Improved Adams Linear Multi-step Method Based on Extended Precise Integration Method

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Summary The extended precise integration method(EPIM) can give the same high precise numerical results as the original PIM but avoid the inverse matrix calculation arising from the non-homogeneous terms of polynomials. In this paper EPIM is applied to constructed high precise numerical algorithms for nonlinear systems. Combining the EPIM with the traditional explicit/implicit Adams linear multi-step method, a series of EPIM-based Adams integration formulas for nonlinear differential equations have been constructed. The EPIM-based Adams linear multi-step method have greatly improved the numerical stability and accuracy of the traditional ones benefiting from the high precise integration for the linear part, which is remarkable for stiff problems. The system matrix of linear part can be chosen and tried arbitrarily and numerical experiments show that the linearization matrix is an effective choice. Finally, numerical simulations illustrate the accuracy, efficiency and applicability of the EPIM-based algorithms.

Introduction

Many engineering problems can be described by a set of first-order ordinary differential equations(ODEs) by the finite element spatial discretization and introducing an appropriate state vector. The ODEs can be formally written as

$$\dot{\boldsymbol{x}} = \tilde{\boldsymbol{f}}(t,\boldsymbol{x}) = \boldsymbol{A}_0\boldsymbol{x} + \boldsymbol{f}(t,\boldsymbol{x}) \ , \quad \boldsymbol{x}(0) = \boldsymbol{x}_0 \tag{1}$$

where $\boldsymbol{x}(t)$ is the unknown state vector and a dot denotes differentiation with respect to time *t*. $\boldsymbol{A}_0$ is the time-invariant matrix and $\boldsymbol{f}$ is the formal non-homogenous term. Numerical integration of Eq.(1) is very important in practice and has attracted much attention during recent decades[1]. Since Zhong[2] proposed the precise integration method(PIM) for the transient analysis of structural dynamics, PIM has attracted many attentions and a series of PIM-based algorithms have been constructed[3,4]. However, difficulties of the inverse matrix calculation arise from non-homogeneous terms. Tan[5] presented an extend-PIM(EPIM) for the response matrices of Duhamel's integration, which not only avoids inverse matrix calculation but also gives high precise numerical results for the polynomial non-homogenous terms. In this paper, a series of numerical integration formulas for nonlinear equations are constructed by combining the EPIM with traditional Adams linear multi-step method. Numerical simulations demonstrate the EPIM-based Adams algorithms are highly accurate and stable, especially for problems of stiffness and oscillatory with high frequencies.

General integration formulas

Nonlinear differential equations can be formally divided into two parts: the time-invariant linear part and non-linear part, as described in Eq.(1). This division may be an entirely mathematical form or represent certain physical problems, such as nonlinear perturbation based on the linear system, etc. The solution of Eq.(1) can be solved by Duhamel's integration in the time interval $[t_k, t_k+\eta]$ (where η denotes time-step, i.e. $t_{k+1} = t_k + \eta$),

$$\boldsymbol{x}_{k+1} = \boldsymbol{\Phi}(\eta)\boldsymbol{x}_k + \int_0^{\eta} \exp(\boldsymbol{A}_0(\eta-\tau)) \cdot \boldsymbol{f}(\boldsymbol{x}, t_k+\tau)\boldsymbol{d}\tau \ , \quad \text{where} \quad \boldsymbol{\Phi}(\eta) = \exp(\boldsymbol{A}_0\eta) \tag{2}$$

Assumed the non-homogeneous term $\boldsymbol{f}(\boldsymbol{x},t)$ is approximated by *m*-order polynomial functions in $[t_k, t_{k+1}]$ as

$$\boldsymbol{f}(\boldsymbol{x}, t_k+\tau) = \boldsymbol{f}_{0,k} + \boldsymbol{f}_{1,k}\tau + \cdots + \boldsymbol{f}_{m,k}\tau^m \ , \quad \tau \in [0,\eta] \tag{3}$$

in which $\boldsymbol{f}_{0,k}, \boldsymbol{f}_{1,k}, \boldsymbol{f}_{2,k}, \cdots$ are the polynomial coefficients. Then the integration formula of Eq.(2) can be written as

$$\boldsymbol{x}_{k+1} = \boldsymbol{\Phi}(\eta)\boldsymbol{x}_k + \boldsymbol{\Phi}_0(\eta)\boldsymbol{f}_{0,k} + \boldsymbol{\Phi}_1(\eta)\boldsymbol{f}_{1,k} + \cdots + \boldsymbol{\Phi}_m(\eta)\boldsymbol{f}_{m,k} \tag{4}$$

where $\boldsymbol{\Phi}_n(\eta)$ is the response matrix of *n*-order polynomial function as[5]

$$\boldsymbol{\Phi}_n(\eta) = \int_0^{\eta} \exp(\boldsymbol{A}_0(\eta-\tau)) \cdot \tau^n \boldsymbol{d}\tau, \quad n = 0,1,2,\cdots m \tag{4a}$$

