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Stability properties of a predictor-corrector implementation of an implicit linear multistep method

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We examine the stability properties of a predictor-corrector implementation of a class of implicit linear multistep methods. The method has recently been described in the literature as suitable for the efficient integration of stiff systems and as having stability regions similar to well known implicit methods. A more detailed analysis reveals that this is not the case.

1. Introduction

In an undergraduate research project that started as a senior capstone project, Meador [2009] became aware of an explicit ODE method that claimed to have desirable stability properties that are usually only enjoyed by implicit methods. The little known method seemed too good to be true. If it had the claimed stability properties, it deserved to be better known and more widely used in applications. In this work we describe what a more careful study of the method revealed. We calculate the correct stability regions of the methods and verify our claims with numerical experiments.

2. Linear multistep methods

A general s-step linear multistep method (LMM) for the numerical solution of the autonomous ordinary differential equation (ODE) initial value problem (IVP)

$$y' = F(y), \qquad y(0) = y_0 \tag{1}$$

is of the form

$$\sum_{m=0}^{s} \alpha_m y^{n+m} = \Delta t \sum_{m=0}^{s} \beta_m F(y^{n+m}), \qquad n = 0, 1, \dots, \tag{2}$$

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where α_m and β_m are given constants. It is conventional to normalize (2) by setting $\alpha_s = 1$. When $\beta_s = 0$ the method is explicit. Otherwise, it is implicit. In order to start multistep methods, the first $s-1$ time levels have to be calculated by a one-step method such as a Runge–Kutta method. Many of the properties of the method (2) can be described in terms of the characteristic polynomials

$$\rho(\omega) = \sum_{m=0}^{s} \alpha_m \omega^s \qquad \text{and} \qquad \sigma(\omega) = \sum_{m=0}^{s} \beta_m \omega^s. \tag{3}$$

The linear stability region of a numerical ODE method is determined by applying the method to the scalar linear equation

$$y' = \lambda y, \qquad y(0) = 1, \tag{4}$$

where λ is a complex number. The exact solution of (4) is $y(t) = e^{\lambda t}$, which approaches zero as $t \to \infty$ if and only if the real part of λ is negative. The set of all numbers $z = \Delta t \lambda$ such that $\lim_{n\to\infty} y^n = 0$ is called the linear stability region of the method. For z in the stability domain, the numerical method exhibits the same asymptotic behavior as (4). For stability, all the scaled eigenvalues of the coefficient matrix of a linear system of ODEs must lie in the stability region. For nonlinear systems, the scaled eigenvalues of the Jacobian matrix of the system must lie within the stability region. A numerical ODE method is A-stable if its region of absolute stability contains the entire left half-plane ($\mathrm{Re}(\Delta t \lambda) < 0$).

For LMMs, the boundary of the stability region is found by the boundary locus method which plots the parametric curve of the function

$$r(\theta) = \frac{\rho(e^{i\theta})}{\sigma(e^{i\theta})}, \qquad 0 \le \theta \le 2\pi, \tag{5}$$

that is, the ratio of the method's characteristic polynomials (3). Standard references on numerical ODEs can be consulted for more details [Butcher 2003; Hairer et al. 2000; Hairer and Wanner 2000; Iserles 1996; Lambert 1973]

3. Implicit LIL linear multistep methods

In this work we consider a class of LMM that has been referred to as local iterative linearization (LIL) in the literature. The s-stage implicit LIL method also has accuracy of order s. The LIL method has been applied to chaotic dynamical systems in [Danca and Chen 2004; Luo et al. 2007]. The convergence, accuracy, and stability properties of the LIL methods were examined in [Danca 2006].

In [Danca and Chen 2004; Danca 2006; Luo et al. 2007], both the implicit and predictor-corrector versions are referred to as LIL methods. However, the stability properties of the methods are very different and we distinguish between the methods by calling the implicit method ILIL, and the predictor-corrector implementation PCLIL.

