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A novel series of solution methods for solving nonlinear stiff dynamic problems

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Abstract A novel type of linear multi-step formulas is proposed for solving initial value problems, such as the problems of multi-body systems and vibration systems and a variety of dynamic problems in engineering. This type of formulas is derived from an eigen-based theory and is characterized by problem dependency since it has problem-dependent coefficients, which are functions of physical properties for defining the problem under analysis and applied step size. These coefficients are no longer limited to be scalar constants but can be constant matrices. The detailed development of a set of problem-dependent formulas is presented, and their numerical properties are intensively explored. These formulas can be explicitly or implicitly implemented in the solution of initial value problems. One of these problem-dependent methods can combine A-stability and explicit formulation together, and thus, it is best suited to solve nonlinear stiff problems, such as problems in chemical kinetics and vibrations, the analysis of control systems and the study of dynamical systems. It is validated that A-stability in conjunction with explicit formulation can save many computational efforts for solving nonlinear stiff dynamic problems when compared to conventional implicit methods. Notice that there exists no conventional method that can simultaneously combine A-stability and explicit formulation.

Keywords Eigen-dependent formula · Problem-dependent formula · Convergence · Consistency · Absolute stability · Nonlinear problems · Stiff dynamic systems

1 Introduction

The use of the laws of Newtonian dynamics to multi-body or vibration systems can lead to a set of second-order ordinary differential equations (ODEs) [1]. They can be converted to a set of first-order ODEs. Although analytical solutions may be found for few simple problems, the number and complex of these equations generally require numerical solutions [2–14], where the computational efficiency and accuracy of the mathematical models will rely on those of the numerical methods for solving ODEs. It is important to select an appropriate numerical method since solutions of these ODEs might be difficult and computationally expensive. Numerical methods have been developed to approximate the solutions of ODEs, and they are classified into two categories of explicit and implicit methods. In general, an explicit method involves no nonlinear iterations for each step in the

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solution of nonlinear ODEs while the step size will be limited due to no possession of A-stability property. On the contrary, an A-stability of an implicit method might have no limitation on a step size while it generally requires nonlinear iterations for each step in the solution of nonlinear ODEs. As a result, A-stability and explicitness seems to repel each other for a numerical method in the solution of nonlinear ODEs. In fact, Dahlquist [15, 16] has proved that there is no explicit method in the linear multi-step methods that can have A-stability.

A difference formula to calculate next step increment is generally required to solve systems of first-order ODEs. The coefficients of difference formulas are generally scalar constants for current numerical methods for solving ODEs. This type of difference formulas is referred as conventional difference formulas for brevity. Unlike the adoption of scalar constant coefficients for conventional difference formulas, a new type of problem-dependent difference formulas is proposed in this work. This type of difference formulas can be derived from an eigen-based theory. In general, three major stages are involved in the development procedure: (1) to decompose a system of coupled first-order ODEs into a system of uncoupled first-order ODEs; (2) to proposed an eigen-dependent difference formula to solve each uncoupled first-order ODE; (3) to convert all the eigen-dependent difference formulas to a problem-dependent difference formula. In general, the first and third stages generally involve an eigen-decomposition technique whereas some critical assumptions are required in the second stage for developing an eigen-dependent difference formula.

A series of problem-dependent difference formulas will be proposed to solve the first-order ODEs. The details of each major stage of the development procedure will be presented. Besides, an insight of each major stage will be disclosed and its correctness will be also justified. It will be shown that the application of the proposed problem-dependent difference formulas to solve ODEs can be either explicitly or implicitly implemented. A problem-dependent method with an explicit implementation can simultaneously combine an A-stability and explicit formulation; thus, it is promising for solving stiff problems arising from engineering science, such as multi-body systems, vibrations, electrical circuits, and chemical reactions. Such stiff problems are often solved by A-stable, implicit methods. To corroborate the numerical properties and feasibility of the proposed problem-dependent methods, some examples are examined, such as a Van der Pol oscillator, a structure vibration problem, and a dynamical system of a nonlinear pendulum. To numerically explore the computational efficiency of the proposed explicit problem-dependent method, a series of mechanical systems, which are stiff, nonlinear problems, are solved.

2 Decomposition of coupled ODEs

A system of n coupled first-order ODEs for modeling a physical or engineering problem can be simply expressed as [17–23]:

$$\mathbf{z}' = \mathbf{g}(x, \mathbf{z}) = \mathbf{Q}\mathbf{z} + \mathbf{f}, \quad \mathbf{z}(x) = \begin{Bmatrix} z_1(x) \\ z_2(x) \\ \mathbf{M} \\ z_n(x) \end{Bmatrix},$$

$$\mathbf{g}(x, \mathbf{z}) = \begin{Bmatrix} g_1(x, \mathbf{z}) \\ g_2(x, \mathbf{z}) \\ \mathbf{M} \\ g_n(x, \mathbf{z}) \end{Bmatrix} \tag{1}$$

where $\mathbf{Q}$ is an $n \times n$ matrix and $\mathbf{f}$ is a vector-valued function of x. The initial value problem for Eq. (1) is to determine a function $\mathbf{z}(x)$ to satisfy Eq. (1) and initial condition of $\mathbf{z}(x_0) = \mathbf{z}_0$.

To decompose coupled Eq. (1) into a series of uncoupled ODEs, it is required to conduct an eigen-analysis of $|\mathbf{Q} - \lambda \mathbf{I}| = 0$ to determine the n eigenvalues and eigenvectors of the matrix $\mathbf{Q}$. If the eigenvalues $\lambda^{(j)}, j = 1, 2, 3, \ldots, n$, of the matrix $\mathbf{Q}$ are distinct, there exists a non-singular eigenvector matrix $\mathbf{S}$ such that:

$$\mathbf{S}^{-1}\mathbf{Q}\mathbf{S} = \mathbf{L} = \begin{bmatrix} \lambda^{(1)} & 0 & \mathbf{L} & 0 \\ 0 & \lambda^{(2)} & \mathbf{L} & 0 \\ \mathbf{L} & \mathbf{L} & \mathbf{L} & \mathbf{L} \\ 0 & 0 & \mathbf{L} & \lambda^{(n)} \end{bmatrix}, \tag{2}$$

$$\mathbf{S} = \begin{bmatrix} \mathbf{s}^{(1)}, & \mathbf{s}^{(2)}, & \mathbf{L} & \mathbf{s}^{(n)} \end{bmatrix}$$

where $\mathbf{s}^{(j)}$ is the j-th eigenvector corresponding to the j-th eigenvalue $\lambda^{(j)}$. Subsequently, the relationships of

$\mathbf{z} = \mathbf{S}\mathbf{y}$ and $\mathbf{f} = \mathbf{S}\mathbf{p}$ are defined. After the substitutions of these relationships into Eq. (1), it becomes:

$$\mathbf{y}' = \mathbf{L}\mathbf{y} + \mathbf{p} \tag{3}$$

Since $\mathbf{L} = \mathbf{S}^{-1}\mathbf{Q}\mathbf{S}$ and is a diagonal matrix, Eq. (3) is a system of the uncoupled first-order ODEs. In general, it can be alternatively expressed in component-wise form and is found to be:

$$y'^{(j)} = \lambda^{(j)}y^{(j)} + p^{(j)}, j = 1, 2, 3, \ldots, n \tag{4}$$

where $y^{(j)}$ and $p^{(j)}$ are the j-th component of $\mathbf{y}$ and $\mathbf{p}$, respectively. Each one of these n equations is completely decoupled from the other $n-1$ equations. Hence, a system of n coupled ODEs is decomposed into a set of n uncoupled ODEs by using an eigen-decomposition technique. If $\mathbf{Q}$ is symmetric, negative semi-definite, one can have $\lambda^{(n)} \leq \lambda^{(n-1)} \leq \cdots \leq \lambda^{(1)} \leq 0$. For simplicity, each uncoupled first-order ODE can be alternatively written as:

$$y' = g(x, y) = \lambda y + p \tag{5}$$

where λ is an eigenvalue of the matrix $\mathbf{Q}$ and p is a function of x. A discrete numerical solution of Eq. (5) can be defined as a set of points (x_i, u_i), which are the approximations to the corresponding point $[x_i, y(x_i)]$ on the solution curve.

3 Development of eigen-dependent difference formula

After decomposing a coupled first-order ODE into a series of uncoupled first-order ODEs, the next stage is to develop an eigen-dependent difference formula to solve each uncoupled first-order ODE, i.e., Eq. (5). The interval of interest $x_0 \leq x \leq x_l$ can be equally divided into l subintervals such that:

$$h = \frac{x_l - x_0}{l}, x_i = x_0 + ih, i = 0, 1, 2, \cdots, l \tag{6}$$

where h is a step size and l is a positive integer. A difference formula is applied to approximate the solution of the first-order ODE as shown in Eq. (5).

3.1 Basic assumptions

An important goal to propose an eigen-dependent difference formula to solve each uncoupled first-order ODE is that an accurate solution must be yielded for slow eigenmodes while no unstable solution must be ensured for fast eigenmodes. This goal is planned to develop a problem-dependent method that can combine A-stability and explicit implementation at the same time. In general, the following assumptions must be made for developing an eigen-dependent difference formula:

(1) A source-dependent term must be included in the eigen-dependent difference formula so that a desired order of accuracy can be achieved.

(2) Since the purpose is to develop an explicit eigen-dependent difference formula, it only involves the previous step data for determining the current step data.

(3) Coefficients of the eigen-dependent difference formula can be rational functions of the product of the initial eigenvalue of the uncoupled first-order ODE and the step size, i.e., the numerator and/or denominator can be a polynomial function of the product of $\Lambda_0 = \lambda_0 h$, where λ_0 is an initial eigenvalue of the corresponding eigenmode.