Eq.(4) presents the integration formula of nonlinear equation based on the response matrices of polynomial functions. Its implementation requires two key points to be well solved. One point is to compute the state transition matrix $\boldsymbol{\Phi}(\eta)$ and response matrices $\boldsymbol{\Phi}_0(\eta), \boldsymbol{\Phi}_1(\eta), \cdots, \boldsymbol{\Phi}_m(\eta)$, which can be obtained by the EPIM[5] avoiding the inverse matrix calculation of $\boldsymbol{A}_0$. The other point is to compute the polynomial coefficients $\boldsymbol{f}_{0,k}, \boldsymbol{f}_{1,k}, \cdots, \boldsymbol{f}_{m,k}$ for approximating non-homogeneous term $\boldsymbol{f}(\boldsymbol{x},t)$. In this paper, the Adams linear multi-step method are used to solve polynomial coefficients. And the corresponding EPIM-based integration formulas of Eq.(4) are also derived.

Multi-step method

Firstly, the derivation based on explicit Adams two-step method is presented in detail. Considering time instances t_{k-2}, t_{k-1}, t_k as the interpolation points, $\boldsymbol{f}(\boldsymbol{x},t)$ in $[t_k, t_{k+1}]$ can be expressed as Eq.(3) with $m=2$, and

$$\boldsymbol{f}_{0,k} = \boldsymbol{f}_k, \ \boldsymbol{f}_{1,k} = \left(\boldsymbol{f}_{k-2} - 4\boldsymbol{f}_{k-1} + 3\boldsymbol{f}_k\right)/2\eta, \ \boldsymbol{f}_{2,k} = \left(\boldsymbol{f}_{k-2} - 2\boldsymbol{f}_{k-1} + \boldsymbol{f}_k\right)/2\eta^2 \tag{5}$$

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in which f_k denotes the value of $f(\boldsymbol{x},t)$ at time instance t_k. Substituting Eq.(5) into Eq.(4), the EPIM-based integration formula is derived as

$$\boldsymbol{x}_{k+1} = \boldsymbol{\Phi}(\eta)\boldsymbol{x}_k + \bar{\boldsymbol{\Phi}}_0(\eta)\cdot \boldsymbol{f}_k + \bar{\boldsymbol{\Phi}}_{-1}(\eta)\cdot \boldsymbol{f}_{k-1} + \bar{\boldsymbol{\Phi}}_{-2}(\eta)\cdot \boldsymbol{f}_{k-2} \tag{6}$$

In the same way, the EPIM-based formula corresponding Eq.(4) based on explicit Adams *m*-step method can be derived as

$$\boldsymbol{x}_{k+1} = \boldsymbol{\Phi}(\eta)\boldsymbol{x}_k + \bar{\boldsymbol{\Phi}}_0(\eta)\cdot \boldsymbol{f}_k + \bar{\boldsymbol{\Phi}}_{-1}(\eta)\cdot \boldsymbol{f}_{k-1} + \cdots + \bar{\boldsymbol{\Phi}}_{-m}(\eta)\cdot \boldsymbol{f}_{k-m} \tag{7}$$

And the EPIM-based formula based on implicit *m*-step method can bederived as

$$\begin{aligned}\boldsymbol{x}_{k+1} = \boldsymbol{\Phi}(\eta)\boldsymbol{x}_k &+ \bar{\boldsymbol{\Phi}}_{+1}(\eta)\cdot \boldsymbol{f}_{k+1} + \bar{\boldsymbol{\Phi}}_0(\eta)\cdot \boldsymbol{f}_k + \bar{\boldsymbol{\Phi}}_{-1}(\eta)\cdot \boldsymbol{f}_{k-1} + \cdots \\ &+ \bar{\boldsymbol{\Phi}}_{-m+1}(\eta)\cdot \boldsymbol{f}_{k-m+1}\end{aligned} \tag{8}$$

where $\bar{\boldsymbol{\Phi}}_0(\eta),\ \bar{\boldsymbol{\Phi}}_{-1}(\eta),\ \cdots,\ \bar{\boldsymbol{\Phi}}_{-m+1}(\eta),\ \bar{\boldsymbol{\Phi}}_{+1}(\eta)$ are determined by the response matrices $\boldsymbol{\Phi}_0(\eta), \boldsymbol{\Phi}_1(\eta), \cdots, \boldsymbol{\Phi}_m(\eta)$. Figure 1(a,b,c) and Figure 1(d,e,f) list the corresponding combination parameters of the EPIM-based explicit and implicit Adams *m*-step method for $m = 1,2,3$, respectively.

