad u_1(t_0) = 0,$$
$$v_1'(t) = -f_y(t, y(t))v_1(t) + \text{function of } t, \quad v_1(t_0) = 0.$$

Here $f_y(t,y(t))$ is the Jacobian of f. Notice that the equation for the weakly stable component $v_1(t)$ has a character opposite that of $y(t)$ and $u_1(t)$.

The expansion (7) shows the distinction between the behavior at even time steps and odd time steps mentioned in Section 1. Gragg showed that the term involving $v_1(t)$ can be removed while retaining an error that can be expanded in powers of h^2 by smoothing at t,

$$S(t;h) = \frac{1}{4}\eta(t-h;h) + \frac{1}{2}\eta(t;h) + \frac{1}{4}\eta(t+h;h). \tag{8}$$

It is easy to see that

$$S(t;h) = y(t) + h^2\left[u_1(t) + \frac{1}{4}y''(t)\right] + \sum_{k=2}^{M} h^{2k}[\tilde{u}_k(t) + (-1)^{(t-t_0)/h}\tilde{v}_k(t)] + O(h^{2M+2}).$$

This replaces the oscillation involving $v_1(t)$ with a smooth term involving $y''(t)/4$ and alters the higher order terms without affecting the nature of the expansion.

It is plausible that removing the leading oscillatory term by smoothing would provide a better extrapolation method, so all the early programs did this. However, as Deuflhard and Bornemann [6, p. 175] say, "Formerly, Gragg's smoothing step was thought to promise a better-behaved discretization. But the resulting improvement in the total computational time observed in practice has been found marginal at best." Shampine and Baca [7] provide a simple explanation: The purpose of extrapolation is to remove successive terms in the asymptotic expansion, so the term involving $v_1(t)$ is removed at the first extrapolation. All the codes do at least one extrapolation, so there is no need to remove it by smoothing. The circumstances we investigate here are different from those of extrapolating the midpoint method, but the asymptotic analysis suggests that smoothing might be helpful. We shall prove that it does not stabilize the midpoint method with restart for eigenvalues on the imaginary axis, but it does provide a worthwhile improvement to the stability of the method, not only on the imaginary axis but also in the left-half complex plane.

3. Limit case

The properties of the restarted midpoint method that we establish in this article are foreshadowed by the limit case of restarting after just one step:

$$y_1 = y_0 + hf(t_0, y_0),$$
$$y_2 = y_0 + 2hf(t_0 + h, y_1).$$

We recognize this as a familiar two-stage, second-order Runge–Kutta formula [5, p. 67] for advancing from t_0 to $t_0 + 2h$. All two-stage, second-order Runge–Kutta formulas have the *same* region of absolute stability that is displayed in many texts, for example [2, p. 109]. The formula has respectable stability in the left-half complex plane. We interpret this as saying that restarting helps stabilize computations with the midpoint method by adding dissipation. Unfortunately, the stability region intersects the imaginary axis only at the origin, so the method is unstable when the local Jacobian has eigenvalues that are purely imaginary. Nevertheless, it is shown in [2, §4.3.1] that when the second-order Adams–Bashforth method is applied to the periodic advection problem, the instability due to such eigenvalues is weak. It is further stated that two-stage, second-order Runge–Kutta methods have the same weak instability. This helps explain why the method might be still useful for imaginary eigenvalues, but the result is established in [2] for step sizes h that go to zero and in this article we are most interested in the stability of the method for "large" h.

4. Stability on the imaginary axis

Because the behavior of the method on the imaginary axis is so important to the midpoint method, we investigate carefully the effects of restarting in this case. We begin with a few observations about stability and the test equation. As illustrated by the representation (6), if all the characteristic roots satisfy $|\xi_k| < 1$, perturbations to y_0 and y_1 tend to zero as the integration proceeds. A transition case is when a characteristic root has magnitude one. This case is especially interesting for the midpoint method because it is true of both roots when $\lambda = \omega i$ and $|h\omega| \leqslant 1$. Clearly initial perturbations are then bounded and the method is stable, but it is also clear that for any given N, the solution y_N might have magnitude bigger than one. This value is the characteristic root for the explicit Runge–Kutta method that results from restarting after N steps, so if the magnitude is greater than 1, the method is unstable. With this in mind, we prove now that *none* of the methods that result from restarting is stable on an interval of the form $[-i\Omega, i\Omega]$ with real $\Omega > 0$.

