Stability Analysis of the Matrix-Free Linearly Implicit Euler Method

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Summary. Implicit time stepping methods are useful for the simulation of large scale PDE systems because they avoid the time step limitations imposed by explicit stability conditions. To alleviate the challenges posed by computational and memory constraints, many applications solve the resulting linear systems by iterative methods where the Jacobian-vector products are approximated by finite differences. This paper explains the relation between a linearly implicit Euler method, solved using a Jacobian-free Krylov method, and explicit Runge-Kutta methods. The case with preconditioning is equivalent to a Rosenbrock-W method where the approximate Jacobian, inverted at each stage, corresponds directly to the preconditioner. The accuracy of the resulting Runge-Kutta methods can be controlled by constraining the Krylov solution. Numerical experiments confirm the theoretical findings.

1 Introduction

Large systems of time dependent partial differential equations (PDEs), arising in multi-physics simulations, are often discretized using the method of lines approach. The independent time and space numerical schemes allow the coupling of multiple physics modules, and provide maximum flexibility in choosing appropriate algorithms. After the semi-discretization in space the system of PDEs is reduced to a system of ordinary differential equations (ODEs)

$$y' = f(y), \quad t_0 \le t \le t_f, \quad y(t_0) = y_0. \tag{1}$$

Here $y(t) \in \mathbb{R}^d$ is the solution vector and y_0 the initial condition. We denote the Jacobian of the ODE function by $J(y) = f_y(y) \in \mathbb{R}^{d\times d}$, and the identity matrix by $\mathbb{I} \in \mathbb{R}^{d\times d}$.

Stability requirements (e.g., the CFL condition for discretized hyperbolic PDEs) limit the time steps allowable by explicit time discretizations of (1). When the fastest time scales in the system (1) are short, e.g., in the presence of fast waves, the stability condition imposes time steps much smaller then those required to achieve the target

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accuracy. The step size limitation by linear stability conditions is referred to as stiffness. In order to overcome this computational inefficiency, it is desirable to use implicit, unconditionally stable discretizations which allow arbitrarily large time steps [2]. Implicit methods have a high cost per step due to the need to solve a (non)linear system of equations.

To reduce the computational and memory costs of direct linear system solvers, and to aid parallelization, iterative Krylov space methods are employed. Furthermore, matrix-free implementations approximate Jacobian vector products by finite differences [4]. This approach avoids additional coding for the Jacobian, preserves the parallel scalability of the explicit model, and has become popular in many applications, e.g., [1, 5, 6]. The hope is that the properties of the implicit time discretization remain unaltered, provided that the iterative solutions are carried out to sufficient accuracy. *We show here that the matrix-free approach does alter the properties of the underlying implicit time stepping method.*

This study treats a linearly implicit method, together with the Krylov subspace iterations for solving the linear system, as a single numerical scheme. The analysis reveals that matrix-free implementations of linearly implicit methods are equivalent to explicit Runge Kutta methods. Consequently, the unconditional stability property of the base method is lost. When preconditioning is used, the matrix-free implicit methods are equivalent to Rosenbrock-W (ROS-W) methods where the approximate Jacobians correspond directly to the preconditioners.

2 The Matrix-Free Linearly Implicit Euler Method

Consider the linearly implicit Euler (LIE) method applied to (1)

$$\big(\mathbb{I} - \Delta t\, J(y_n)\big) \cdot w = f(y_n), \quad y_{n+1} = y_n + \Delta t \cdot w. \tag{2}$$

When the linear system is solved exactly (modulo roundoff errors) by LU factorization the method (2) is unconditionally stable, and thus suitable for the solution of stiff systems. For many PDEs semi-discretized in the method of lines framework, however, the dimension of the linear system (2) is very large, and the computational and memory costs associated with a direct solution are prohibitive. Moreover, the construction of the explicit Jacobian matrix J is difficult when the space discretization is based on a domain decomposition approach. To alleviate these problems, a popular approach is to solve (2) by matrix-free iterative methods. We seek to analyze the impact that this approximate solutions have on the stability and accuracy of the implicit time stepping scheme. *Our approach is to treat the original discretization (2) together with the iterations as a single numerical method applied to solve the ODE (1).*

To be specific, we solve the linear system in (2) by a Krylov space method. The initial guess is $y_{n+1} = y_n$, i.e., $w = 0$. After m iterations the following m-dimensional Krylov space is built:

$$\mathscr{K}_m = \text{span}\left\{ f(y_n), \ldots, \big(\mathbb{I} - \Delta t\, J(y_n)\big)^{m-1} f(y_n) \right\}.$$