(4) A scalar constant term must be included in the polynomial function of the numerator and that of the denominator. This is intended to ensure that an eigen-dependent coefficient can degenerate into an asymptotic scalar constant as the product $|\Lambda_0| = |\lambda_0 h|$ tends to zero and infinity. Hence, the eigen-dependent difference formula will become a conventional difference formula in both extreme cases.

(5) The maximum power of Λ_0 in the numerator must be no more than that of the denominator so that a stable calculation can be guaranteed for fast eigenmodes.

A series of eigen-dependent difference formulas will be developed based on these assumptions and they will be also explored subsequently.

An approximating difference formula to define the increment of y is generally required for solving Eq. (5), and the Taylor series expansion is often adopted to derive this formula. As a result, many linear multi-step formulas have been developed to solve a system of coupled first-order ODEs. The following general form will be used to develop a linear multi-step, eigen-dependent difference formula:

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$$u_{i+1} = u_i + h\left(\sum_{k=1}^{m} \beta_k v_{i+1-k} + \psi_{i+1}\right) \quad (7)$$

where $u_{i+1} \approx y(x_{i+1})$, $v_{i+1} \approx y'(x_{i+1})$, and $\beta_1, \beta_2, \ldots, \beta_m$ are the coefficients of $v_i, v_{i-1}, \ldots, v_{i+1-m}$. In addition, ψ_{i+1} is a function of the source term. It will be shown later that the term ψ_{i+1} must be included in the general formulation of an eigen-dependent difference formula so that a desired order of accuracy can be obtained. This source-dependent term has never been seen in the conventional linear multi-step formulas. The eigen-dependent coefficient β_k is assumed to be:

$$\beta_k = \frac{b_k}{1 + a_m \Lambda_0} \quad \text{for} \quad k = 1, 2, \ldots, m \quad (8)$$

where m is a total number of step data $v_i, v_{i-1}, v_{i-2}, \ldots$ for calculating u_{i+1}. The eigenvalue λ as shown in Eq. (5) is generally different from λ_0 for a nonlinear first-order ODE since it may vary with x. It is evident that β_k is a rational function of Λ_0, where the numerator and denominator are polynomial functions of Λ_0. Besides, b_1 to b_m and a_m are scalar constant coefficients. The maximum power of Λ_0 in the numerator is found to be 0 and is less than that in the denominator of 1. A scalar constant term b_k is taken for the numerator and that of 1 is taken in the denominator for simplicity.

It is found that β_k will tend to b_k in the limit $|\Lambda_0| \rightarrow 0$ while it will approach zero in the limit $|\Lambda_0| \rightarrow \infty$. The former implies that the proposed eigen-dependent formula will degenerate into a conventional formula form, whose coefficients are scalar constants, for slow eigenmodes. On the other hand, the latter implies that there will be no unstable solutions for the fast eigenmodes due to $\beta_k = 0$. As a result, it seems possible to achieve the goal to develop an eigen-dependent difference formula that can simultaneously combine an A-stability and an explicit formulation together.

3.2 Determination of coefficient

Since a numerical method is required to be convergent, convergence must be satisfied for an eigen-dependent difference formula. The convergence of the proposed eigen-dependent difference formulas can be proved by using the Dahlquist equivalence theorem

[15], which states that a linear multi-step formula is convergent if and only if it is zero-stable and consistent. Thus, consistency and zero-stability can be used to determine the coefficients of the proposed eigen-dependent difference formulas. It is clear that β_k must be appropriately determined so that desired numerical properties, such as A-stability and desired order of accuracy, can be achieved. The proposed eigen-dependent difference formula can be applied to solve the corresponding uncoupled first-order ODE and then a Proposed Eigen-dependent Method is formulated and will be abbreviated as PEM for brevity.

To verify that PEM is consistent and zero-stable can be considered as an alternative way to prove the convergence of PEM based on the Dahlquist equivalence theorem. Besides, consistency of a numerical method can be confirmed by its order of accuracy and this order of accuracy can be, in general, determined from a local truncation error. As a result, the local truncation error of PEM can be applied to determine the coefficients β_k so that a desired order of accuracy can be achieved. A local truncation error of a numerical method is generally defined as the error experienced in each step by using an approximating difference equation to replace the differential equation. Hence, the local truncation error for PEM can be written as:

$$E_i = \frac{y_{i+1} - y_i}{h} - \left(\sum_{k=1}^{m} \beta_k g_{i+1-k} + \psi_{i+1}\right) \quad (9)$$

A local truncation error is limited by $|E_i| \leq \alpha h^\beta$ where α is a constant and is independent of h. It is consistent if $\beta > 0$ and β is referred as the rate of convergence or the order of accuracy.

An explicit expression of the local truncation error for PEM can be obtained after substituting y_{i+1}, g_{i+1}, g_{i-1}, $\ldots$ and g_{i+1-m} into it. Each of the terms can be expanded by a finite Taylor series if $y(x)$ and $g[x, y(x)]$ is continuously differentiable up to any required order. As a result, they can be generally written as:

$$y_{i+1} = y_i + hy_i' + \frac{1}{2!}h^2 y_i'' + \frac{1}{3!}h^3 y_i''' + \cdots = y_i + hg_i + \frac{1}{2!}h^2 g_i' + \frac{1}{3!}h^3 g_1'' + \cdots$$

$$g_{i+1-k} = g_i - [(k-1)h]g_i' + \frac{1}{2!}[(k-1)h]^2 g_i'' - \frac{1}{3!}[(k-1)h]^3 g_i''' + \cdots$$
$$(10)$$

where $k = 1, 2, \ldots, m$ for developing a set of eigen-dependent difference formulas correspondingly. As a result, the local truncation error of PEM is found to be:

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$$E_i = \psi_{i+1} - \left(\frac{a_m}{1+a_m\Lambda_0}\right)(p_{i+1}-p_i) + \left(\frac{1}{1+a_m\Lambda_0}\right)[1-(b_1+b_2+\cdots+b_m)]g_i$$
$$+ \left(\frac{1}{1+a_m\Lambda_0}\right)\left\{\frac{1}{1!}a_m + \frac{1}{2!} + \frac{1}{1!}\left[b_2 + 2^1b_3 + 3^1b_3\cdots+(m-1)b_m\right]\right\}hg_i'$$
$$+ \left(\frac{1}{1+a_m\Lambda_0}\right)\left\{\frac{1}{2!}a_m + \frac{1}{3!} - \frac{1}{2!}\left[b_2 + 2^2b_3 + 3^2b_3\cdots+(m-1)^2b_m\right]\right\}h^2g_i''$$
$$+ \left(\frac{1}{1+a_m\Lambda_0}\right)\left\{\frac{1}{3!}a_m + \frac{1}{4!} + \frac{1}{3!}\left[b_2 + 2^3b_3 + 3^3b_3\cdots+(m-1)^3b_m\right]\right\}h^3g_i'''$$
$$+ \left(\frac{1}{1+a_m\Lambda_0}\right)\left\{\frac{1}{4!}a_m + \frac{1}{5!} - \frac{1}{4!}\left[b_2 + 2^4b_3 + 3^4b_3\cdots+(m-1)^4b_m\right]\right\}h^4g_i^{(4)} + \cdots$$

$$(11)$$

To be a consistent linear multi-step method, the local truncation error of PEM is necessitated to at least possess the first-order accuracy. This implies that all the error terms with an order of h less than 1 must be eliminated from Eq. (11). Hence, the second and third terms on the right side of Eq. (11) must disappear since they have a zero order of h. It is manifested from Eq. (11) that the second term is the only source-dependent error term, and thus, it can be completely taken out by using the assumed source-dependent term ψ_{i+1}. It is straightforward to find that the term of ψ_{i+1} is:

$$\psi_{i+1} = \frac{a_m}{1+a_m\Lambda_0}(p_{i+1}-p_i) \qquad (12)$$

Apparently, there is no way to remove the second term on the right side of Eq. (11) if the source-dependent term ψ_{i+1} is excluded from the general formulation of the proposed difference formula, i.e., Eq. (7). A series of eigen-dependent difference formulas can be derived from Eq. (11) if the coefficients of a_m and $b_1, b_2, \ldots, b_m$ are appropriately determined. For brevity, PEM-m is used to represent a m-step proposed eigen-dependent difference formula, where the m-step data of $v_i, v_{i-1}, v_{i-2},\ldots$ and v_{i-m+1} are adopted to determine u_{i+1}. As an example, PEM-1 can be achieved if only the previous step data u_i and v_i are used to approximate u_{i+1} in Eq. (7). In this case, Eq. (7) will reduce to $u_{i+1} = u_i + h(\beta_1 v_i + \psi_{i+1})$ and its corresponding local truncation error in Eq. (11) will be simplified to be:

$$E_i = \psi_{i+1} - \left(\frac{a_1}{1+a_1\Lambda_0}\right)(p_{i+1}-p_i) + \frac{1-b_1}{1+a_1\Lambda_0}g_i$$
$$+ \frac{a_1+\frac{1}{2}}{1+a_1\Lambda_0}hg_i' + \frac{\frac{1}{2}a_1+\frac{1}{6}}{1+a_1\Lambda_0}h^2g_i'' + O(h^3)$$

$$(13)$$

Clearly, an order of accuracy 1 can be obtained if $b_1 = 1$ is adopted in addition to the satisfaction of

Eq. (12). As a result, the local truncation error for PEM-1 becomes:

$$E_i = \frac{a_1+\frac{1}{2}}{1+a_1\Lambda_0}hg_i' + \frac{\frac{1}{2}a_1+\frac{1}{6}}{1+a_1\Lambda_0}h^2g_i'' + O(h^3) \qquad (14)$$

This equation reveals that PEM-1 can have the first-order accuracy for a general value of a_1. Thus, its consistency is verified. The second-order accuracy can be further achieved for PEM-1 if $a_1 = -\frac{1}{2}$ is taken, and the corresponding local truncation error is found to be $E_i = -\frac{1}{12}h^2g_i''/(1-\frac{1}{2}\Lambda_0) + O(h^3)$.