4.1. Small step sizes

We begin by working out some details for the solution (6). To study stability for the homogeneous test equation (4), we can assume that $y_0 = 1$. The forward Euler method is used to compute the starting value y_1, so $y_1 = 1 + z$. We consider the behavior of y_n when $\lambda = (h\omega)i$ for real ω. It will be convenient to write $\delta = \sqrt{1 - (h\omega)^2}$. The two characteristic roots are then $\xi_{1,2} = (h\omega)i \pm \delta$ and solving for the α, β that yield the given y_0, y_1 results in

$$y_n = \left(\frac{\delta + 1}{2\delta}\right)\xi_1^n + \left(\frac{\delta - 1}{2\delta}\right)\xi_2^n. \tag{9}$$

For a given number of steps N, we now ask how $|y_N|$ behaves as $h\omega \to 0$. Because $\delta \sim 1 - (h\omega)^2/2$, we have $\alpha \sim 1 + (h\omega)^2/4$ and $\beta \sim -(h\omega)^2/4$. Also $\xi_1 \sim (h\omega)\, i + 1 - (h\omega)^2/2 \sim 1 + (h\omega)i$. This implies that $\xi_1^N \sim 1 + N(h\omega)i$. Similarly, $\xi_2 \sim -1 + (h\omega)i$ and $\xi_2^N \sim (-1)^N(1 - N(h\omega)i)$. All together, we have $y_N \sim 1 + N(h\omega)i$. The square of the magnitude $|y_N|^2 \sim 1 + N^2(h\omega)^2$ as $h\omega \to 0$.

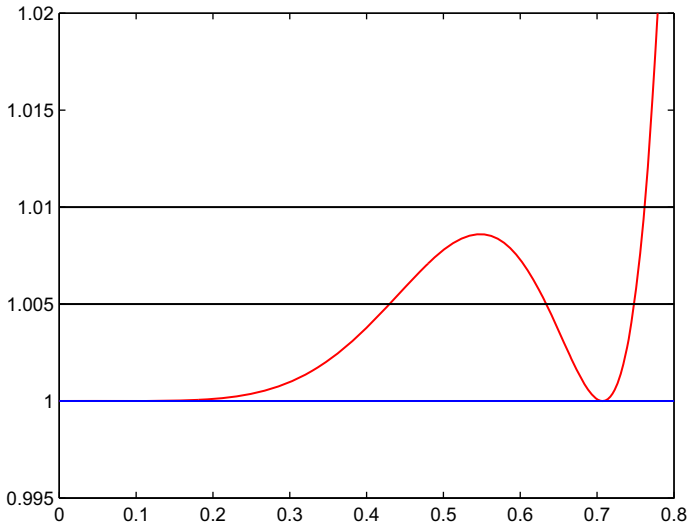

Fig. 1. Stability on imaginary axis with smoothing, $N = 4$.

This says that for any given number of steps N, we have $|y_N| > 1$ for all $z = (h\omega)i$ that are sufficiently small in magnitude. That is, the stability region of the method that restarts after N steps does not include any interval of the form $[-\Omega i, \Omega i]$ with real $\Omega > 0$.

We argue now that smoothing does not alter the qualitative behavior of the restarted midpoint method on the imaginary axis. Consider the Runge–Kutta formula obtained by starting with the forward Euler method, taking N steps with the midpoint method, and smoothing the result by Gragg's scheme (8). We have already seen that for the test equation with $\lambda = (h\omega)i$, the numerical solution $y_N \sim 1 + N(h\omega)i$ as $h\omega \to 0$. It then follows that $S(t;\ h) \sim 1 + N(h\omega)i$, which is to say that to leading order, the behavior of the smoothed result is the same as that of y_N itself. And, we have just seen that asymptotically $|y_N| > 1$ for all N, hence the scheme is unstable on all intervals of the form $[-\Omega i, \Omega i]$ with real $\Omega > 0$.

4.2. Why doesn't it blow up?

In view of the results just established, we must ask why computations with the leapfrog method do not blow up when there are eigenvalues on the imaginary axis. In Section 3 we cited an investigation that shows the instability to be weak for the case of $N = 2$ when no smoothing is done. In Section 4.1 we proved that for all sufficiently small $h\omega$, the growth factor is bigger than 1. In our experiments for a range of N and both smoothing and not smoothing, the growth factor has been bigger than 1 for *all* $h\omega$. In this section we investigate numerically the size of the growth factor.

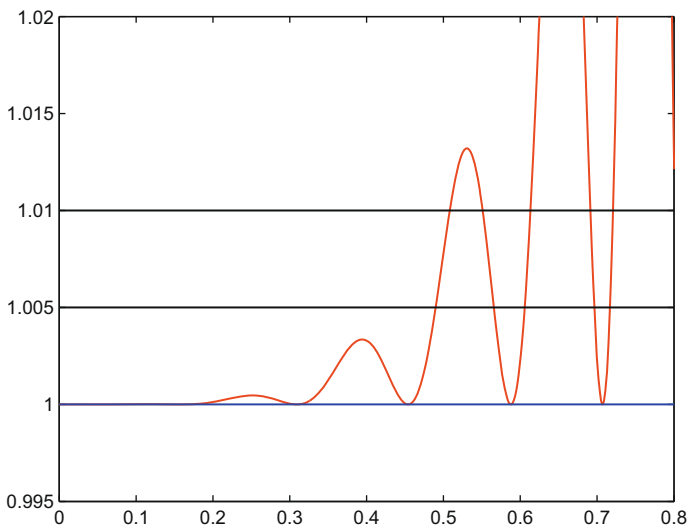

Fig. 2. Stability on imaginary axis with smoothing, $N = 20$.

