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Journal of Computational Physics 187 (2003) 95–109

JOURNAL OF COMPUTATIONAL PHYSICS

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Telescopic projective methods for parabolic differential equations

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Received 28 November 2001; received in revised form 1 February 2003; accepted 7 February 2003

Abstract

Projective methods were introduced in an earlier paper [C.W. Gear, I.G. Kevrekidis, Projective Methods for Stiff Differential Equations: *problems with gaps in their eigenvalue spectrum*, NEC Research Institute Report 2001-029, available from http://www.neci.nj.nec.com/homepages/cwg/projective.pdf Abbreviated version to appear in SISC] as having potential for the efficient integration of problems with a large gap between two clusters in their eigenvalue spectrum, one cluster containing eigenvalues corresponding to components that have already been damped in the numerical solution and one corresponding to components that are still active. In this paper we introduce iterated projective methods that allow for explicit integration of stiff problems that have a large spread of eigenvalues with no gaps in their spectrum as arise in the semi-discretization of PDEs with parabolic components.

Keywords: Integration; Stiff; Explicit; Stability; Legacy codes

1. Introduction

In [1] we introduced the projective method which is based on the following very simple idea: any stable method (the inner integrator) is used to integrate a problem over a number of small steps and then a *projective* [2] step uses polynomial extrapolation to compute an approximation to the solution far ahead of the inner integration steps. The first k steps of the inner integrator serve to damp the fast components in the solution. The projective step then uses the result of the last step and the results from the next q inner steps to extrapolate forward. This is shown in Fig. 1 with $k = 2$ and $q = 1$. It is clear that the slope of the chord through y_2 and y_3 in Fig. 1 is a first-order approximation to the derivative, so we call this example a Projective Forward Euler (PFE) method.

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[1] Supported in part by AFOSR (Dynamics and Control program, Dr. Mark Jacobs and Dr. Belinda King).
[2] The term *projective method* was used rather than *extrapolation method* because the latter term has already been used for another class of methods. *Projective* should be associated with *projectile* and not be confused with the mathematical term *projection*.

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doi:10.1016/S0021-9991(03)00082-2

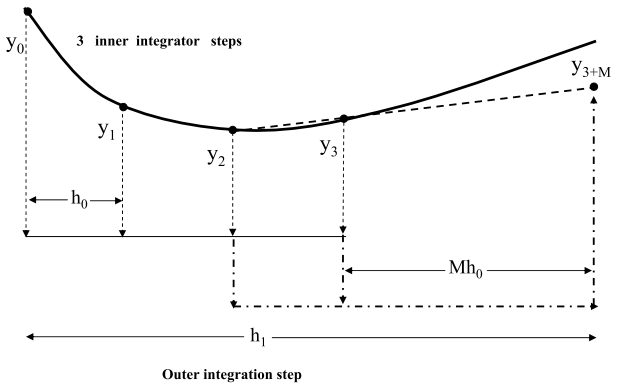

Fig. 1. Projective Forward Euler method with $k = 2$ and $q = 1$.

The combination of the inner steps and the projective step effectively constitutes another integrator which we call the *outer* integrator. It was shown that this integrator could be constructed so that it was absolutely stable (hereafter referred to as "stable") if the eigenvalues of the problem Jacobian matrix were in one of two regions, one corresponding to rapidly decaying components handled very stably by the inner step and one corresponding to an approximation to the stability region of the outer integrator (the Forward Euler in the example of Fig. 1). Thus, for problems with a large gap between the time constants of the fast inactive components and the time constants of the slow active components (those still causing changes in the solution) one is able to project forward over large steps, commensurate with the slow components, and gain speed (i.e., increase average step size). In the example shown in Fig. 1 we use three inner integration steps of length h_0 to cover a distance $h_1 = (3 + M)h_0$. If we assume that the inner integration step represents the bulk of the work (because, for example, evaluations of the derivatives are very expensive) and that it is not possible to use a larger step size in the inner integrator, then we can define the speedup of the projective method as *the number of inner integration steps needed to integrate over the interval directly divided by the number used when combined with the projective step.* Thus the PFE method in Fig. 1 has a speedup of

$$S = (3 + M)/3.$$

We are particularly interested in the application of these methods when the inner integrator is a legacy code that performs one time step. Often it is extremely difficult to modify such codes because they represent many years of development, employ numerous devices such as split steps, and the original developers may have long since left.

In this paper we consider an obvious extension of the projective method: Since the outer, or projective integrator can be viewed as just another integrator, why not use it as the inner integrator in yet a further projective integrator, and so on, ad infinitum? This is illustrated in Fig. 2 which has two projective levels. Note that in this illustration the speedup of the 2nd level method is $[(3 + M)/3]^2$ since we cover a distance $(3 + M)^2 h$ with nine inner integrations.

The methods resulting from this iteration of the projective step can have two quite different sets of properties. In one case they can handle problems that have multiple gaps – that is, whose eigenvalues lie in one of a number of well-separated regions of the complex plane. In the second case we can choose the method parameters so that its stability region includes a large section of the negative real axis and neighboring points in the complex plane – methods we will call "$[0, 1]$ stable" for reasons that will be apparent later. This is the case that is applicable to parabolic equations and will be discussed in this paper. The multiple gap case is discussed in [2].