A series of eigen-dependent difference formulas can be derived from Eq. (11) by applying the same procedure, and the results are shown in Table 1. The value of a_m is found to be $a_1 = -\frac{1}{2}$, $a_2 = -\frac{5}{12}$ and $a_3 = -\frac{9}{24}$ corresponding to PEM-1 to PEM-3. The last column of this table shows the A-stability interval of each eigen-dependent difference formula and will be investigated later. The column of E_i reveals that the dominant error term increases from the second-order to fourth-order accuracy corresponding to PEM-1 to PEM-3. For comparison, the conventional formulas of the Adams–Moulton Method (AMM) are also listed in this table correspondingly. It is disclosed by the second column that PEM has an explicit eigen-dependent difference formula while AMM has an implicit difference formula since it involves the current step data v_{i+1} to determine u_{i+1}.

Some discrepancies can be found between the coefficients β_k for PEM and γ_k for AMM in Table 1. Clearly, β_k is an eigen-dependent coefficient while γ_k is a scalar constant coefficient. It is also found that the numerator of β_1 is equal to the sum of γ_1 and γ_2 for each corresponding difference formula, whereas the other β_k of the numerator is equivalent to γ_{k+1} correspondingly. The column of E_i exhibits that PEM and AMM have the same order of accuracy for a specific m. In fact, the only difference in the coefficient of E_i is the denominator of $1+a_m\Lambda_0$ for PEM and 1 for AMM. The last column reveals that the A-stability interval for each difference formula of PEM is the same as that of AMM. This will be validated later. Hence, it is expected that the performance of PEM in the solution of an uncoupled first-order ODE will resemble that of AMM due to almost the same stability and accuracy properties.

It is of interest to assess the performance of each eigen-dependent difference formula for both slow and

Table 1 PEM and AMM as well as their numerical properties

m	PEM-m	$\beta_k = \frac{b_k}{1+a_m\Lambda_0}$	$\psi_{i+1} = \frac{a_m(p_{i+1}-p_i)}{1+a_m\Lambda_0}$	E_i	A-Stability
1	$u_{i+1} = u_i + h\left(\sum_{k=1}^{1}\beta_k v_{i+1-k} + \psi_{i+1}\right)$	$\beta_1 = \frac{1}{1-\frac{1}{2}\Lambda_0}$	$\frac{\frac{1}{2}(p_{i+1}-p_i)}{1-\frac{1}{2}\Lambda_0}$	$\frac{-\frac{1}{12}}{1-\frac{1}{2}\Lambda_0}h^2 y'''(x_i)$	$-\infty \le \Lambda_0 \le 0$
2	$u_{i+1} = u_i + h\left(\sum_{k=1}^{2}\beta_k v_{i+1-k} + \psi_{i+1}\right)$	$\beta_1 = \frac{\frac{13}{12}}{1-\frac{5}{12}\Lambda_0}$, $\beta_2 = \frac{-\frac{1}{12}}{1-\frac{5}{12}\Lambda_0}$	$\frac{\frac{5}{12}(p_{i+1}-p_i)}{1-\frac{5}{12}\Lambda_0}$	$\frac{-\frac{1}{24}}{1-\frac{5}{12}\Lambda_0}h^3 y^{(4)}(x_i)$	$-6le\Lambda_0 \le 0$
3	$u_{i+1} = u_i + h\left(\sum_{k=1}^{3}\beta_k v_{i+1-k} + \psi_{i+1}\right)$	$\beta_1 = \frac{\frac{28}{24}}{1-\frac{9}{24}\Lambda_0}$, $\beta_2 = \frac{-\frac{5}{24}}{1-\frac{9}{24}\Lambda_0}$, $\beta_3 = \frac{\frac{1}{24}}{1-\frac{9}{24}\Lambda_0}$	$\frac{\frac{9}{24}(p_{i+1}-p_i)}{1-\frac{9}{24}\Lambda_0}$	$\frac{-\frac{19}{720}}{1-\frac{9}{24}\Lambda_0}h^4 y^{(5)}(x_i)$	$-3 \le \Lambda_0 \le 0$

m	AMM-m	γ_k	E_i	A-Stability
1	$u_{i+1} = u_i + h\sum_{k=0}^{1}\gamma_{k+1}v_{i+1-k}$	$\gamma_1 = \frac{1}{2}$, $\gamma_2 = \frac{1}{2}$	$-\frac{1}{12}h^2 y'''(x_i)$	$-\infty \le \Lambda_0 \le 0$
2	$u_{i+1} = u_i + h\sum_{k=0}^{2}\gamma_{k+1}v_{i+1-k}$	$\gamma_1 = \frac{5}{12}$, $\gamma_2 = \frac{8}{12}$, $\gamma_3 = \frac{-1}{12}$	$-\frac{1}{24}h^3 y^{(4)}(x_i)$	$-6le\Lambda_0 \le 0$
3	$u_{i+1} = u_i + h\sum_{k=0}^{3}\gamma_{k+1}v_{i+1-k}$	$\gamma_1 = \frac{9}{24}$, $\gamma_2 = \frac{19}{24}$, $\gamma_3 = \frac{-5}{24}$, $\gamma_4 = \frac{1}{24}$	$-\frac{19}{720}h^4 y^{(5)}(x_i)$	$-3 \le \Lambda_0 \le 0$

fast eigenmodes since these formulas have the characteristic of eigen dependency. Hence, the limiting cases of $|\Lambda_0| \to 0$ and $|\Lambda_0| \to \infty$ are investigated for each eigen-dependent difference formula of PEM and the results are summarized in Table 2. These two limiting cases can imply the behaviors of the slow and fast eigenmodes, respectively. As an example, in the limit $|\Lambda_0| \to 0$, the one-step proposed eigen-dependent difference formula for PEM becomes:

$$u_{i+1} = \lim_{\Lambda_0 \to 0}\left[u_i + \frac{1}{1-\frac{1}{2}\Lambda_0}hv_i + \frac{\frac{1}{2}}{1-\frac{1}{2}\Lambda_0}h(p_{i+1}-p_i)\right]$$
$$\approx u_i + hv_i + \frac{1}{2}h(p_{i+1}-p_i)$$
(15)

The similar calculating procedure can be also used to obtain the results for the two-step to four-step proposed eigen-dependent difference formulas. It is manifested from Table 2 that the coefficients of each eigen-dependent difference formula are no longer eigen-dependent but become scalar constants in the limiting case of $|\Lambda_0| \to 0$. In fact, each eigen-

dependent difference formula degenerates like a conventional difference formula except for an extra source-dependent term. It is interesting to find that each degenerate difference formula as shown in the second column of Table 2 is analogous to that of AMM as shown in Table 1. In fact, PEM and AMM have the same coefficients for most terms of each corresponding difference formula except that the coefficient of the term of v_i for PEM is equal to the sum of the coefficients of the terms of v_i and v_{i+1} for AMM.

On the other hand, it can be found that in the limiting case of $|\Lambda_0| \to \infty$ the formulation of the proposed eigen-dependent difference formula for PEM-1 will reduce to:

$$u_{i+1} = \lim_{\Lambda_0 \to \infty}\left[u_i + \frac{1}{1-\frac{1}{2}\Lambda_0}hv_i + \frac{\frac{1}{2}}{1-\frac{1}{2}\Lambda_0}h(p_{i+1}-p_i)\right]$$
$$\approx u_i$$
(16)

where u_{i+1} is approximated by u_i. This indicates that u_{i+1} approaches u_0 in the limit $|\Lambda_0| \to \infty$. Hence,

Table 2 Limiting cases of PEM

PEM	$\Lambda_0 \to 0$	$\Lambda_0 \to \infty$
PEM-1	$u_{i+1} \approx u_i + hv_i + \frac{1}{2}h(p_{i+1}-p_i)$	$u_{i+1} \approx u_i$
PEM-2	$u_{i+1} \approx u_i + \frac{13}{12}hv_i - \frac{1}{12}hv_{i-1} + \frac{5}{12}h(p_{i+1}-p_i)$	$u_{i+1} \approx u_i$
PEM-3	$u_{i+1} \approx u_i + \frac{28}{24}hv_i - \frac{5}{24}hv_{i-1} + \frac{1}{24}hv_{i-2} + \frac{9}{24}h(p_{i+1}-p_i)$	$u_{i+1} \approx u_i$

there will be no unstable solution in each step of the solution. This approximation is found not only for that of PEM-1 but also for the other eigen-dependent difference formulas of PEM as shown in Table 2. This approximation result implies that although the contribution from the fast eigenmodes might not be accurately obtained it will not be abnormally amplified to contaminate or even to destroy a total solution. This study of extreme cases indicates that the slow eigenmodes can be accurately integrated, which can be confirmed by the dominant error term listed in the column E_i of Table 1, while a stable calculation is guaranteed for fast eigenmodes. This study of the two limiting cases is indicative for the solution behaviors of slow and fast eigenmodes. Notice that a further exploration of a general value of Λ_0 is still needed and will be conducted later.

3.3 Zero stability

The proof of convergence is the most important aspect in the evaluation of a linear multi-step method. The consistency of PEM is verified through the study of the local truncation error. Hence, the next step is to substantiate that each eigen-dependent difference formula of PEM can possess zero stability for the complete verification of convergence.