In the matrix-free approach, the basis is constructed recursively and the Jacobian-vector products are approximated by finite differences

$$\ell_i = \ell_{i-1} - \Delta t\, \varepsilon^{-1}\, f(y_n + \varepsilon\, \ell_{i-1}) + \Delta t\, \varepsilon^{-1}\, \ell_1\,, \quad i = 2, \ldots, m\,. \tag{3}$$

We assume that the same scaling factor ε is used to compute the finite differences in all iterations. (The analysis can be easily extended to the case where a different ε is used in each iteration.) Denote

$$k_1 = f(y_n)\,; \quad k_i = f\left(y_n + \varepsilon \ell_{i-1}\right)\,, \ \ i = 2, \cdots, m\,. \tag{4}$$

The recurrence (3) can be expressed in terms of k_i as:

$$k_i = f\left(y_n + \Delta t\, \left(\Delta t^{-1}\, \varepsilon + (i-2)\right) k_1 - \Delta t \sum_{j=2}^{i-1} k_j\right), \ i = 2, \ldots, m. \tag{5}$$

The solution $w = \sum_{i=1}^{m} \alpha_i\, \ell_i \in \mathscr{K}_m$ can be expressed in terms of k_i's:

$$w = \left(\sum_{i=1}^{m} \alpha_i + \Delta t\, \varepsilon^{-1} \sum_{i=2}^{m} (i-1)\, \alpha_i\right) k_1 - \Delta t\, \varepsilon^{-1} \sum_{i=2}^{m} \left(\sum_{j=i}^{m} \alpha_j\right) k_i\,. \tag{6}$$

Equations (5) and (6), together with the relation $y_{n+1} = y_n + \Delta t\, w$, are compared with the m-stage explicit Runge Kutta (ERK) method [3]

$$k_i = f\left(y_n + \sum_{j=1}^{i-1} a_{ij}\, k_j\right), \ i = 1, \ldots, m\,; \quad y_{n+1} = y_n + \Delta t \sum_{i=1}^{m} b_i\, k_i\,.$$

The comparison reveals the following.

Theorem 1. *The matrix-free LIE (2) method is equivalent to an explicit Runge Kutta method. The number m of Krylov iterations defines the number of Runge Kutta stages.*

Equations (5) and (6) define the coefficients of the ERK method:

$$a_{i,1} = \Delta t^{-1} \varepsilon + (i-2)\,; \ a_{i,j} = -1\,, \ \text{for} \ \ i = 2, \cdots, m\,, \ \ j = 2, \cdots, i-1\,;$$

$$b_1 = \sum_{j=1}^{m} \alpha_j + \Delta t\, \varepsilon^{-1} \sum_{j=2}^{m} (j-1)\, \alpha_j\,; \quad b_i = -\Delta t\, \varepsilon^{-1} \sum_{j=i}^{m} \alpha_j\,, \quad i = 2, \ldots, m\,.$$

2.1 Stability Considerations

The solution of the linear system (under the initial guess $w = 0$) is part of the Krylov space $\mathscr{K}_m$ and can be represented by a matrix polynomial

$$w = p_{m-1}\left(\mathbb{I} - \Delta t\, J(y_n)\right) \cdot f(y_n)\,.$$

The matrix-free LIE method applied to the Dahlquist test problem $y' = \lambda\, y$, $y(0) = 1$, gives the following solution:

$$y_{n+1} = y_n + \Delta t\, w = \left(1 + z\, p_{m-1}(1-z)\right) y_n = R(z)\, y_n\,,$$

with $z = \Delta t\, \lambda$. The stability function of the equivalent ERK method is the degree m polynomial $R(z) = 1 + z\, p_{m-1}(1-z)$.

Theorem 2. *The stability region of the LIE method, with a Krylov matrix-free linear solver, is necessarily finite. The unconditional stability of the original LIE method is lost.*

Similar considerations hold for Krylov space methods that use an orthogonal basis of the Krylov space, built by Arnoldi iterations [7].

2.2 Accuracy Considerations

The method accuracy is difficult to assess, as the coefficients depend on the time step. The relation between the finite difference scaling factor ε and the time step Δt is important in determining accuracy.

Assume that the finite difference scaling factor is a constant fraction of the time step, $\varepsilon/\Delta t = \text{const}$. This is a reasonable assumption: in order to increase accuracy one decreases both Δt, to reduce the truncation error, and ε, to reduce the finite difference error. (Of course, for very small ε the finite difference error becomes again large due to roundoff.) Also assume that the coefficients $\alpha_1, \ldots, \alpha_m$ do not depend on ε or Δt.