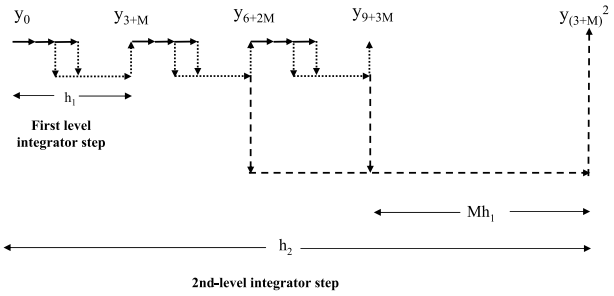

Fig. 2. A two-level projective integrator.

In the next section we will briefly review the stability analysis of projective methods and their important properties so that we can discuss $[0, 1]$ stable methods in the third section.

2. Stability analysis

The usual linear stability analysis of time-stepping methods discusses stability in the $h\lambda$-plane, where h is the time step and λ is an eigenvalue of the local linearization of the problem. We are applying a projective step to any inner integrator (we may have, for example, a legacy code that performs one time step in a manner we do not fully understand). Since the nature of the inner integrator affects the stability and since we wish to analyze the stability of the projective process independently of the details of the inner integrator, we analyze stability as a function of the error amplification, ρ, of the inner integrator, where $\rho = \rho(h_0\lambda)$ and h_0 is the time step of the inner integrator. For example, if the inner integrator were *exact* then $\rho = \exp(h_0\lambda)$, while if the inner integrator were Forward Euler, $\rho = (1 + h_0\lambda)$. (Of course, we cannot have an exact numerical integrator unless the problem is particularly simple, but it is possible that a legacy code or a more detailed simulation model provides an almost exact integration over one step for the range of problems considered, albeit at a heavy computational cost.) Note that if the inner integrator is the forward Euler (FE) method, then the ρ-plane is simply a unit translation of the more conventional $h\lambda$-plane since in that case $\rho = 1 + h_0\lambda$.

The projective method consists of two processes: an inner integrator and a projective step. For example, the PFE method completes one outer step over a distance $h_1 = (M + k + 1)h_0$ from y_n as follows:

1. Form y_{n+i} for $i = 1, 2, \ldots, k + 1$ starting from y_n using an inner integrator.
2. Form

$$y_{n+k+1+M} = (M + 1)y_{n+k+1} - My_{n+k}. \tag{1}$$

If the inner integrator has a one step error amplification of ρ, then, as discussed in [1], the error amplification of one outer step of the PFE is

$$\sigma = [(M + 1)\rho - M]\rho^k. \tag{2}$$

It was shown in [1] that the stability region of this method breaks into two separate pieces whenever M is more than about three times k. In other words, for larger M the method is only valuable for problems with a gap in their spectrum. This is illustrated in Fig. 3 which shows the absolute stability region in the ρ-plane for PFE method with $k = 2$ and $M = 9$, that is, the method consists of three inner steps of size h_0 followed by a linear projective step over a distance of $9h_0$ from the last two computed values. The above example covers 12 steps for each three derivative evaluations, so the speedup is 4 but there has to be a gap in the problem spectrum for this parameter choice to be stable for the problem.

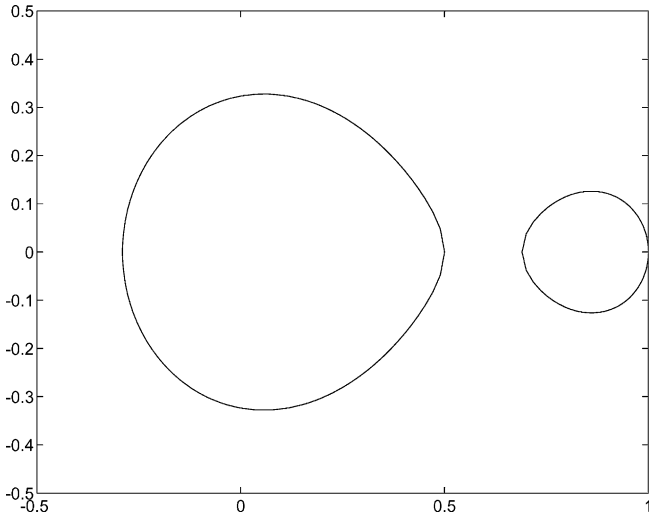

Fig. 3. Complex ρ-plane stability for P2–1–9 method.

In contrast, if M is smaller, a single region of absolute stability is obtained, as illustrated in Fig. 4, which is the stability region for the same method but with $M = 5$. However, this method has a speedup of only 8/3.

Note that the stability region in Fig. 4 includes all of the real axis in the ρ-plane from 0 to 1. We will call this a $[0, 1]$ stability region and call such methods *[0,1] stable*. If the inner integrator is the Forward Euler method, $\rho = 1 + h_0\lambda$ so any real $\lambda \in [-1/h_0, 0]$ maps into $\rho \in [0, 1]$. Similar results apply to most explicit methods. Hence $[0, 1]$-stable methods are potentially useful when problems have a spread of eigenvalues along or near the negative real axis.