A numerical method is zero-stable if the solution remains bounded as $h \to 0$. In this limiting case, an m-step eigen-dependent difference formula as given in Eq. (7) will reduce to $u_{i+1} - u_i = 0$. This recurrence equation completely determines the characteristic behavior of the linear multi-step method. The method is said to be zero-stable if all solutions to $u_{i+1} - u_i = 0$ remain bounded. As a result, to determine whether a m-step eigen-dependent method of PEM is zero-stable, one can assume that the solution to the recurrence equation has the form of $u_n = u_0 w^n$. After substituting this solution into $u_{i+1} - u_i = 0$, the result is found to be $u_0 w^n (w - 1) = 0$. Clearly, $w = 0$ and 1 are the two zeros of the equation $u_{i+1} - u_i = 0$. Consequently, it is affirmed that each eigen-dependent difference formula of PEM is zero-stable. This proof of zero stability in addition to the verification of consistency for each eigen-dependent difference formula of PEM, the convergence of PEM is validated [24].

4 A-stability

The stability of the proposed eigen-dependent difference formulas for PEM was studied in the extreme case of $h \to 0$, $n \to \infty$, nh fixed. In addition to this extreme case, it is also important to further explore the performance of each eigen-dependent difference formula for a general value of $h > 0$ and $n \to \infty$. In numerical ODEs, a variety of different forms of stability that have been defined and they are related to a concept of stability in the dynamical systems sense [15–23, 25–29]. It seems that A-stability is the most basic one. In general, the result of the study of the A-stability of a numerical method can provide information that is very useful for choosing an appropriate step size in the solution of nonlinear first-order ODEs. It is important to adopt an A-stable method when solving a stiff equation.

The canonical model problem, which will lead to an exponentially decaying solution, can be generally written as:

$$y' = \lambda_0 y, \quad x > 0, \quad y(0) = y_0 \neq 0 \tag{17}$$

where $\lambda_0 = a + ib$ and $a < 0$ is assumed. A theoretical solution of this canonical model problem can be analytically derived and is found to be:

$$y(x) = y_0 e^{ax} e^{ibx} \tag{18}$$

Thus, $|y(x)| \leq e^{ax}$ as $x \geq 0$, yielding $\lim_{x \to \infty} y(x) = 0$. For simplicity, λ_0 can be degenerated into a negative, real number.

If the proposed linear multi-step, eigen-dependent difference formula as shown in Eq. (7) is applied to solve the canonical model problem, as shown in Eq. (17), the following approximating difference equation can be obtained:

$$u_{i+1} - u_i - \sum_{k=1}^{m} \Lambda_0 \beta_k u_{i+1-k} = 0 \tag{19}$$

A solution u_n of this approximating difference equation can be alternatively written as a linear combination of the powers of the roots of the corresponding stability polynomial. As a result, the stability polynomial is found to be:

$$\pi(w, \Lambda_0) = w^{n+1} - w^n - \Lambda_0 \sum_{k=1}^{m} \beta_k w^{n+1-k} \tag{20}$$

If all the roots of this equation have modulus less than 1, then u_n will converge to zero for $h > 0$ and n→∞. In general, a linear multi-step method is A-stable for a specified Λ_0 if and only if all the roots w_i of Eq. (20) can satisfy $|w_i| < 1$ for that Λ_0. Otherwise, the linear multi-step method is A-unstable. An interval of $\alpha_{min} \leq \Lambda_0 \leq \alpha_{max}$ in the real line is called the A-stability interval of the linear multi-step method if it is A-stable for all Λ_0 in this interval.

To investigate the stability properties of PEM, the Routh-Hurwitz criterion [30] is adopted. As an example, for PEM-1, Eq. (20) becomes:

$$\pi(w, \Lambda_0) = w^{n+1} - w^n - \Lambda_0 \beta_1 w^n$$
$$= w^n \left[w - \left(1 + \frac{\Lambda_0}{1 - \frac{1}{2}\Lambda_0} \right) \right] \quad (21)$$

The roots of $\pi(w, \Lambda_0) = 0$ are a zero root and:

$$w = 1 + \frac{\Lambda_0}{1 - \frac{1}{2}\Lambda_0} \quad (22)$$

To meet the requirement of $|w| \leq 1$, it is straightforward to have:

$$-\infty \leq \Lambda_0 \leq 0 \quad (23)$$

Thus, PEM-1 may have A-stability. The most important consequence of the A-stability property is that there is no limitation on the step size. This property is very important and generally desired in the solution of multi-body and other engineering systems, since the user is only required to concern with the step size for accuracy and not for stability. Using the same the stability analysis procedure for PEM-1, both PEM-2 and PEM-3 are also analyzed and the results of A-stability interval for the m-step of PEM are listed in the last column of Table 1.

It is more common to consider an A-stability region in the complex plane of $\Lambda_0 = \lambda_0 h$. This implies that λ_0 can be a complex number while the step size h is positive and real. As a result, the A-stability regions for the m-step of PEM are plotted in Fig. 1. If the expression of $\lambda_0 = a + ib$ is adopted, the real and imaginary parts of Λ_0 are denoted by ah and bh, respectively. In Fig. 1, it is found that the A-stability region for PEM-1 is the open left half complex plane while that for PEM-2 to PEM-3 is the interior region bounded by each curve. It is manifested from PEM that the increase of the order of accuracy will decrease the A-stability region. An A-stable method, such as

PEM-1, may be defined as a method whose A-stability region is the complete left half complex plane including the imaginary axis.

Comparing the A-stability interval of m-step of PEM as shown in the last column of Table 1 to that of AMM, they are found to be the same for each m-step of the two methods correspondingly. In addition, the A-stability region of each m-step of PEM as shown in Fig. 1 is also the same as that of AMM. As a result, the same stability property and similar local truncation error of each m-step of the two methods might imply that PEM can have almost the same performance as that of AMM in the solution of first-order ODEs although their formulations are different, where PEM is *explicit* while AMM is *implicit*. It will be shown next that PEM not only can be explicitly implemented but also implicitly implemented.

5 Explicit or implicit implementation

In the original development of PEM, an initial eigenvalue is intentionally adopted to determine the eigen-dependent coefficients so that it can have an explicit formulation. Thus, it is classified as an explicit method. However, it may become an implicit method if the current eigenvalue is applied to replace the initial eigenvalue for determining the eigen-dependent coefficients. The feasibility of applying a current eigenvalue to derive an implicit PEM will be verified next. An explicit PEM will be abbreviated as PEM-E while an implicit PEM is abbreviated as PEM-I for brevity.

Equation (9) can be also applied to develop a series of eigen-dependent difference formulas for PEM by using a current eigenvalue instead of an initial eigenvalue for determining the eigen-dependent coefficients. Unlike the adoption of Eq. (8), the coefficient β_k can be alternatively written in the form of:

$$\beta_k = \frac{b_k}{1 + a_m \Lambda_{i+1}} \quad \text{for} \quad k = 1, 2, \ldots, m \quad (24)$$

where $\Lambda_{i+1} = \lambda_{i+1} h$ and λ_{i+1} is the eigenvalue corresponding to the current step, i.e., the $(i + 1)$-th step. The only difference between Eqs. (8) and (24) is that λ_0 is replaced by λ_{i+1}. Applying the same procedure to develop PEM-E, where Eq. (8) is adopted, a series of similar eigen-dependent difference formulas for PEM-I can be also derived based on Eq. (24). The proof of convergence for PEM-I can be completed by using the

Fig. 1 A-stability region for PEM
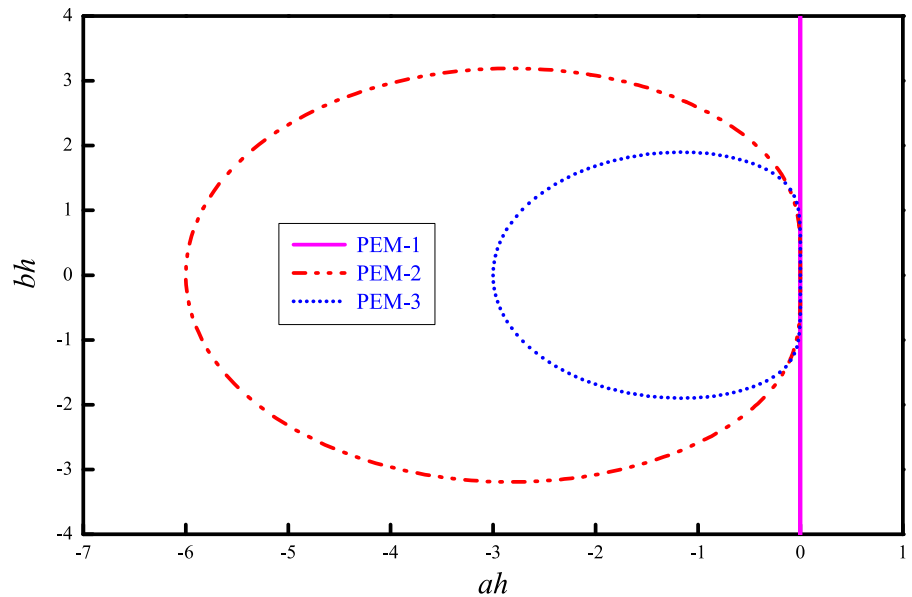
same way for PEM-E. As a summary, the use of an initial eigenvalue can be applied to derive PEM-E while a current eigenvalue can be used to derive PEM-I. Besides, PEM-E and PEM-I will have the similar numerical properties, such as A-stability interval and order of accuracy.

Since a current eigenvalue is applied to determine the eigen-dependent coefficients for PEM-I and these eigen-dependent coefficients cannot be known as a prior, the use of the eigen-dependent difference formula to solve first-order ODEs cannot be explicitly implemented. In fact, Eq. (7) with the eigen-dependent coefficients that are determined from a current eigenvalue can be written as:

$$(1 + a_m \Lambda_{i+1})(u_{i+1} - u_i) = h \sum_{k=1}^{m} b_k v_{i+1-k} + a_m h(p_{i+1} - p_i) \qquad (25)$$

This equation is nonlinear since u_{i+1} is a function of λ_{i+1} (or Λ_{i+1}). Thus, an iteration procedure is required to be adopted for solving u_{i+1}. As a result, the eigen-dependent difference formulas of this type will be classified as implicit formulas. Consequently, PEM-I is an implicit method.