In this case the accuracy can be assessed using the classical approach. The order conditions depend on the Krylov space coefficients α as follows:

$$\text{Order 1:} \quad \sum_{i=1}^{m} b_i = \sum_{j=1}^{m} \alpha_j = 1\,, \tag{7a}$$

$$\text{Order 2:} \quad \sum_{i=1}^{m} b_i c_i = -\sum_{i=2}^{m} (i-1)\,\alpha_i = \frac{1}{2}\,. \tag{7b}$$

Neither condition (7a) nor (7b) are automatically satisfied by the Krylov iterative methods. In particular,

Lemma 1. *The first order accuracy of the matrix-free LIE is not automatic when $\varepsilon/\Delta t = const$. Additional constraints need to be imposed on the Krylov solution coefficients.*

Consider now the case where ε is constant (does not depend on Δt). Assume that the coefficients $\alpha_1, \ldots, \alpha_m$ do not depend on ε or Δt. A necessary condition for the method to be accurate of order p is that its stability function approximates the exponential, $R(z) = e^z + \mathcal{O}\left(z^{p+1}\right)$. The stability function does not depend on either ε or Δt. The conditions (7a) and (7b) on the Krylov solution coefficients $\alpha_1, \ldots, \alpha_m$, which are sufficient when $\varepsilon = const \cdot \Delta t$, seem to be necessary in the case $\varepsilon = const$.

In the general case the Krylov solution coefficients $\alpha_1, \ldots, \alpha_m$ do depend on Δt. For $\Delta t \to 0$ we have that $w \to f(y_n)$ and therefore $\alpha_1 \to 1$, $\alpha_2, \alpha_3, \ldots \to 0$. Asymptotically the condition (7a) holds. Moreover, the number of iterations m also depends on Δt through the convergence speed. Consequently, it is difficult to extend the classical accuracy analysis to matrix-free linearly implicit methods. It seems reasonable, however, to modify the Krylov method and impose at least condition (7a) on the Krylov coefficients.

3 Preconditioned Iterations

Consider the case where a preconditioner matrix M is used to speed up the iterations. The linear system (2) becomes

$$M^{-1}\left(\mathbb{I}-\Delta t\, J(y_n)\right)\cdot k = M^{-1} f(y_n)\,.$$

The Krylov space constructed in this case is

$$\mathscr{K}_m = \text{span}\left\{ f(y_n)\ \ \ldots,\ \left(M^{-1}\left(\mathbb{I}-\Delta t\, J(y_n)\right)\right)^{m-1} M^{-1} f(y_n)\right\}.$$

In the matrix-free approach the following basis is constructed recursively

$$\begin{aligned}
&\ell_1 = M^{-1} f(y_n)\,,\\
&\ell_i = M^{-1}\ell_{i-1} - \Delta t\,\varepsilon^{-1}\, M^{-1} f\left(y_n+\varepsilon\,\ell_{i-1}\right) + \Delta t\,\varepsilon^{-1}\,\ell_1\,,\quad i=2,\ldots,m\,.
\end{aligned}$$

Denote $k_1 = \Delta t\,\ell_1$ and $k_i = \Delta t\,\ell_1 - \varepsilon\,\ell_i$ for $i=2,\cdots,m$. We have

$$\begin{aligned}
M\,k_1 &= \Delta t\, f(y_n) \qquad\qquad (8)\\
M\,k_i &= \Delta t\, f\left(y_n + k_1 - k_{i-1}\right) + k_{i-1} - k_1\,,\quad i=2,\ldots,m\,.
\end{aligned}$$

Consider, for comparison, a Rosenbrock-W (ROW) method in the implementation-friendly formulation [2, Sect. IV.7]

$$\left[\mathbb{I}-\Delta t\,\gamma\widehat{J}_n\right] k_i = \Delta t\,\gamma f\left(y_n + \sum_{j=1}^{i-1} a_{ij}\,k_j\right) + \gamma\sum_{j=1}^{i-1} c_{ij}\,k_j\,,$$

$$y_{n+1} = y_n + \sum_{i=1}^{s} m_i\,k_i\,. \qquad (9)$$

Here $\widehat{J}_n \approx J(y_n)$ is an approximation of the exact Jacobian at the current step. We identify the method coefficients $\gamma = 1$ and

$$c_{i,1} = -1\,;\ \ c_{i,i-1} = 1\,;\ \ a_{i,1} = 1\,;\ \ a_{i,i-1} = -1\,,\quad i=2,\cdots,m\,.$$

From the solution $w = \sum_{i=1}^{m}\alpha_i\,\ell_i = \sum_{i=1}^{m} b_i\,k_i \in \mathscr{K}_m$ we identify the weights

$$b_1 = \alpha_1\,\Delta t^{-1} + \varepsilon^{-1}\sum_{j=2}^{m}\alpha_j\,;\quad b_i = -\varepsilon^{-1}\,\alpha_i\,,\ \ i=2,\ldots,m\,.$$