The disadvantage of $[0, 1]$-stable methods is that we have shown that their speedup cannot be much larger than three. In the next section we show how the projective methods can be applied recursively to achieve $[0, 1]$ stability regions with greater speedup.

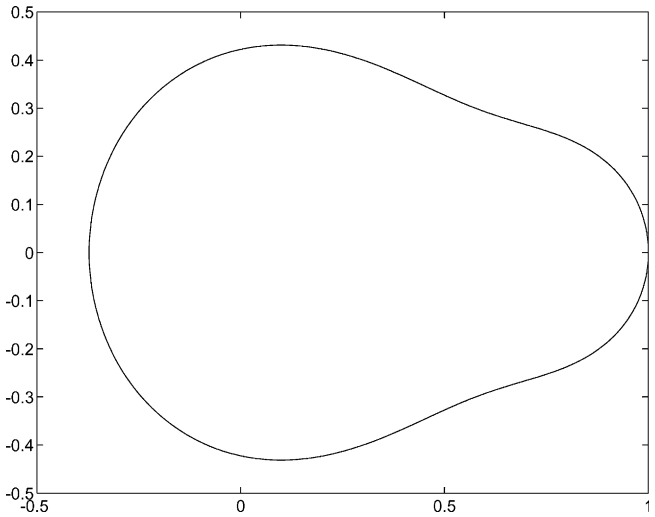

Fig. 4. Complex ρ-plane stability for P2–1–5 method.

In the generalized projective method we iteratively apply a new outer projective step to the results of the previous outer step. To express the general form, it is convenient to change notation slightly. Write one step of the inner integrator as

$$y_{s+1} = \Phi_0(y_s)$$

so that one step of the outer integrator (for the PFE method) starting from a value z_r is

1. Set $y_0 = z_r$.
2. Form $y_i = \Phi_0(y_{i-1})$ for $i = 1, 2, \ldots, k+1$.
3. Form $z_{r+1} = (M+1)y_{k+1} - My_k$.

We now refer to this as the *first level* outer integrator, and write it as

$$z_{r+1} = \Phi_1(z_r).$$

The mth level outer integrator, Φ_m, is defined recursively by

1. If $m = 0$, Φ_m is the inner integrator.
2. If $m > 0$ then $\Phi_m(z)$ is defined by the process
   2.1. Set $y_0 = z$;
   2.2. Form $y_i = \Phi_{m-1}(y_{i-1})$ for $i = 1, 2, \ldots, k+1$;
   2.3. Form $\Phi_m(z) = (M+1)y_{k+1} - My_k$.

Although we have used recursion for its definition, the method is applied *iteratively*, that is, from the bottom up. We start with an inner integrator and, after sufficient steps ($k+1$ in the discussion above) have been taken, we take a level-1 outer step. After sufficient level-1 steps (each of which involves multiple level-0, or inner, steps) have been taken, we take a level-2 outer step, and so on. Each successive outer level "looks forward" or *telescopes* over many inner levels. Hence we call it a *Telescopic Projective*, or TP, method.

For now, we will consider the stability of the fixed step, constant k–M TP method. We will assume that ρ for the inner method is constant. (This is equivalent to the standard linear, constant coefficient analysis assumption. Showing that a method is stable for such problems is not sufficient to show stability for more general problems without significant additional assumptions, but methods that are not linearly stable are seldom worth using for any problems!)

We define the stability region of the TP method to be the set of ρ such that all outer integrators are stable. Suppose the amplification of one step of the mth outer integrator is σ_m. Then we have

$$\sigma_{m+1} = [(M+1)\sigma_m - M]\sigma_m^k, \quad m = 0, 1, \ldots, \tag{3}$$

where $\sigma_0 = \rho$. Hence the stability region of the TP method is the set of ρ such that the iteration

$$\rho \leftarrow [(M+1)\rho - M]\rho^k \tag{4}$$

remains in the unit disk [3]. This is the same as ρ remaining bounded since, if $|\sigma_m| > 1$ Eq. (3) implies

$$|\sigma_{m+1}| - 1 > (M+1)(|\sigma_m| - 1)$$

from which it follows that σ_m diverges for $M > 0$.

In practice, of course, we do not use an infinite number of iterations of the projective operation. If we stop after any given number of iterations, the resulting stability region will contain the stability region of

[3] Formally this will be a fractal set, but all that is important for our purposes is that the set contains one (or more) connected regions of stability.

the infinitely iterated method as defined above. Hence, if a linear problem's eigenvalues are in the stability region as defined above, the use of any finite number of iterations will result in a linearly stable method.

In the above example, we have used the same value of M and k at each level of recursion and a constant inner step size. That would not be the case in a practical automatic code where the outermost integrator should use a step size *and order* automatically determined to be consistent with the current behavior of the system and accuracy requirements. At the same time, an automatic integrator should detect when the step size needed for stability is smaller than the step size possible for accuracy and limit the step to maintain stability. (This has been detected in ODE codes in the past and used to make a decision to switch to more expensive stiff methods.) In a projective method the step size must be limited to maintain stability since we want to continue using explicit methods. At the same time, we get an estimate of the critical eigenvalues – those limiting the step for stability. As the step size limitation becomes more severe, the order of the method should be reduced (lower order methods provide a larger integration step per function evaluation when stability is the limiting factor). When the possible step size for accurate integration is sufficiently larger than that for stability, an additional outer level of integration can be added, leaving the older outer level as an intermediate level at order one – since this provides sufficient accuracy at its smaller step. The new outer integrator can use a higher-order method as before. In fact, the outer integrator can even be an ''implicit method'' solved by Predictor–Corrector iteration, as discussed in [1]. Such methods usually have better accuracy than explicit methods. (This brief discussion leaves out many details that are the subject of ongoing research.)