Using the notation $f^n = F(y^n)$, the first four ILIL formulas follow. The $s = 1$ ILIL formula

$$y^{n+1} - y^n = \Delta t f^{n+1} \tag{6}$$

coincides with the implicit Euler method. For $s = 2$ the ILIL algorithm is

$$y^{n+2} - \frac{4}{3}y^{n+1} + \frac{1}{3}y^n = \Delta t\left(\frac{25}{36}f^{n+2} - \frac{1}{18}f^{n+1} + \frac{1}{36}f^n\right); \tag{7}$$

for $s = 3$,

$$y^{n+3} - \frac{5}{3}y^{n+2} + \frac{13}{15}y^{n+1} - \frac{1}{5}y^n = \Delta t\left(\frac{26}{45}f^{n+3} - \frac{1}{9}f^{n+2} + \frac{4}{45}f^{n+1} - \frac{1}{45}f^n\right); \tag{8}$$

and for $s = 4$,

$$y^{n+4} - 2y^{n+3} + \frac{8}{5}y^{n+2} - \frac{26}{35}y^{n+1} + \frac{1}{7}y^n = \Delta t\left(\frac{6463}{12600}f^{n+4} - \frac{523}{3150}f^{n+3} + \frac{383}{2100}f^{n+2} - \frac{283}{3150}f^{n+1} + \frac{223}{12600}f^n\right). \tag{9}$$

The characteristic polynomial coefficients of the ILIL methods are listed in Table 1. The stability regions of the ILIL methods of orders 1 through 4 are shown in Figure 1 (left). The stability regions are exterior to the curves. The innermost curve is associated with the first-order method and the stability region shrinks as the order of the method increases. The first- and second-order methods are A-stable, while the third and fourth-order methods do not include all of the left half-plane. It is well known that the order of an A-stable LMM cannot exceed 2 [Lambert 1973].

	$s=1$	$s=2$	$s=3$	$s=4$
α_0/β_0	$-1/0$	$\frac{1}{3}/\frac{1}{36}$	$\frac{-1}{5}/\frac{-1}{45}$	$\frac{1}{7}/\frac{223}{12600}$
α_1/β_1	$1/1$	$\frac{-4}{3}/\frac{-1}{18}$	$\frac{13}{15}/\frac{4}{45}$	$\frac{-26}{35}/\frac{-283}{3150}$
α_2/β_2	-	$1/\frac{25}{36}$	$\frac{-5}{3}/\frac{-1}{9}$	$\frac{8}{5}/\frac{383}{2100}$
α_3/β_3	-	-	$1/\frac{26}{45}$	$-2/\frac{-523}{3150}$
α_4/β_4	-	-	-	$1/\frac{6463}{12600}$

Table 1. Coefficients of the characteristic polynomials (3) for the ILIL algorithms.

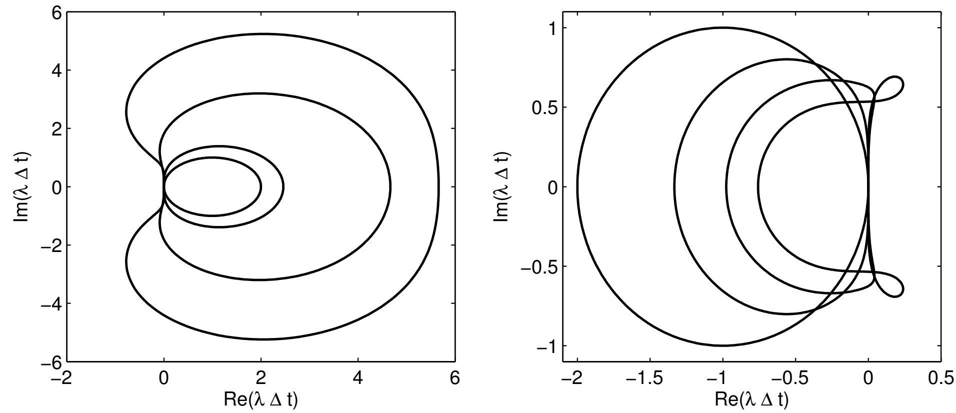

Figure 1. Left: Implicit LIL methods have stability regions consisting of the exterior of the plotted curves. Right: Predictor-corrector implemented LIL methods have bounded stability regions in the interior of the plotted curves.