In summary, the use of an eigen-dependent difference formula to solve first-order ODEs can be either explicitly or implicitly implemented, such as PEM. An initial eigenvalue is used to determine the eigen-dependent coefficients for explicit eigen-dependent difference formulas while for implicit eigen-dependent difference formulas, a current eigenvalue is adopted. An explicit implementation is preferred over an implicit implementation for a numerical method since an explicit implementation will involve no nonlinear iterations for each step, and thus, it can save many computationally efforts in contrast to an implicit implementation.

6 Transformation from eigen-dependent to problem-dependent formulas

Apparently, there will exist three steps to solve a system of coupled first-order ODEs if using an eigen-dependent method, such as PEM. They are: (1) to decompose the coupled first-order ODEs into a set of uncoupled first-order ODEs; (2) to use an eigen-dependent difference formula to solve each uncoupled first-order ODE; and (3) to apply a mode superposition technique to sum up the solutions of all the eigen-modes. Clearly, each step will involve the eigenvalues and/or eigenvectors of the coupled first-order ODE. Hence, an eigen-analysis of the system of the coupled first-order ODEs must be performed first so that the eigenvalues and eigenvectors can be achieved. It is simple to conduct an eigen-analysis for a single first-order ODE. However, it will become time consuming for a large system of the coupled first-order ODEs.

Consequently, it is infeasible to apply an eigen-dependent method to solve a system of coupled first-order ODEs in practical applications.

An eigen-analysis can be avoided if the system of coupled first-order ODEs is directly solved and all the eigen-dependent difference formulas are converted into a problem-dependent difference formula, where the eigen-dependent coefficient β_k is no longer a function of Λ_0 but a function of the product of the initial physical property for defining the problem, such as $\mathbf{Q}_0$ in Eq. (1), and step size. To convert all the eigen-dependent difference formulas for solving each uncoupled first-order ODE to a problem-dependent difference formula for solving the system of coupled first-order ODEs can be completed by means of a reverse procedure of an eigen-decomposition technique. As a result, the problem-dependent method can be explicitly written as:

$$\mathbf{v}_{i+1} = \mathbf{Q}_{i+1}\mathbf{u}_{i+1} + \mathbf{f}_{i+1}$$
$$\mathbf{u}_{i+1} = \mathbf{u}_i + h\left(\sum_{k=1}^{m} \mathbf{B}_k \mathbf{v}_{i+1-k} + \boldsymbol{\psi}_{i+1}\right) \qquad (26)$$

where $\mathbf{B}_k$ and $\boldsymbol{\psi}_{i+1}$ for PEM-E and PEM-I can be expressed as:

$$\begin{cases} \mathbf{B}_k = (\mathbf{D}_0)^{-1} b_k \\ \boldsymbol{\psi}_{i+1} = (\mathbf{D}_0)^{-1} a_m(\mathbf{f}_{i+1} - \mathbf{f}_i) \end{cases}, \quad \text{for PEM - E}$$

$$\begin{cases} \mathbf{B}_k = (\mathbf{D}_{i+1})^{-1} b_k \\ \boldsymbol{\psi}_{i+1} = (\mathbf{D}_{i+1})^{-1} a_m(\mathbf{f}_{i+1} - \mathbf{f}_i) \end{cases}, \quad \text{for PEM - I}$$

$$(27)$$

where $\mathbf{D}_0 = \mathbf{I} + a_m h \mathbf{Q}_0$ and $\mathbf{D}_{i+1} = \mathbf{I} + a_m h \mathbf{Q}_{i+1}$; a_m and b_k are summarized in Table 1 for PEM; and $k = 1, 2, \ldots, m$ for a m-step method. Notice that $\mathbf{Q}_0$ is the initial matrix at the beginning of the solution procedure, while $\mathbf{Q}_{i+1}$ is the matrix at the $(i + 1)$-th step and might vary with the change of x for a system of coupled, nonlinear first-order ODEs. The first line of Eq. (26) is a set of coupled first-order ODEs and the second line is a problem-dependent difference formula for solving the set of the coupled first-order ODEs. Since the reverse procedure of an eigen-decomposition technique is used to derive the problem-dependent method, a series of eigen-dependent methods can be yielded after the decomposition of the problem-dependent method.

An initial matrix $\mathbf{Q}_0$ is adopted to determine the problem-dependent coefficients for PEM-E as shown in the first line of Eq. (27). In contrast, a current matrix $\mathbf{Q}_{i+1}$ is applied to determine the problem-dependent coefficients for PEM-I as shown in the second line of Eq. (28). The matrix $\mathbf{Q}_{i+1}$ might be different from $\mathbf{Q}_0$ since it will vary with x for a system of nonlinear ODEs. Both lines of Eq. (26) can be simultaneously decoupled only if $\mathbf{Q}_{i+1}$ and $\mathbf{Q}_0$ have the same eigenvalues and eigenvectors, i.e., $\mathbf{Q}_{i+1}$ is identical to $\mathbf{Q}_0$. Hence, the decomposition of Eq. (26) can be conducted if PEM-E is chosen to solve a system of linear first-order ODEs whereas PEM-I can be adopted to solve a set of linear or nonlinear first-order ODEs since $\mathbf{Q}_{i+1}$ is found in both the first and second lines of Eq. (26). Notice that a simultaneous decomposition of the two lines of Eq. (26) implies that the method follows the development procedure, and thus, it can inherit the numerical properties of stability and accuracy, i.e., convergence.

It is important to show that PEM-E can still give a reliable solution for a system of nonlinear first-order ODEs although an eigen-decomposition technique cannot simultaneously decompose the coupled first-order ODEs under analysis and problem-dependent difference formula due to different eigenvalues and eigenvectors between $\mathbf{Q}_0$ and $\mathbf{Q}_{i+1}$. The feasibility of using PEM-E to accurately solve a system of coupled, nonlinear first-order ODEs can be verified next. This verification is for a single step but not for a complete solution procedure since $\mathbf{Q}_{i+1}$ may vary with x for each step for nonlinear first-order ODEs. However, it is still indicative for a complete solution procedure since it consists of each step. Besides, two extreme cases of $|\Lambda_0| \to 0$ and $|\Lambda_0| \to \infty$ will be considered. It is evident that the extreme case of can $|\Lambda_0| \to 0$ imply the behaviors of slow eigenmodes, while those of fast eigenmodes are implied by the extreme case of $|\Lambda_0| \to \infty$.

If PEM-I is applied to solve a nonlinear problem, the solution of the $(i + 1)$-th step is described next. After decomposing $\mathbf{Q}_{i+1}$, one can have $\Lambda_{i+1}^{(j)} = \lambda_{i+1}^{(j)} \times h$, for $j = 1, 2, \ldots n$, where the superscript (j) denotes the j-th eigenmode. Hence, the j-th eigenmode solution is conceptually computed by:

$$u_{i+1}^{(j)} = u_i^{(j)} + h\left[\sum_{k=1}^{m} \frac{b_k}{1 + a_m\Lambda_{i+1}^{(j)}} v_{i+1-k}^{(j)} + \frac{a_m}{1 + a_m\Lambda_{i+1}^{(j)}}\left(p_{i+1}^{(j)} - p_i^{(j)}\right)\right] \tag{28}$$

However, for using PEM-E, Eq. (28) will become:

$$u_{i+1}^{(j)} = u_i^{(j)} + h\left[\sum_{k=1}^{m} \frac{b_k}{1 + a_m\Lambda_0^{(j)}} v_{i+1-k}^{(j)} + \frac{a_m}{1 + a_m\Lambda_0^{(j)}}\left(p_{i+1}^{(j)} - p_i^{(j)}\right)\right] \tag{29}$$

where PEM-E adopts $\Lambda_0^{(j)}$ to replace $\Lambda_{i+1}^{(j)}$ in the difference formula. This implies that the use of Eqs. (28) and (29) to solve nonlinear first-order ODEs may result in different solutions. However, the difference is insignificant and both PEM-I and PEM-E can still provide reliable solutions. This will be proved next.

Two extreme cases of $|\Lambda_0| \to 0$ and $|\Lambda_0| \to \infty$ that are in correspondence to the behaviors of slow and fast eigenmodes are considered. Although the difference between $\mathbf{Q}_{i+1}$ and $\mathbf{Q}_0$ for first-order nonlinear ODEs leads to different eigen-dependent difference formulas for each eigenmode as shown in Eqs. (28) and (29), respectively, slow eigenmode solutions can be still accurately calculated. This is because that Eqs. (28) and (29) become the same in the limit $|\Lambda_0| \to 0$ due to $1 + a_m\Lambda_0^{(j)} \approx 1$ and $1 + a_m\Lambda_{i+1}^{(j)} \approx 1$. As a result, they become:

$$u_{i+1}^{(j)} \approx u_i^{(j)} + h\left[\sum_{k=1}^{m} b_k v_{i+1-k}^{(j)} + a_m\left(p_{i+1}^{(j)} - p_i^{(j)}\right)\right] \tag{30}$$

This equation is almost the same as a conventional difference formula since it has scalar constant coefficients. Thus, the solution of this eigenmode can be as accurate as a conventional method if the scalar constant coefficients, i.e., a_m and b_k, are properly determined.