In many ways, the proposed methods are similar to the explicit Runge–Kutta methods with extended ranges of stability (see [3–5]). Indeed, one outermost step (which is taken to be the collection of inner-level steps plus the projective operation) can be expressed in the Runge–Kutta formalism if the innermost integrator is a conventional explicit integrator. However, there are several significant differences. First, if the innermost integrator is a legacy code that is not a simple explicit integrator, the RK formalism no longer applies. Second, the method coefficients of an RK method are precomputed to achieve certain stability regions (and accuracy) and it does not seem feasible to change these coefficients in ''mid step.'' In contrast, in the proposed methods, the step sizes of integrators at any level can be dynamically selected based on current estimates of errors and significant eigenvalues. A third difference is that it is possible to accommodate ''noisy'' inner integrators, as would happen if the inner integrator were actually a Monte Carlo simulation. (This can be done by estimating the chord or other low-degree polynomial from a large number of integration steps.)

3. Stability and speedup of TP methods

One way to compute the stability region is to map the unit circle under the inverse of the mapping (4) for a number of iterations. Actually, then we have the boundary of the stability region of only that many applications of the TP method. Since the region shrinks at each iteration (and starts from the finite unit disk) it must converge and in practice we quickly get a reasonable approximation to the infinitely iterated region. Fig. 5 shows the stability region for 10 iterations of the P2–1–3 method [4]. With $k = 2$ three inner integrations are used to cover one first-level outer integration step of length $6h_0$ so its speedup is 2. Each successive outer integration provides an additional doubling of the speedup, so after 10 iterations we have an speedup of $2^{10} = 1024$. However, by this time, the outer step size is $6^{10}h_0$ which

[4] The designation Pk–q–M method means that k initial steps are used, a further q steps are used to generate a qth order extrapolate through the last $q + 1$ points, and the extrapolation is over M steps.

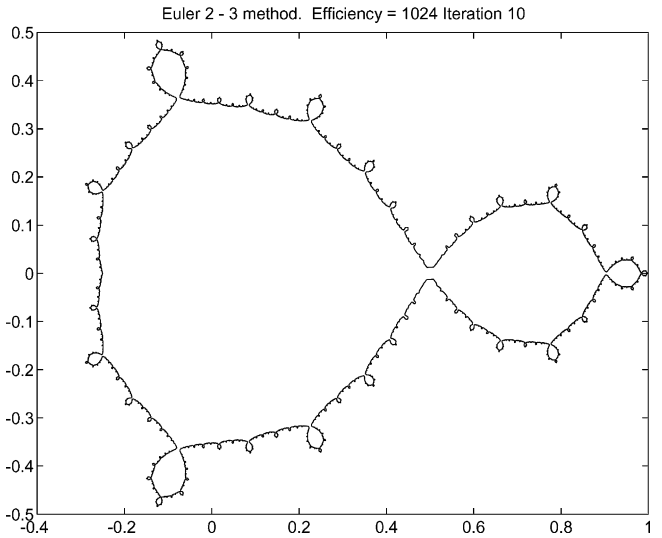

Fig. 5. Stability region for P2–1–3 method after 10 iterations.

may well too large for accurate integration of the active components! Thus, the speedup will be limited by the relative speed of the fastest components compared to the active components. This will be discussed in the analysis below.

Fig. 5 suggests that the real axis from about −0.25 to +1.0 is inside the stability region – although we have not shown that errors in calculation of the figure or further iterates do not change that conclusion. Can we always guarantee that a section of the real axis of the ρ-plane including $[0,1]$ is always in the stability region so this method is $[0,1]$ stable? The answer is that for any $k \geqslant 1$ and extrapolation order $q \geqslant 1$ (using the last $q+1$ values) there exists an $M_{k,q}$ such that all $\rho \in [0,1]$ are stable for any $M \leqslant M_{k,q}$. We will prove that statement at the end of this section.

The M chosen for Fig. 5 is the largest consistent with $[0,1]$ stability for $k=2, q=1$. Fig. 5 suggests that the boundary of the stability region touches the real axis in the interval $[0,1]$. That is true, because M has its maximum value. Inevitably, when one chooses the "best" value of one parameter, the limit is pushed on other criteria. We can keep the interior of $[0,1]$ in the interior of the stability region by choosing a value of M smaller than the maximum allowed. For example, Fig. 6 shows the stability region for 10 iterations of the P2–1–2 method. However, the speedup of each projective step is 5/3 rather than the two of the P2–1–3 method.

Table 1 gives the values of $M_{k,q}$ for $1 \leqslant k \leqslant 10$ and $1 \leqslant q \leqslant 5$. (The way these can be calculated is indicated at the end of this section.)