(a) Explicit

	$\boldsymbol{\Phi}_0$	$\boldsymbol{\Phi}_1/\eta$
$\bar{\boldsymbol{\Phi}}_{-3}$		
$\bar{\boldsymbol{\Phi}}_{-2}$		
$\bar{\boldsymbol{\Phi}}_{-1}$		-1
$\bar{\boldsymbol{\Phi}}_{0}$	1	1

(b)

	$\boldsymbol{\Phi}_0$	$\boldsymbol{\Phi}_1/\eta$	$\boldsymbol{\Phi}_2/\eta^2$
$\bar{\boldsymbol{\Phi}}_{-3}$			
$\bar{\boldsymbol{\Phi}}_{-2}$		1/2	1/2
$\bar{\boldsymbol{\Phi}}_{-1}$		-2	-1
$\bar{\boldsymbol{\Phi}}_{0}$	1	3/2	1/2

(c)

	$\boldsymbol{\Phi}_0$	$\boldsymbol{\Phi}_1/\eta$	$\boldsymbol{\Phi}_2/\eta^2$	$\boldsymbol{\Phi}_3/\eta^3$
$\bar{\boldsymbol{\Phi}}_{-3}$		$-1/3$	$-1/2$	$-1/6$
$\bar{\boldsymbol{\Phi}}_{-2}$		3/2	2	1/2
$\bar{\boldsymbol{\Phi}}_{-1}$		-3	$-5/2$	$-1/2$
$\bar{\boldsymbol{\Phi}}_{0}$	1	11/6	1	1/6

(d) Implicit

	$\boldsymbol{\Phi}_0$	$\boldsymbol{\Phi}_1/\eta$
$\bar{\boldsymbol{\Phi}}_{-2}$		
$\bar{\boldsymbol{\Phi}}_{-1}$		
$\bar{\boldsymbol{\Phi}}_{+1}$		1
$\bar{\boldsymbol{\Phi}}_{0}$	1	-1

(e)

	$\boldsymbol{\Phi}_0$	$\boldsymbol{\Phi}_1/\eta$	$\boldsymbol{\Phi}_2/\eta^2$
$\bar{\boldsymbol{\Phi}}_{-2}$			
$\bar{\boldsymbol{\Phi}}_{-1}$		$-1/2$	1/2
$\bar{\boldsymbol{\Phi}}_{+1}$		1/2	1/2
$\bar{\boldsymbol{\Phi}}_{0}$	1	0	-1

(f)

	$\boldsymbol{\Phi}_0$	$\boldsymbol{\Phi}_1/\eta$	$\boldsymbol{\Phi}_2/\eta^2$	$\boldsymbol{\Phi}_3/\eta^3$
$\bar{\boldsymbol{\Phi}}_{-2}$		1/6	0	$-1/6$
$\bar{\boldsymbol{\Phi}}_{-1}$		-1	1/2	1/2
$\bar{\boldsymbol{\Phi}}_{+1}$		1/3	1/2	1/6
$\bar{\boldsymbol{\Phi}}_{0}$	1	1/2	-1	$-1/2$

Figure 1 Parameters of EPIM-based explicit And implicit Adams m-step method
(a,b,c): parameters of explicit method
(d,e,f): parameters of implicit method

Numerical Simulations

Example 1: The problem of Fermi-Pasta-Ulam[6] is used to compare the numerical accuracy and stability of the EPIM-based explicit/implicit Adams linear multi-step methods and the traditional ones. The nonlinear equations can be expressed in the form of Eq.(1) with $\boldsymbol{x} = [q_1, q_2, \dot{q}_1, \dot{q}_2]^{\mathrm{T}}$

$$\boldsymbol{A}_0 = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -\omega^2 & \omega^2 & 0 & 0 \\ \omega^2 & -\omega^2 & 0 & 0 \end{bmatrix}, \quad \boldsymbol{f}(\boldsymbol{x},t) = \begin{Bmatrix} 0 \\ 0 \\ -q_1^3 \\ -q_2^3 \end{Bmatrix}$$

This is a typical nonlinear stiff problem when ω is large.

In numerical computations, let $\omega = 50$ and the initial value $\boldsymbol{x}(0) = [1, 1.1, 0, 0]^{\mathrm{T}}$. When the time step is set as $\eta = 0.001$, numerical results of the EPIM-based algorithms are about four significant digits more than ones of the corresponding traditional explicit/implicit Adams method. To further testify the numerical stability, the simulation time is extended to 400s. Figure 2 shows the reference result and the results obtained from the present EPIM-based implicit Adams 3-step method for long time simulations. It can be seen that the results coincide with the reference results even for larger time step. While the numerical results of traditional implicit Adams 3-step method diverge rapidly with the same time step $\eta = 0.01$.

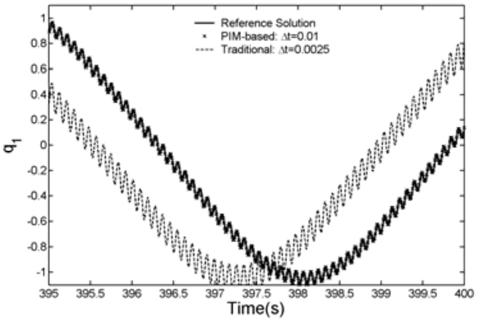

Figure 2 Comparisons of argument q_1 for long time computation

Conclusions

EPIM enhance the numerical stability and extend the scope of application of PIM. In this paper a series of EPIM-based algorithms for nonlinear system are constructed combining with the traditional explicit/implicit Adams linear multi-step method, where the system matrix of linear part can be chosen and tried arbitrarily. In contrast to traditional Adams algorithms, the EPIM-based Adams algorithms greatly improved the numerical accuracy and stability, especially for stiff problems. Numerical simulations illustrate the numerical accuracy, efficiency and applicability of the proposed method.

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