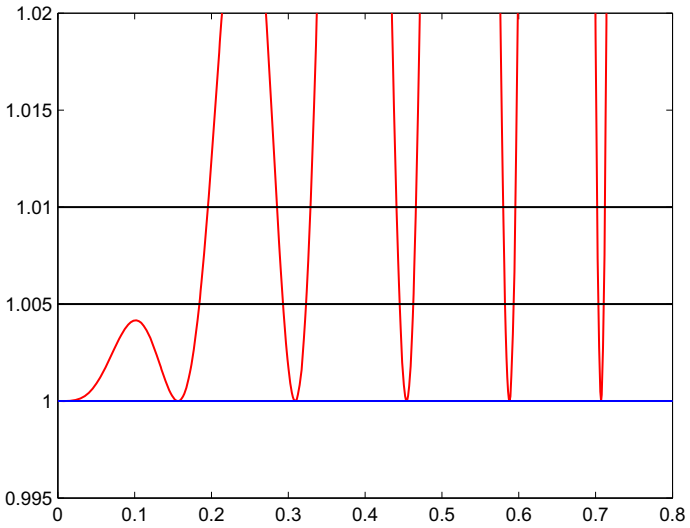

Fig. 3. Stability on imaginary axis without smoothing, $N = 20$.

Figs. 1 and 2 show the growth factor as a function of $h\omega$ for the methods resulting from smoothing at $N = 4$ and $N = 20$ steps, respectively. The method with $N = 20$ corresponds roughly to five steps of the method with $N = 4$. Correspondingly if the growth factor with $N = 4$ is $1 + g$, we must compare a growth after five steps of $(1 + g)^5 \approx 1 + 5g$ to the growth factor for the method with $N = 20$. When this is taken into account, we recognize that the behavior on the imaginary axis is considerably improved by increasing N. We might have expected this as the method then resembles more the midpoint method which is stable for $h\omega \leqslant 1$. Of course, the behavior of the growth factor is not at all uniform, so it is appropriate to consider an interval for which the growth is modest. For example, if a growth of no more than half a percent is acceptable, we could say that the method with smoothing and $N = 20$ is stable in practice for $h\omega < 0.5$, an interval nearly half the interval of stability of the underlying midpoint method. Our attention has been directed to intervals where the method is "almost" stable, but as the plots suggest, there are $h\omega$ in the interval where the midpoint method is stable for which restarting leads to explosive growth.

Our computations have shown that smoothing improves considerably stability on the imaginary axis. For example, Figs. 2 and 3 show that smoothing has increased the interval on which growth is no more than half a percent from roughly $h\omega < 0.2$ to $h\omega < 0.5$. It is little trouble to smooth along with restarting, so we recommend it. Moreover, as we discuss in the next section, smoothing is also helpful as regards dissipation.

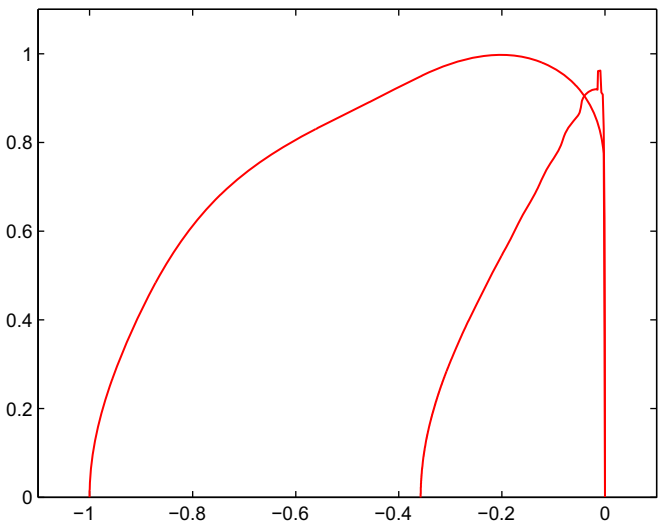

Fig. 4. Stability with smoothing: $N = 4$ (larger region) and $N = 20$.

5. Dissipation

Though the stability region of the limit case discussed in Section 3 does not include the imaginary axis, it is otherwise quite satisfactory. We have plotted stability regions for a wide range of N with and without smoothing. For both possibilities the size of the region decreases as N increases. This is to be expected because as N is increased, the method behaves more like the underlying midpoint method. However, even for relatively large N, restarting provides a useful amount of dissipation. The two regions plotted in Fig. 4 are representative. When smoothing is not done, the regions are similar, but they are not as big and the boundaries are less smooth. We recommend smoothing, so we display here stability regions only for this variant.

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