Clearly, the larger M, the greater the speedup of the method because it integrates over a greater distance for a given number of inner integration steps. The speedup of the first level of the projective step using the maximum value $M = M_{k,q}$ consistent with $[0,1]$ stability is shown in Table 2.

Table 3 shows the speedup of the method after five iterations. It also shows the step size ratio – that is, the size of the 5th-level outer step as a multiple of h_0. Although the speedups appear to increase significantly as k increases, in practice the largest outer step size will be limited, and the size of the outer step also increases with k. The effect is to make smaller values of k more efficient as shown below. After the mth level of iteration we have a speedup of

$$S_m = S_1^m = [(k+q+M)/(k+q)]^m.$$

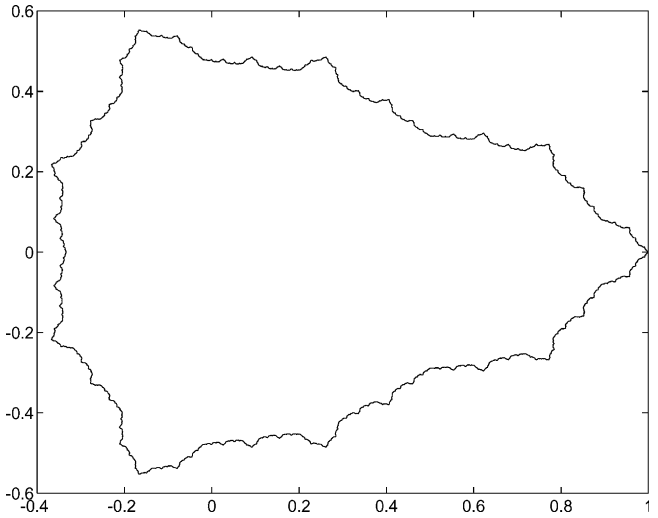

Fig. 6. Stability region for P2–1–2 method after 10 iterations.

Table 1
Values of $M_{k,q}$

k	q				
	1	2	3	4	5
1	2.00	3.56	1.57	2.94	1.50
2	3.00	5.92	2.25	4.68	2.14
3	6.66	8.27	4.34	6.40	3.92
4	8.32	10.60	5.35	8.11	4.82
5	12.21	12.93	7.47	9.82	6.59
6	14.24	15.27	8.66	11.52	7.62
7	18.22	17.60	10.78	13.23	9.37
8	20.48	19.93	12.07	14.93	10.48
9	24.48	22.25	14.18	16.63	12.21
10	26.91	24.58	15.55	18.37	13.38

Table 2
Values of speedup $(M_{k,q} + k + q)/(k + q)$

k	q				
	1	2	3	4	5
1	2.00	2.19	1.39	1.59	1.25
2	2.00	2.48	1.45	1.78	1.31
3	2.66	2.65	1.72	1.91	1.49
4	2.66	2.77	1.76	2.01	1.54
5	3.04	2.85	1.93	2.09	1.66
6	3.04	2.91	1.96	2.15	1.69
7	3.28	2.96	2.08	2.20	1.78
8	3.28	2.99	2.10	2.24	1.81
9	3.45	3.02	2.18	2.28	1.87
10	3.45	3.05	2.20	2.31	1.89

Table 3
Values of speedup and step size ratio for 5 iterations

k	Speedup		Step ratio	
	$q=1$	$q=2$	$q=1$	$q=2$
1	32.0	50.4	1024	3766
2	32.0	93.8	3125	1.1×10^4
3	133.2	130.7	1.3×10^4	2.6×10^4
4	133.2	163.1	2.6×10^4	5.2×10^4
5	259.6	188.0	6.0×10^4	9.3×10^4
6	259.6	208.7	1.0×10^5	1.5×10^5
7	379.6	227.2	1.8×10^5	2.4×10^5
8	379.6	239.0	2.8×10^5	3.7×10^5
9	488.8	251.2	4.4×10^5	5.4×10^5
10	488.8	263.9	6.3×10^5	7.7×10^5

By this time the outermost step size is

$$h_m = (k+q+M)^m h_0.$$

The largest outer step size that can be used will be limited [5] by the time constant of the active components in the solution – the outer integrator must limit its step size for their accurate integration. Let us suppose that this time scale is Dh_0 – that is, we can use an outer integrator with step size no larger than D times that of the inner integrator for accuracy. Consequently, we have

$$(k+q+M)^m \leqslant D$$

or the largest m is given by

$$m \approx \log(D)/\log(k+q+M). \tag{5}$$

With this number of iterations of the outer integrator, a total of $N_{k,q,M} = (k+q)^m$ inner integrations will have been used in one level-m outer step, or

$$N_{k,q,M} = (k+q)^{\log(D)/\log(k+q+M)} = D^{\log(k+q)/\log(k+q+M)}. \tag{6}$$

Let us define $p_{k,q,M}$ to be the exponent of D in Eq. (6). Since D inner integration steps would be used to integrate over the interval if no projective steps were done, the speedup is

$$S = D/N_{k,q,M} = D^{1-p_{k,q,M}}.$$

The smaller the value of $p_{k,q,M}$ the greater the speedup. Since $p_{k,q,M}$ decreases as M increases, the smallest $p_{k,q,M}$ occurs when M is as large as possible (consistent with stability). That value of $M = M_{k,q}$ is shown in Table 1. Thus, $p_{k,q} = p_{k,q,M_{k,q}}$ is the smallest p consistent with $[0,1]$ stability. Its value is shown in Table 4. We see that $p_{k,q}$ increases with k, indicating that the speedup decreases as k increases.