4. LIL predictor-corrector

Two types of methods that are commonly used to solve the nonlinear difference equations of implicit methods are functional iteration and Newton's method. A third approach, which does not involve solving nonlinear equations, that can be used to implement an implicit ODE method is a predictor-corrector approach. An explicit formula, the predictor, is used to get a preliminary approximation $\hat{y}^{n+s}$ of y^{n+s}. Then the corrector step uses formulas like the implicit LIL methods (6)–(9), with $\hat{y}^{n+s}$ in place of y^{n+s} when calculating f^{n+s}, to get a more accurate approximation of y^{n+s}. The predictor-corrector approach turns the implicit method into one that is implemented in the manner of an explicit method. However, the stability properties of the predictor-corrector method will be inferior to those of the original implicit method. The predictors for the PCLIL methods are listed in Table 2.

s	order s LIL predictor
1	$\hat{y}^{n+1} = y^n$
2	$\hat{y}^{n+2} = 2y^{n+1} - y^n$
3	$\hat{y}^{n+3} = 3y^{n+2} - 3y^{n+1} + y^n$
4	$\hat{y}^{n+4} = 4y^{n+3} - 6y^{n+2} + 4y^{n+1} - y^n$

Table 2. The predictor stages for the predictor-corrector LIL algorithms.

Applying the PCLIL methods to the stability test problem (4) reveals that the α coefficients of the characteristic polynomial (3) remain the same as the implicit LIL methods. However, the β coefficients are modified to be $\hat{\beta}$ which lead to different stability regions. The $\hat{\beta}$ coefficients for the PCLIL methods are listed in Table 3. The details of finding the $\hat{\beta}$ coefficients are illustrated with the second-order PCLIL method:

$$\begin{aligned}\alpha_2 y^{n+2} + \alpha_1 y^{n+1} + \alpha_0 y^n &= \Delta t\big(\beta_2 f^{n+2} + \beta_1 f^{n+1} + \beta_0 f^n\big)\\ &= \Delta t\big(\beta_2 \lambda(2y^{n+1} - y^n) + \beta_1 \lambda y^{n+1} + \beta_0 \lambda y^n\big)\\ &= \Delta t\big((\beta_1 + 2\beta_2)\lambda y^{n+1} + (\beta_0 - \beta_2)\lambda y^n\big)\\ &= \Delta t\big(\hat{\beta}_1 f^{n+1} + \hat{\beta}_0 f^n\big).\end{aligned}$$

The stability regions for the PCLIL methods of orders 1 through 4 are shown in the right image of Figure 1. Since the stability regions consist of the regions that are interior to the curves, PCLIL methods are not A-stable. It is well known that A-stable explicit LMMs do not exist [Nevanlinna and Sipilä 1974].

5. Numerical examples

Many problems arising from various fields result in systems of ODEs that have a property called stiffness. A formal definition can be formulated (see [Lambert 1973], for example), but the essence of a stiff problem can be explained by the fact the coefficient matrix of a linear ODE system (or Jacobian matrix of a nonlinear ODE system) has some eigenvalues with large negative real parts. Thus, explicit methods with their bounded stability regions may be required to take much smaller time steps for stability than are necessary for accuracy. Implicit methods, particularly A-stable methods, with their unbounded stability regions are well suited for stiff problems.

	$s=1$	$s=2$	$s=3$	$s=4$
$\hat{\beta}_0$	1	$-\frac{2}{3}$	$\frac{5}{9}$	$\beta_0 - \beta_4$
$\hat{\beta}_1$	0	$\frac{4}{3}$	$-\frac{74}{45}$	$\beta_1 + 4\beta_4$
$\hat{\beta}_2$	-	0	$\frac{73}{45}$	$\beta_2 - 6\beta_4$
$\hat{\beta}_3$	-	-	0	$\beta_3 + 4\beta_4$
$\hat{\beta}_4$	-	-	-	0

Table 3. Modified β coefficients of the characteristic polynomials (3) for the LIL algorithms implemented as predictor-correctors.