Meanwhile, in the limiting case of $|\Lambda_0| \to \infty$, the asymptotic values of $1 + a_m\Lambda_0^{(j)} \approx \infty$ as well as $1 + a_m\Lambda_{i+1}^{(j)} \approx \infty$ are found. As a result, Eqs. (28) and (29) also become the same and reduce to:

$$u_{i+1}^{(j)} \approx u_i^{(j)} \quad \Rightarrow \quad u_{i+1}^{(j)} \approx u_0^{(j)} \tag{31}$$

Hence, there is no excessive amplitude growth or even instability in the fast eigenmode solutions for both PEM-I and PEM-E. Although the difference in

eigenvalues between $\mathbf{Q}_{i+1}$ and $\mathbf{Q}_0$ will result in different fast eigenmode solutions for PEM-I and PEM-E, the accuracy of a total solution will be almost unaffected by fast eigenmode solutions. This is because that (1) The maximum power of Λ_0 in the numerator of the eigen-dependent coefficients is 0 and is less than that of the denominator of 1. Thus, the eigen-dependent coefficients will approach 0, resulting Eq. (31), in the limit $|\Lambda_0| \to \infty$. As a result, stable solutions with no excessive amplitude growth can be yielded for fast eigenmodes. (2) The contributions from fast eigenmodes to the total solution are insignificant for stiff problems, where the total solution of the problem under analysis is dominated by slow eigenmodes.

As a summary, it is corroborated that slow eigenmode solutions can be accurately obtained as a conventional method if the scalar constants of a_m and b_k are appropriately determined for PEM since the eigen-dependent difference formulas will degenerate to conventional difference formulas for slow eigenmodes. Besides, no excessive amplitude growth or instability for fast eigenmodes is ensured since an approximate solution of $u_{i+1}^{(j)} = u_i^{(j)}$ is found for each fast eigenmode. Hence, PEM is best suited to solve stiff problems.

In Eq. (26), $\mathbf{B}_k$ and ψ_{i+1} are no longer eigen-dependent but problem-dependent. As a result, "problem-dependent" is adopted instead of "eigen-dependent" for PEM. It is beneficial for PEM in computing efficiency if all the eigen-dependent difference formulas can be converted to a problem-dependent difference formula since an eigen-analysis of the coupled first-order ODEs for each step can be avoided, and thus, there is no necessity to involve a superposition technique to sum up each eigenmode solution to obtain a total solution. Notice that although an eigen-decomposition concept is adopted to provide a fundamental basis for developing the problem-dependent formula, there is no involvement of any eigen-decomposition in a complete step-by-step solution procedure.

7 Implementation

To substantiate the numerical properties of PEM and its performance in the solution of initial value

problems, some numerical examples will be examined. Hence, it must be implemented for solving a system of first-order ODEs, where both the explicit and implicit implementations will be schematically sketched.

7.1 Explicit implementation

The detailed implementation of PEM-E is described next. The adoption of PEM-E to solve a system of first-order ODEs can be generally written as shown in Eq. (26), where $\mathbf{Q}_{i+1}$ is the matrix corresponding to the instantaneous state at the end of the $(i + 1)$-th step and is generally different from $\mathbf{Q}_0$ for a system of nonlinear first-order ODEs. In addition, $\mathbf{B}_k$ and ψ_{i+1} are defined in the first line of Eq. (28). Since $\mathbf{u}_{i+1}$ in the second line of Eq. (26) is a function of the previous step data only, it can be directly calculated and is numerically equivalent to solve the equation of:

$$(\mathbf{I} + a_m h \mathbf{Q}_0)(\mathbf{u}_{i+1} - \mathbf{u}_i) = h\left[\sum_{k=1}^{m} b_k \mathbf{v}_{i+1-k} + a_m(\mathbf{f}_{i+1} - \mathbf{f}_i)\right]$$
(32)

A direct elimination method can be applied to solve this equation. In general, a direct elimination method consists of a triangulation and a substitution for each step and a triangulation will consume most computational efforts of the step. The triangulation of the matrix $\mathbf{I} + a_m h \mathbf{Q}_0$ is required to be conducted only once at the beginning since $\mathbf{I} + a_m h \mathbf{Q}_0$ is invariant for a whole solution procedure. Subsequently, $\mathbf{v}_{i+1}$ can be calculated from the first line of Eq. (26). This solution procedure will involve no nonlinear iterations for each step, and the triangulation of $\mathbf{I} + a_m h \mathbf{Q}_0$ is executed only once. As a result, a lot of CPU demand can be saved when compared to an implicit method, where an iteration procedure is needed for each step. This solution procedure can be conducted repeatedly until the desired solution history is obtained.

7.2 Implicit implementation

In addition to an explicit implementation for PEM-E, an implicit implementation for PEM-I is described next. In Eq. (26), the second line is an implicit problem-dependent formula if $\mathbf{B}_k$ and ψ_{i+1} are defined in the second line of Eq. (27). In this case, $\mathbf{u}_{i+1}$ in the second line of Eq. (26) is not only a function of the previous step data but also the current step data. It can be alternatively expressed as:

$$(\mathbf{I} + a_m h \mathbf{Q}_{i+1})(\mathbf{u}_{i+1} - \mathbf{u}_i) = h\left[\sum_{k=1}^{m} b_k \mathbf{v}_{i+1-k} + a_m(\mathbf{f}_{i+1} - \mathbf{f}_i)\right]$$
(33)

This equation is slightly different from Eq. (32) due to the use of $\mathbf{Q}_{i+1}$ to replace $\mathbf{Q}_0$. It must be solved iteratively for each step since $\mathbf{Q}_{i+1}$ is a function of $\mathbf{u}_{i+1}$ for a coupled nonlinear first-order ODEs. After obtaining $\mathbf{u}_{i+1}$, $\mathbf{v}_{i+1}$ can be also determined from the first line of Eq. (26). Clearly, an explicit implementation of PEM-E involves no nonlinear iterations for each step while an iteration procedure is generally needed for PEM-I for using an implicit implementation.

8 Numerical examples

Although PEM-m has been shown to possess almost the same numerical properties, such as A-stability and order of accuracy, as those of AMM-m, for solving linear first-order ODEs, it is of interest to examine the actual performance between PEM-m and AMM-m in the solution of first-order ODEs. Some first-order ODEs with a variety of different types of nonlinearity will be solved. In fact, six test problems are examined in this section. The examples in 8.1 and 8.2 are linear ODEs while those in 8.3 to 8.6 are nonlinear ODEs. Example 1 and 2 are intentionally devised to be linear ODEs. This is because they have theoretical solutions so that the numerical properties of PEM can be validated. Meanwhile, the examples considered in 8.3 to 8.6 all are highly nonlinear ODEs, such as the well-known stiff problem of the Van der Pol oscillator, a nonlinear vibration of building including a free vibration analysis and a forced vibration analysis, a 360° nonlinear pendulum and a series of nonlinear mechanical systems including the three systems of 250, 500 and 1000 first-order ODEs. These examples are used to validate the feasibility PEM in the solution of highly nonlinear first-order ODEs. Besides, the numerical properties of stability and accuracy can be also affirmed by the various types of different nonlinear examples. Since PEM-1 can integrate explicit formulation as well as A-stability, it is also of interest to explore its computational efficiency for

solving nonlinear first-order stiff ODEs in contrast to a conventional implicit method of AMM-1. The investigation of the computational efficiency can be revealed by the example in 8.6. Notice that explicit PEM-1 and implicit AMM-1 have almost the same A-stability and accuracy properties.

8.1 A linear non-stiff system

An initial value problem is solved by using a problem-dependent formula. A linear first-order ODE with a specified initial value is considered and can be written as:

$$y'(x) = 10y(x) - 10\cos(x) - \sin(x), y(0) = 1 \quad (34)$$

A theoretical solution to this initial value problem is found to be $y(x) = \cos(x)$. This initial value problem is solved by explicit implementations of PEM-1 to PEM-3, as listed in Table 1. Besides, the methods of AMM-1 to AMM-3 are also adopted to solve the problem for comparison. Notice that PEM is an explicit method, while AMM is an implicit method. In addition, there will be no difference between PEM-E and PEM-I in the solution of linear first-order ODEs.

Numerical solution for Eq. (34) is plotted in Fig. 2, where "Exact" is the theoretical solution of $y(x) = \cos(x)$. In Eq. (34), an eigenvalue of $\lambda_0 = -10$ is found and it is invariant. A step size of $h = 0.1$ is adopted for each analysis. As a result, $\Lambda_0 = \lambda_0 h = -1$ is found, which implies that the stability conditions for AMM-1 to AMM-3 and PEM-1 to PEM-3 are satisfied since their stability interval are $-\infty \le \Lambda_0 \le 0$, $-6 \le \Lambda_0 \le 0$ and $-3 \le \Lambda_0 \le 0$, correspondingly, as listed in Table 1. It is seen that the solutions calculated from PEM-m are not only the same as those determined from AMM-m but also overlap together with the exact solutions in each plot of this figure. This indicates that PEM-m can give a numerical solution as accurate as that of AMM-m for solving a linear first-order ODE. The numerical accuracy of PEM-m and AMM-m can be further explored by computing the absolute error of each step in each analysis and the variation of the absolute error with x for PEM-m is shown in Fig. 3. For comparison, that for AMM-m is also plotted in each plot of the figure, correspondingly. Each plot of Fig. 3 discloses that the curve of PEM-m coincides together with that of AMM-m. Hence, it can be drawn that PEM-m will

have the same numerical solution as that of AMM-m in the solution of linear first-order ODEs if the same step size is adopted. Besides, it is also found that a more accurate solution can be achieved as m increases for both PEM-m and AMM-m. This can be manifested from the comparison of the amount of absolute error in Fig. 3a–d. This phenomenon is also consistent with the analytical prediction of the order of accuracy as listed in Table 1.