It is interesting to compare this technique with the explicit Runge–Kutta (RK) methods with extended stability ranges discussed in [3–5]. Let m be the maximum iteration level we can use, as given by Eq. (5). If we view a single level-m outer step of the TP method as if it were a single RK step, it uses $s = D^{p_{k,q}}$ inner integrations, or *stages* assuming one function evaluation per inner step, to cover an outer step size of

[5] The step size needed for accurate integration of a component like $\exp(\lambda t)$ by a conventional explicit method is always smaller than that needed for stability since the former is concerned with the accurate approximation of $\exp(h\lambda)$ whereas the latter is concerned only with the approximation being less than one in magnitude (for λ in the negative half plane).

Table 4
Values of $p_{k,q}$

k	q				
	1	2	3	4	5
1	0.50	0.58	0.81	0.78	0.89
2	0.61	0.60	0.81	0.76	0.88
3	0.59	0.62	0.76	0.75	0.84
4	0.62	0.64	0.77	0.75	0.84
5	0.62	0.65	0.76	0.75	0.82
6	0.64	0.66	0.77	0.75	0.82
7	0.64	0.67	0.76	0.75	0.81
8	0.65	0.68	0.76	0.75	0.81
9	0.65	0.68	0.76	0.76	0.81
10	0.66	0.69	0.77	0.76	0.81

$H = Dh_0$. Assume that the inner integration is explicit and its step size is $h_0 \approx 1/|\mathrm{Re}(\lambda)|$ where $\mathrm{Re}(\lambda)$ is the most negative real part of any eigenvalue. Then the method is stable for real eigenvalues λ as negative as given by $H|\lambda| \approx D = s^{1/p_{k,q}}$. For the case $k = 1$ and $q = 1$ from Table 4 we have the stability range $\approx s^2$. This compares with the stability range given in [5] of Cs^2, although the RK methods achieved that with a larger C and also for second-order methods. In that sense, those RK methods are superior, but, as we noted earlier, they are less flexible for problems whose eigenvalues may be changing during a step and generally cannot be used with legacy codes as the inner integrator. This is because the parameters in the RK methods were chosen to maximize their stability regions at the expense of simplicity and flexible choice of internal step sizes and order.

3.1. Existence of [0,1] stability regions

We will now prove that for any positive integers k and q such that the Pk–q–M TP method is $[0, 1]$ stable for all M less than some maximum $M_{k,q}$. We will do this by demonstrating that there is a line segment $[-\beta, 1]$ with $0 \leqslant \beta < \infty$ that maps into itself under (4) and thus remains bounded. This section can be skipped by the reader uninterested in the details of the proof.

3.1.1. Case $q = 1$, first order

Let us first consider $k = 1$ and the plot of σ versus real ρ in Eq. (2). It is illustrated in Fig. 7. In general, let it be the map

$$\sigma(\rho) = f(M, \rho).$$

In this case, it is a quadratic function that has a minimum at

$$\rho_{\min} = 0.5M/(M + 1)$$

and does not exceed +1 for $\rho \in [-\beta, 1]$. If the minimum of σ is $-\gamma = \sigma(\rho_{\min})$ and if $\gamma \leqslant \beta$ then the interval $[-\beta, 1]$ maps into itself. In this case, trivial algebra shows this to be true for $0 \leqslant M \leqslant 2$.

It is convenient to consider a requirement equivalent to $\gamma < \beta$ that is more useful for larger k and q. First note that the minimum γ is a function of M for any pair k and q. In this case we have

$$\gamma(M) = \frac{1}{M + 1}\left[\frac{M}{2}\right]^2.$$

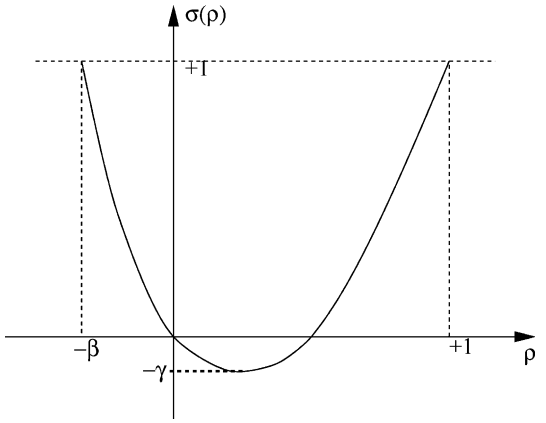

Fig. 7. Real σ–ρ map, $k = 1, q = 1$.

The equivalent requirement is that the map of $-\gamma$ does not exceed 1, or

$$f(M,\gamma) = (M+1)\gamma^2 + M\gamma \leqslant 1 \tag{7}$$

$f(M,\gamma(M))$ is an increasing function of M for positive M. Hence, condition (7) is satisfied for all M in the interval $[0, M_{\max}]$, where $M_{\max}$ is the smallest positive solution of $f(M,\gamma(M)) = 1$, namely 2.