Linear example. We consider the linear ODE system

$$\begin{aligned} y_1' &= -21y_1 + 19y_2 - 20y_3, & y_1(0) &= 1, \\ y_2' &= 19y_1 - 21y_2 + 20y_3, & y_2(0) &= 0, \\ y_3' &= 40y_1 - 40y_2 - 40y_3, & y_3(0) &= -1, \end{aligned} \tag{10}$$

which may be considered stiff. The coefficient matrix

$$A = \begin{bmatrix} -21 & 19 & -20 \\ 19 & -21 & 20 \\ 40 & -40 & -40 \end{bmatrix} \tag{11}$$

has eigenvalues $\lambda_1 = -2$, $\lambda_2 = -40 + 40i$, and $\lambda_3 = -40 - 40i$.

In Figure 2 the stability region of the third-order ILIL is the outside of the dashed curve and the stability region of the third-order PCLIL is the interior of solid curve. The eigenvalues of the linear ODE system (10) scaled by $\Delta t = 0.017$ are in the left image and scaled by $\Delta t = 0.012$ in the right image.

The unstable PCLIL solution of the $y_1(t)$ component of the system using $\Delta t = 0.017$ is shown in the left image in Figure 3 and the stable solution using $\Delta t = 0.012$ is shown on the right. The system can be integrated with the implicit LIL methods with any size time step and the method will remain stable.

Note that for linear problems it is possible to derive an explicit expression from the implicit LIL formulas and that an iterative method is not required. For example,

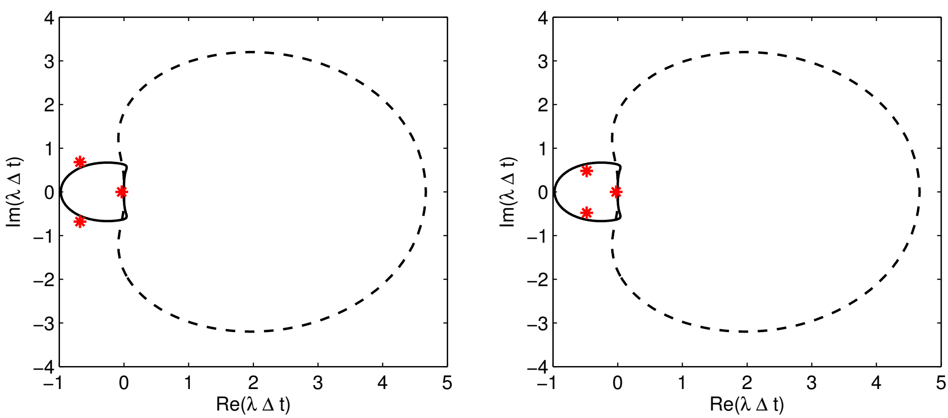

Figure 2. Color dots indicate the eigenvalues of the linear ODE system (10) scaled by $\Delta t = 0.017$ (left) and $\Delta t = 0.012$ (right). The third-order ILIL is stable for eigenvalues outside the dashed curve, and the third-order PCLIL for those inside the solid curve.