8.2 A linear stiff system

A subclass of the initial value problems involving rapidly decaying transient solutions might arise in a wide variety of engineering applications, such as problems in chemical kinetics, the study of spring and damping systems and the analysis of control systems. This type of problems is known as stiff problems [2, 3, 6, 7, 10, 22, 25]. Stiff ODEs generally involve a large dispersion of eigenvalues and these eigenvalues refer to the rate of decay. Since PEM can combine A-stability and explicit formulation, it is very promising for solving stiff problems. Thus, it is applied to solve the following initial value problem:

$$\begin{Bmatrix} y'_1 \\ y'_2 \end{Bmatrix} = \begin{bmatrix} 0 & 1 \\ -10000 & -10001 \end{bmatrix} \begin{Bmatrix} y_1 \\ y_2 \end{Bmatrix} \quad (35)$$

The initial conditions are taken to be $y_1(0) = 5$ and $y_2(0) = -5$. The eigenvalues of this system are found to be $\lambda_0^{(1)} = -1$ and $\lambda_0^{(2)} = -10^4$, where the two eigenvalues are widely separated. In fact, the stiffness ratio is found to be as large as $\lambda_0^{(2)}/\lambda_0^{(1)} = 10^4$ and thus the system is stiff. The theoretical solutions are found to be:

$$y_1(x) = 5e^{-x}, y_2(x) = -5e^{-x} \quad (36)$$

It is found that $|y_1(x)| = |y_2(x)|$.

Both AMM-m and PEM-m are chosen to solve Eq. (35) with the specified initial conditions. Numerical results obtained from AMM-m and PEM-m are plotted in Fig. 4. In each plot of this figure, "Exact" is used to denote the solution is theoretically obtained. In Fig. 4a, both AMM-1 and PEM-1 can provide the solutions that almost coincide with the exact solution for both $h = 0.1$ and 0.5. This indicates that AMM-1 and PEM-1 can have an A-stability since an accurate solution can be achieved although the maximum value of Λ_0 is as large as -5000 for $h = 0.5$. This is in good

Fig. 2 Numerical solutions for a linear first-order differential equation
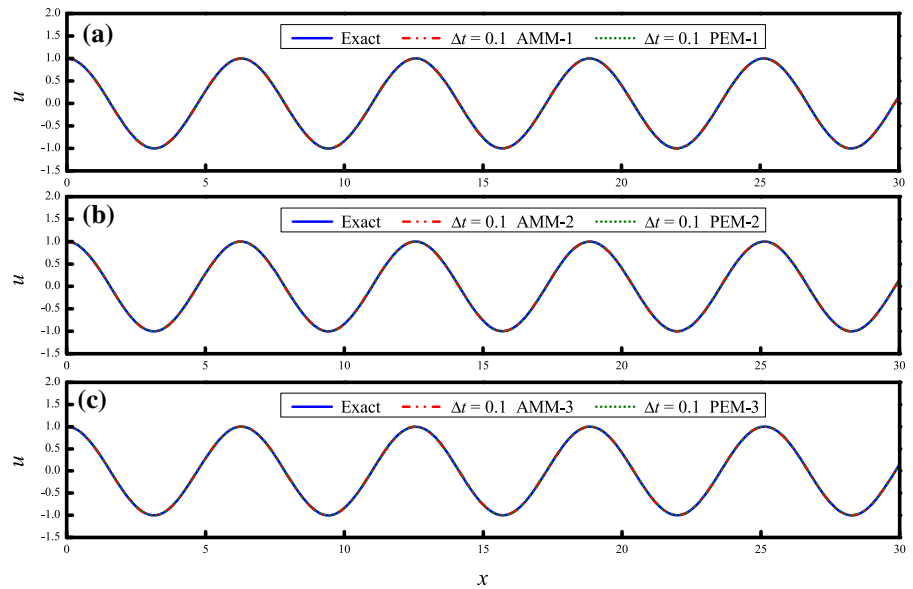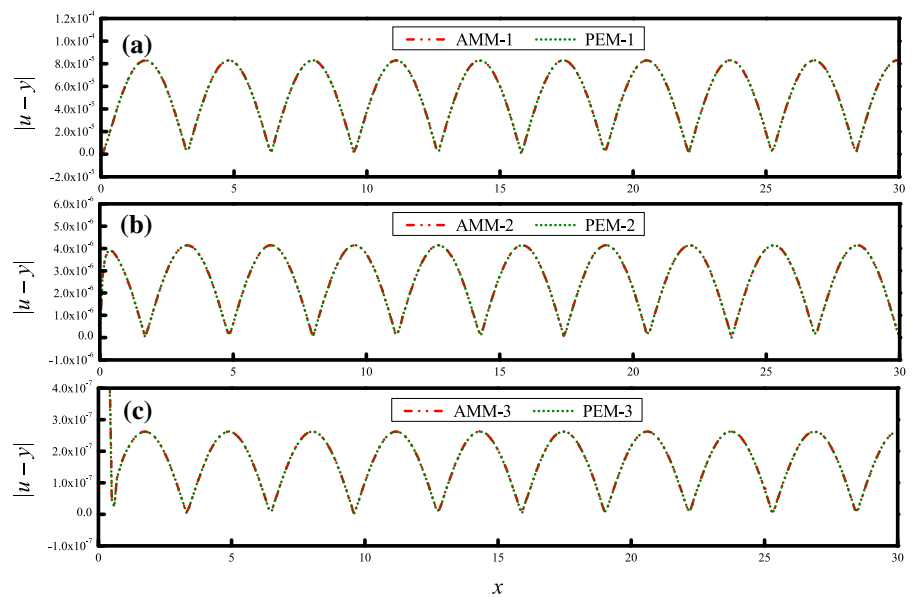

Fig. 3 Comparisons of absolute errors between AMM and PEM

agreement with the A-stability interval of $-\infty \le \Lambda_0 \le 0$, which is given in Table 1 for both AMM-1 and PEM-1. Further verifications of the A-stability interval for other AMM-m and PEM-m are also conducted. As an example, for AMM-2 and PEM-2, they can have an A-stability interval of $-6 \le \Lambda_0 \le 0$. The step sizes $h = 5.9 \times 10^{-4}$ and 6.1×10^{-4} are used to solve Eq. (35) and the results are shown in Fig. 4b. The step size of $h = 5.9 \times 10^{-4}$ can result in an accurate solution while that of $h = 6.1 \times$

10^{-4} leads to an unstable solution although there only exists a slight difference in step size. This is because that $h = 5.9 \times 10^{-4}$ and 6.1×10^{-4} are in correspondence to $\Lambda_0^{(2)} = \lambda_0^{(2)} h = -5.9$ and $\Lambda_0^{(2)} = \lambda_0^{(2)} h = -6.1$. Clearly, $\Lambda_0^{(2)} = -5.9$ is within the A-stability interval of $-6 \le \Lambda_0 \le 0$ and thus a reliable solution is achieved while $\Lambda_0^{(2)} = -6.1$ is outside the A-stability interval and thus instability occurs. A very similar phenomenon is also found in Fig. 4c.

Fig. 4 Numerical solutions obtained from AMM-m and PEM-m for a stiff problem
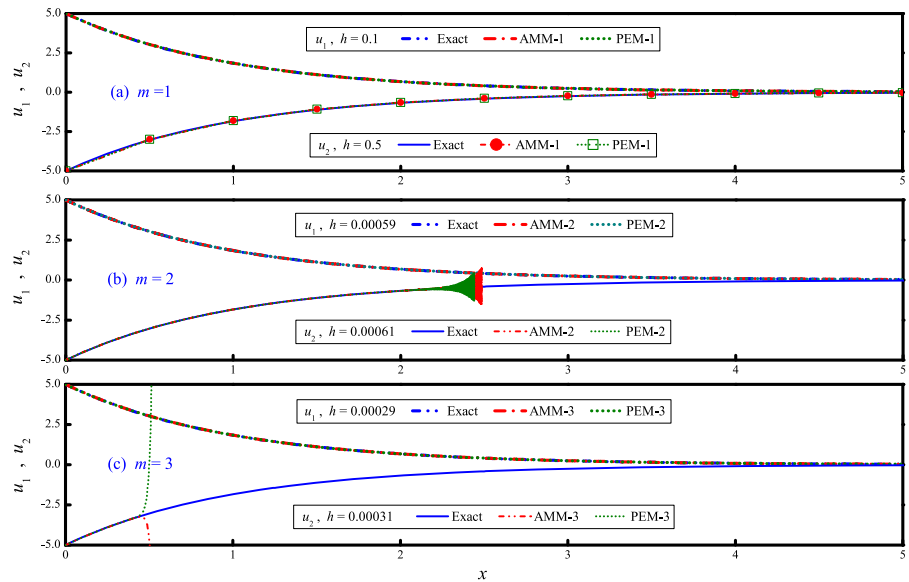
It is manifested from this example that an A-stability property is very important for a solution method in the solution of stiff problems. Although PEM-2 to PEM-3 and AMM-2 to AMM-3 can have better accuracy than PEM-1 and AMM-1, they possess no A-stability and thus they might be limited in the solution of stiff problems. Evidently, both PEM-1 and AMM-1 are promising for solving stiff problems due to an A-stability property.

8.3 A Van der Pol oscillator

The Van der Pol oscillator [31, 32] is an oscillator with nonlinear damping. It has been used to explore the properties of nonlinear oscillators and various oscillatory phenomena in biological and physical fields, such as the action potential in neurons, analyses of electrical circuits and models of the heartbeat. The Van der Pol equation can be generally written as:

$$\ddot{u} - \mu(1 - u^2)\dot{u} + u = 0 \tag{37}$$

where u is a dynamical variable and is a function of the time t. The parameter μ is a positive scalar constant and it generally indicates the strength of the damping and nonlinearity. After taking $v = \dot{u}$, the second-order ODE of Eq. (37) can be converted to a system of first-order ODEs as:

$$\left\{ \begin{matrix} \dot{u} \\ \dot{v} \end{matrix} \right\} = \begin{bmatrix} 0 & 1 \\ -1 & \mu(1 - u^2) \end{bmatrix} \left\{ \begin{matrix} u \\ v \end{matrix} \right\} \tag{38}$$

In general, a stiff system can be simulated for a large value of μ. In this study, $\mu = 100$ is taken and the initial conditions of $u(0) = 2.0$ and $v(0) = 0.0$ are adopted. The two eigenvalues of the system are widely separated and are found to be -3.33×10^{-3} and -300, resulting the stiffness ratio of $Re\left|\lambda_0^{(2)}\right|/Re\left|\lambda_0^{(1)}\right| = 9 \times 10^5$.