If k is odd and larger than 1, the plot of $\sigma(\rho)$ is very similar to Fig. 7 except that there is a multiple zero at the origin. In this case we find that the minimum occurs at

$$\rho_{\min} = \frac{kM}{(k+1)(M+1)}$$

and

$$\gamma = -\sigma(\rho_{\min}) = \left[\frac{M}{k+1}\right]^{k+1}\left[\frac{k}{M+1}\right]^{k}.$$

The condition equivalent to Eq. (7) is

$$f_k(M,\gamma) = \gamma^k[(M+1)\gamma + M] \leqslant 1. \tag{8}$$

In Eq. (8) f is an increasing function of M so we find that the condition is satisfied for all M in the interval $[0, M_{\max}]$, where $M_{\max}$ is the smallest positive solution of $f_k(M,\gamma(M)) = 1$.

If k is even, the plot changes to that shown in Fig. 8. Now the condition on γ is that it must be less than β, where $-\beta$ is the value at which the graph of $\sigma(\rho)$ intersects the line $\sigma = \rho$ in the lower left quadrant. This is equivalent to

$$\gamma^k[(M+1)\gamma + M] \leqslant \gamma$$

or, if we define $f_k(M,\gamma)$ for even k as

$$f_k(M,\gamma) = \gamma^{k-1}[(M+1)\gamma + M$$

and by Eq. (8) for odd k, the condition for each $k \geqslant 1$ is

$$f_k(M,\gamma) \leqslant 1.$$

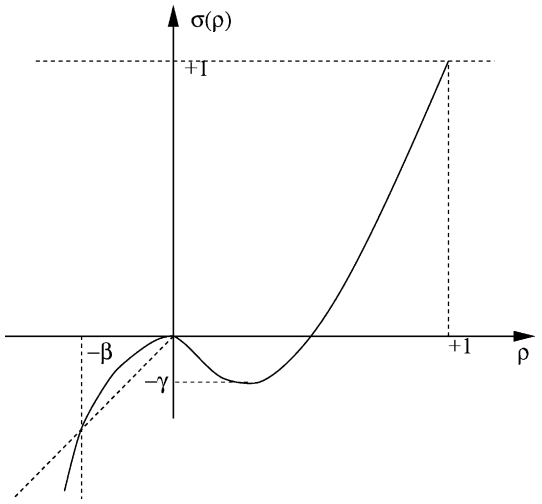

Fig. 8. Real σ–ρ map, k even, $q = 1$.

3.1.2. Case $q = 2$, second order

When $q = 2$ the extrapolation formula leads to

$$\sigma(\rho) = \rho^k \left[\frac{(M+1)(M+2)}{2} \rho^2 - M(M+2)\rho + \frac{M(M+1)}{2} \right].$$

If $k = 1$ the σ–ρ graph is as shown in Fig. 9. Because its slope at $\rho = 0$ exceeds +1, no part of the negative real axis can be stable. However, as long as σ does not lie outside of $[0, 1]$ for $\rho \in [0, 1]$ then the method has a $[0, 1]$ stability region. By simple algebra we note that

$$\sigma(\rho) = \left[\frac{(M+1)M + 2}{2} \right] (\rho - \rho_1)(\rho - \rho_2)\rho,$$

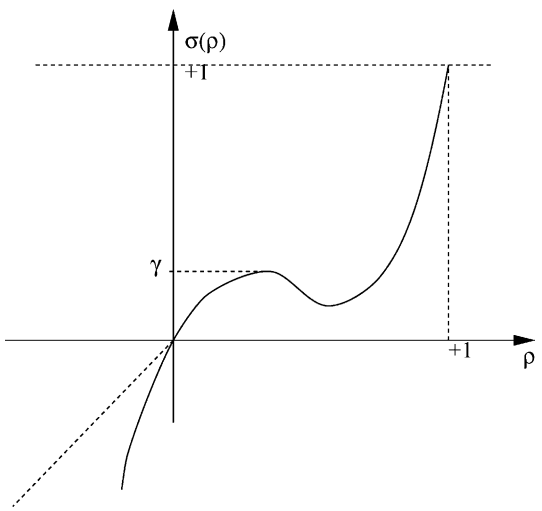

Fig. 9. Real σ–ρ map, $k = 1, q = 2$.

where

$$\rho_i = \frac{M(M+2) \pm \sqrt{-M(M+2)}}{(M+1)(M+2)}.$$

Thus the only real zero of σ is at $\rho = 0$ so σ is everywhere positive for $\rho > 0$. Hence the method has a $[0,1]$ stability region as long as the local maximum does not exceed one. The maximum occurs at

$$\rho_0 = \frac{2M(M+2) - \sqrt{(M-1)M(M+2)(M+3)}}{3M(M+2)}$$

for $M > 1$ and the largest M for which we have a $[0,1]$ stability region is the smallest value of M for which $\sigma(\rho_0) = 1$.

If k is even, the graph takes the form in Fig. 10. In this case the method has a $[0,1]$ stability region if the local maximum does not exceed 1 and then the stability region includes the segment $[-\beta, 1]$ of the real axis.