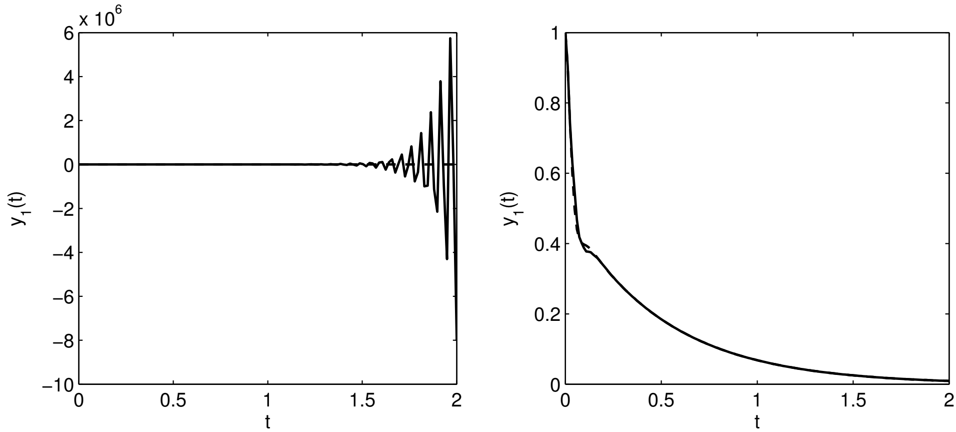

Figure 3. Left: unstable PCLIL solution of the $y_1(t)$ component of the system (10) using $\Delta t = 0.017$. Right: stable solution using $\Delta t = 0.012$.

the second-order implicit LIL method applied to the linear ODE system (10) can be evaluated as

$$y^{n+1} = \Big(I - \frac{25\Delta t}{36}A\Big)^{-1}\Big(\frac{4}{3}I - \frac{\Delta t}{18}A\Big)y^n + \Big(I - \frac{25\Delta t}{36}A\Big)^{-1}\Big(\frac{-1}{3}I - \frac{\Delta t}{36}A\Big)y^{n-1},$$

where I is the 3×3 identity matrix.

Nonlinear example. We consider the Rabinovich–Fabrikant (RF) equations, a set of differential equations in three variables with two constant parameters a and b:

$$\begin{aligned} x' &= y(z - 1 + y^2) + ax, \\ y' &= x(3z + 1 - x^2) + ay, \\ z' &= -2z(b + xy). \end{aligned}$$

PCLIL methods have been used extensively in the study of this system [Danca and Chen 2004; Luo et al. 2007; Danca 2006].

In our numerical work, we encountered severe stability issues while using the PCLIL methods with certain settings of the parameters. For instance, with $a = 0.33$ and $b = 0.5$, a very small step size of $\Delta t = 0.0001$ was needed to stably integrate the system to $t = 200$ with the fourth-order PCLIL method. The resulting attractor is shown in Figure 4. The fourth-order ILIL method was implemented and was an improvement in many cases. However, due to the method not being A-stable, we still had stability problems for some parameter settings.

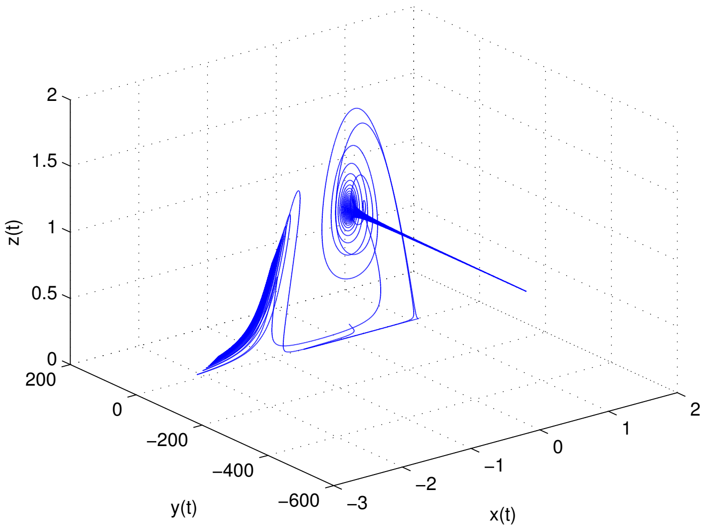

Figure 4. Phase plots of the Rabinovich–Fabrikant equations for parameter settings $a = 0.33$ and $b = 0.5$.

We note that the most efficient method that we found for our numerical exploration of the RF system was an implicit Runge–Kutta method. Using the 4-stage, eighth-order accurate, A-stable Gauss method [Butcher 1964; Ehle 1968; Hairer and Wanner 2000; Sanz-Serna and Calvo 1994], we were able to accurately approximate the attractor in Figure 4 with a step size as large as $\Delta t = 0.2$.