The preconditioner defines the Jacobian approximation in the ROW method,

$$M = \mathbb{I}-\Delta t\,\gamma\widehat{J}_n \quad\Rightarrow\quad \widehat{J}_n = \Delta t^{-1}\left(\mathbb{I}-M\right).$$

Theorem 3. *The preconditioned matrix-free LIE is equivalent to a linearly-implicit ROW method. The choice of the preconditioner, besides accelerating convergence, improves the stability of the matrix-free LIE method. The preconditioner defines the Jacobian approximation in the ROW method.*

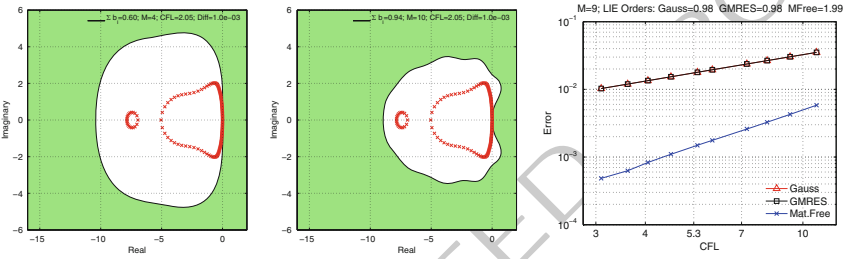
Note that the general approach can be applied to ROW methods [2, Sect. IV.7] by solving the linear system of each stage with an iterative matrix free algorithm. The resulting scheme is an explicit Runge Kutta method (or a ROW method) with $\sum_{i=1}^{s} m_i$ stages.

4 Numerical Results

Consider the one dimensional scalar advection-diffusion equation

$$u_t + (a\,u)_x = D\,u_{xx},\; u(x,t=0) = u_0(x)\,. \tag{10}$$

A spectral discontinuous Galerkin spatial discretization is used with 20 elements and polynomials of order 8. The diffusive term discretization is stabilized using the internal penalty method [8]. The LIE time stepping is used with the matrix-free GMRES solver [7].



(a) D=0.001, m=4 (b) D=0.001, m=10 (c) D=0.001, m=9

Fig. 1. (**a**) and (**b**) The ERK stability regions for different numbers of GMRES iterations. (**c**) The accuracy of the LIE scheme using various approaches to invert the Jacobian matrix. The GMRES weights are restricted by (7b) such as to obtain a second order method. Advection-diffusion equation (10), $\Delta t = CFL$, $\varepsilon = 10^{-6}\,\Delta t$

In Fig. 1a, b, the stability regions generated by the GMRES iterations are plotted for a varying number of Krylov vectors. The regions grow quickly and encompass the eigenvalues of the discrete advection-diffusion operator. Subsequent iterations improve solution accuracy but do not improve linear stability. Additional experiments (not reported here due to space constraints) reveal that the stability region of the resulting ERK method adapts to the eigenvalues of different discrete operators.

To verify the analysis in (7), we consider three different ways of computing the inverse of the linear Jacobian. The first is by Gauss elimination (LU), the second uses GMRES with the full Jacobian, and the third employs matrix-free GMRES iterations. In the last approach the GMRES coefficients are restricted by (7b) such as to obtain a second order time discretization method. Figure 1c shows the work-precision diagram for these approaches. The Gaussian elimination and traditional GMRES solutions display first order converge, while the constrained GMRES solution displays second order convergence.

5 Conclusions

Implicit time integration methods are becoming widely used in the the simulation of time dependent PDEs, as they do not suffer from CFL stability restrictions. While

implicit methods can use much larger time steps than explicit methods, their computational cost per step is also higher. The computational time is dominated by the solutions of (non)linear systems of equations that define each stage of a (linearly) implicit method. The implicit code is more effective only when the gains in step size offset the extra cost.

To reduce the computational overhead of LU decomposition, to alleviate memory requirements, and to aid parallelization, iterative Krylov space methods are used to solve the large linear systems. A matrix-free implementation approximates the required Jacobian vector products by finite differences.

This paper studies the effect of the matrix-free iterative solutions on the properties of the numerical integration method. The analysis reveals that matrix-free linearly implicit methods can be viewed as explicit Runge Kutta methods. Their stability region is finite, and the unconditional stability property of the original implicit method is lost. The equivalent Runge Kutta method is nonlinear, in the sense that its weights depend on the time step and on the stage vectors. This makes the accuracy analysis difficult. Order conditions of the equivalent explicit Runge Kutta method can be fulfilled by imposing additional conditions on the Krylov solution coefficients. For preconditioned matrix-free iterations the overall time stepping process is equivalent to a Rosenbrock-W method, where the preconditioner determines the Jacobian approximation. Future work will address the effect of a finite number of Krylov iterations on the stability and accuracy of the overall scheme, in the case where an analytical Jacobian is used.

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