If $k > 1$ and is odd, the graph takes the form shown in Fig. 11. While this is similar to Fig. 9, the high order contact at the origin means that there is the section of the negative real axis $[-\beta, 0]$ that maps into itself where $-\beta$ is the intersect of the line $\sigma = \rho$ and the graph. Again, for M less than the critical value at which the local maximum is +1 the method has a $[0,1]$ stability region.

3.1.3. Case $q > 2$

The earlier figures illustrate the general features for all q. If $k + q$ is even, σ is positive when ρ is negative, as in Figs. 7 and 10. However, there may be more maxima and minima than shown, so the conditions are that no maxima exceed +1 and no minima be less than $-\beta$. If $k + q$ is odd, σ is negative when ρ is negative, as in Figs. 8, 9, and 11. In this case, the conditions are that no maxima exceed +1 and that no minima be less than $-\beta$. (When k is one and q is even, we have the case in Fig. 9 and β is effectively zero.)

In the general case we have

$$\sigma(\rho) = \rho^k \frac{M(M+1)\cdots(M+q)}{q!} \int_0^1 t^{M-1}(\rho - t)^q \, \mathrm{d}t \tag{9}$$

for the qth order extrapolation. (This can be derived by tedious algebra or verified by expansion as a power series in ρ.) It uses the fact that the qth order extrapolant is simply the qth order polynomial through the last $q + 1$ points $k, k + 1, \ldots, k + q$, and then $\sigma(\rho)$ is obtained by substituting ρ^{k+i} for the $k + i$ data value.

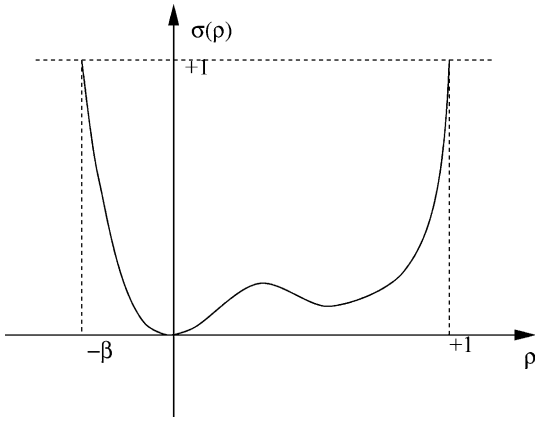

Fig. 10. Real σ–ρ map, k even, $q = 2$.

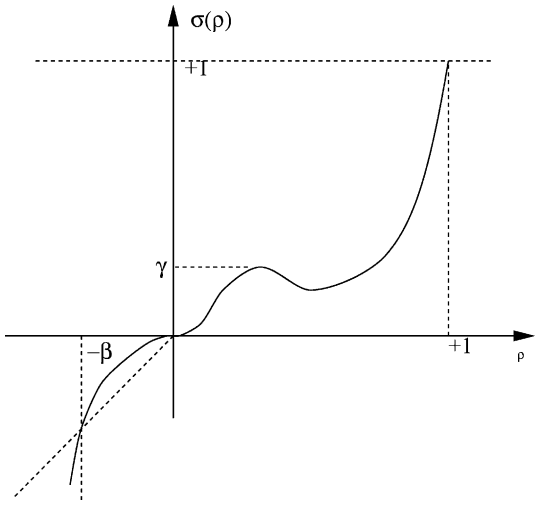

Fig. 11. Real σ–ρ map, $k \geqslant 3$ and odd, $q = 2$.

Since $\sigma(\rho)$ (given by Eq. (9)) is a polynomial in ρ whose coefficients are continuous (and differentiable) functions of M, we only need to verify that the method is $[0,1]$ stable for one value of M. Then we know that it is $[0,1]$ stable for all values of M up to the first that violates the criteria discussed above. When $M = 0$ we have $\sigma(\rho) = \rho^{k+q}$ and it is trivially true, hence we have $[0,1]$ stability for some non-negative M.

From the expression in Eq. (9) we see that σ is positive for all positive ρ when q is even. Hence for these cases we need only look at local maxima in the interval $[0,1]$ and ensure that they do not exceed 1. When q is odd, we must compute both the positive local maxima and the negative local minima and ensure that (i) the largest maxima does not exceed 1, and (ii) the smallest local minima, $-\gamma$, is such that the map $\sigma(-\gamma)$ is less than one if $k+q$ is even, or is less than γ is $k+q$ is odd. These criteria were used in an iteration to compute the $M_{k,q}$ shown in Table 1. (In fact, for the k and q considered, there was only one local minimum and no local maximum when q was odd, and only one local maximum when q was even.)

4. Conclusion

We have shown how the projective method can be iterated to achieve larger regions of absolute stability. Some simple numerical examples are given in [2] where it is also shown how to handle problems with multiple gaps in their eigenspectrum. A combination of these two objectives could be used to have fewer gaps and larger stability regions where needed. While the methods discussed do not appear to be as efficient as Runge–Kutta methods designed to have extended stability regions, telescopic methods can be used with legacy codes, they can be applied to "noisy integrators" such as Monte Carlo simulations, they are conceptually much simpler, and it appears that it will be much easier to design an automatic code to adapt to the clusters of eigenvalues in a specific problem. We are working on a code to do that, but it is too early to report on specifics.

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