6. Conclusions

Previously, the predictor-corrector implementation of the LIL method has been analyzed in [Danca 2006] where of the PCLIL method it was said that "The time stability of LIL method is more efficient than that of other known algorithms and is comparable with time stability of the Gear's algorithm" and that the LIL method is suitable for stiff problems. Additionally, in [Danca and Chen 2004; Luo et al. 2007] the PCLIL was applied to chaotic dynamical systems that had stiff characteristics and was presented as a method well suited to this type of problem. As we have shown here, this is not the case. The PCLIL methods are explicit and have bounded stability regions that decrease in area as the order of the method increases. The PCLIL methods are not well suited for stiff problems as they will require very small time steps in order to remain stable. It is possible that in the previous application to nonlinear chaotic systems that very small time steps were always used for accuracy purposes and thus stability issues were not encountered.

References

[Butcher 1964] J. C. Butcher, "Implicit Runge–Kutta processes", *Math. Comp.* **18** (1964), 50–64. MR 28 #2641 Zbl 0123.11701

[Butcher 2003] J. C. Butcher, *Numerical methods for ordinary differential equations*, John Wiley & Sons Ltd., Chichester, 2003. MR 2004e:65069 Zbl 1040.65057

[Danca 2006] M.-F. Danca, "A multistep algorithm for ODEs", *Dyn. Contin. Discrete Impuls. Syst. Ser. B Appl. Algorithms* **13**:6 (2006), 803–821. MR 2007k:65097 Zbl 1111.65065

[Danca and Chen 2004] M.-F. Danca and G. Chen, "Bifurcation and chaos in a complex model of dissipative medium", *Internat. J. Bifur. Chaos Appl. Sci. Engrg.* **14**:10 (2004), 3409–3447. MR 2107556 Zbl 1129.37314

[Ehle 1968] B. L. Ehle, "High order A-stable methods for the numerical solution of systems of D.E.'s", *Nordisk Tidskr. Informationsbehandling* (*BIT*) **8** (1968), 276–278. MR 39 #1119

[Hairer and Wanner 2000] E. Hairer and G. Wanner, *Solving ordinary differential equations, II: Stiff and differential-algebraic problems*, Spinger Series in Computational Math. **14**, Springer, 2000.

[Hairer et al. 2000] E. Hairer, S. Norsett, and G. Wanner, *Solving ordinary differential equations, I: Nonstiff problems*, Spinger Series in Computational Math. **8**, Springer, 2000.

[Iserles 1996] A. Iserles, *A first course in the numerical analysis of differential equations*, Cambridge Texts in Applied Mathematics, Cambridge University Press, Cambridge, 1996. MR 1384977 (97m:65003)

[Lambert 1973] J. D. Lambert, *Computational methods in ordinary differential equations*, Wiley, New York, 1973. MR 54 #11789 Zbl 0258.65069

[Luo et al. 2007] X. Luo, M. Small, M.-F. Danca, and G. Chen, "On a dynamical system with multiple chaotic attractors", *Internat. J. Bifur. Chaos Appl. Sci. Engrg.* **17**:9 (2007), 3235–3251. MR 2008k:37081 Zbl 1185.37081

[Meador 2009] C. Meador, "A comparison of two 4th-order numerical ordinary differential equation methods applied to the Rabinovich–Fabrikant equations", 2009, http://www.scottsarra.org/math/papers/ClydeMeador_SeniorCapstone_2009.pdf.

[Nevanlinna and Sipilä 1974] O. Nevanlinna and A. H. Sipilä, "A nonexistence theorem for explicit A-stable methods", *Math. Comp.* **28** (1974), 1053–1056. MR 50 #1515 Zbl 0293.65055

[Sanz-Serna and Calvo 1994] J. M. Sanz-Serna and M. P. Calvo, *Numerical Hamiltonian problems*, Applied Mathematics and Mathematical Computation **7**, Chapman & Hall, London, 1994. MR 95f:65006 Zbl 0816.65042

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