The result calculated from AMM-1 with $h = 0.0001$ is considered as a reference solution for comparisons. Both PEM-E-1 and PEM-I-1 as well as AMM-1 are applied to solve Eq. (38) by using $h = 0.001$ and 0.003. Figure 5 displays the calculated results. The results calculated from all the three methods with $h = 0.001$ are almost the same and coincide together with the reference solution as shown in Fig. 5a. On the other hand, those obtained from these methods with $h = 0.003$ slightly deviate from the reference solution, where the result obtained from PEM-I-1 is almost the same as that obtained from AMM-1, while the solution obtained from PEM-E-1 exhibits a slightly less error in contrast to AMM-1 and PEM-I-1. This example validates that PEM-E-1 and PEM-I-1 can have almost the same performance as that of AMM-1 in the solution of nonlinear stiff systems.

Fig. 5 Numerical solutions
of Van der Pol equations for
using AMM-1 and PEM-1
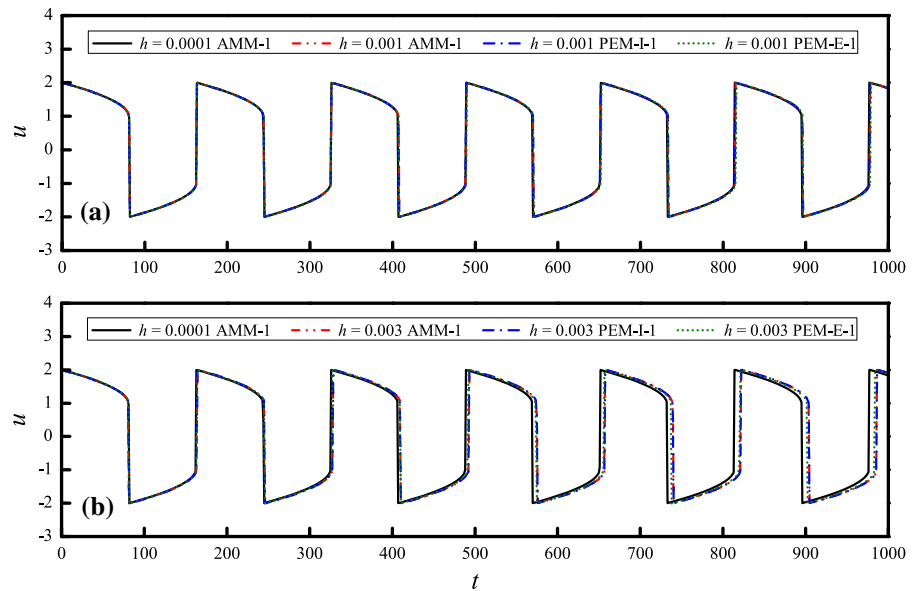
8.4 A structure vibration system

For a four-story building, its beams and floor systems
are assumed to be rigid in flexure and thus there is no
rotation of a horizontal section at the floor levels.
Hence, it can be simulated as a shear building and then
its governing equations of motion can be largely
simplified. For a shear building, the horizontal
displacement at each story floor can be chosen as a
degree of freedom for modeling the building. As a
result, a system of second-order ODEs can be adopted
to govern the dynamic behaviors of the building and
can be written as:

$$\mathbf{M\ddot{u}} + \mathbf{C\dot{u}} + \mathbf{Ku} = \mathbf{f} \tag{39}$$

where $\mathbf{u} = \left\{\begin{matrix} u_1 & u_2 & u_3 & u_4 \end{matrix}\right\}^{\mathrm{T}}$; $\mathbf{M}$, $\mathbf{C}$ and $\mathbf{K}$ are the
mass, viscous damping, and stiffness matrices, respec-
tively; and $\mathbf{f}$ is an external force vector. In general, the
mass and stiffness matrices $\mathbf{M}$ and $\mathbf{C}$ are constant
matrices while the stiffness matrix $\mathbf{K}$ may vary due to
geometric and/or material nonlinearity. Equation (39)
can be transformed into a system of first-order ODEs
by adopting $\mathbf{v} = \dot{\mathbf{u}}$. As a result, it is found to be:

$$\begin{bmatrix} \mathbf{M} & \mathbf{0} \\ \mathbf{0} & \mathbf{M} \end{bmatrix} \begin{bmatrix} \dot{\mathbf{u}} \\ \dot{\mathbf{v}} \end{bmatrix} + \begin{bmatrix} \mathbf{0} & \mathbf{M} \\ -\mathbf{K} & -\mathbf{C} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{f} \end{bmatrix} \tag{40}$$

where $\mathbf{v} = \left\{ v_1 \ v_2 \ v_3 \ v_4 \right\}^T$. Figure 6 shows structural
and vibrational properties of the shear building.
Clearly, the stiffness of each story will reduce after

the frame deforms. Besides, the initial natural fre-
quencies of Eq. (39) are found to be $\omega_0^{(k)}$ for $k = 1, 2, 3, 4$ as shown in Fig. 6. On the other hand, the
initial eigenvalues of $\lambda_0^{(k)}$ for $k = 1, 2, \ldots, 8$ can be
found from Eq. (40). The relation between the initial
natural frequency and initial eigenvalue is found to be
$\omega_0^{(k)} = \left| \pm \lambda_0^{(k)} \right|$. In general, $\omega^{(k)}$ is the natural fre-
quency of Eq. (39) for the k-th mode and the
eigenvalues for Eq. (40) are found to be $\pm \lambda^{(k)} i$
correspondingly. Since each story stiffness will reduce
due to deformation, the system of first-order ODEs
will become nonlinear. In this study, $\mathbf{C} = \mathbf{0}$ is taken
for simplicity. The first and fourth mode shapes of the
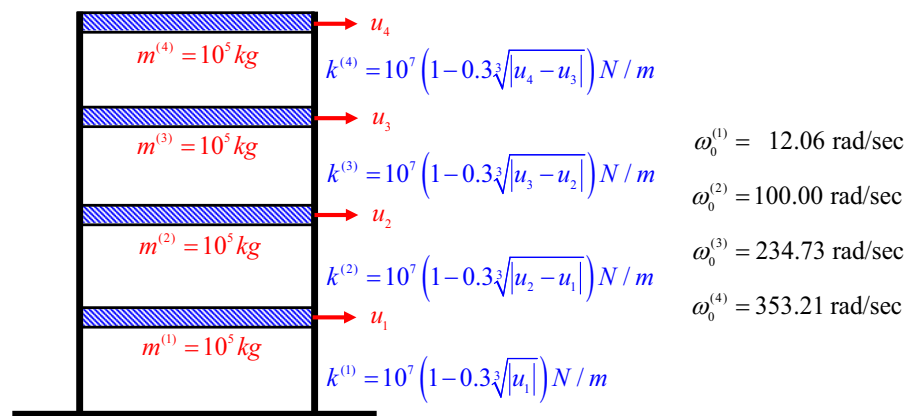building are found to be:

$$\phi_1 = \begin{Bmatrix} 0.347 \\ 0.653 \\ 0.879 \\ 1.000 \end{Bmatrix}, \quad \phi_4 = \begin{Bmatrix} -1.879 \\ 2.879 \\ -2.532 \\ 1.000 \end{Bmatrix},$$
$$\mathbf{u}(0) = \phi_1 + \frac{1}{10}\phi_4 = \begin{Bmatrix} 0.159 \\ 0.941 \\ 0.626 \\ 1.100 \end{Bmatrix} \tag{41}$$

where ϕ_1 and ϕ_4 denote the first and fourth modes of
the shear building and $\mathbf{u}(0)$ is an initial displacement
vector and is made up of first and fourth modes.

At first, the free vibration solutions to the initial
conditions of $\mathbf{v}(0)$, as given in Eq. (41), in addition to

Fig. 6 A four-story shear building and its vibration properties

$m^{(4)} = 10^5\,kg$

u_4

$k^{(4)} = 10^7\left(1 - 0.3\sqrt[3]{|u_4 - u_3|}\right)N/m$

u_3

$m^{(3)} = 10^5\,kg$

$k^{(3)} = 10^7\left(1 - 0.3\sqrt[3]{|u_3 - u_2|}\right)N/m$

$\omega_0^{(1)} = 12.06$ rad/sec

u_2

$m^{(2)} = 10^5\,kg$

$k^{(2)} = 10^7\left(1 - 0.3\sqrt[3]{|u_2 - u_1|}\right)N/m$

$\omega_0^{(2)} = 100.00$ rad/sec

$\omega_0^{(3)} = 234.73$ rad/sec

u_1

$m^{(1)} = 10^5\,kg$

$\omega_0^{(4)} = 353.21$ rad/sec

$k^{(1)} = 10^7\left(1 - 0.3\sqrt[3]{|u_1|}\right)N/m$

$\mathbf{v}(0) = \mathbf{0}$ are calculated. In this case, $\mathbf{f} = \mathbf{0}$ is taken. The result obtained from AMM-1 with $h = 0.0001$ is considered as a reference solution for comparison. On the other hand, AMM-1, PEM-I-1, and PEM-E-1 are also used to carry out calculations by using the step sizes of $h = 0.001$ and 0.003. Numerical results are plotted in Fig. 7. It is seen in Fig. 7a that the three methods with $h = 0.001$ result in almost the same solution, and this result is reliable in contrast to the reference solution. On the other hand, the result obtained from PEM-I-1 with $h = 0.003$ seems to coincide together with that of AMM-1 as shown in Fig. 7b while the solution calculated from PEM-E-1 slightly deviates from this solution. Evidently, the results obtained from $h = 0.003$ for all the three methods show more numerical errors when compared to those calculated from $h = 0.001$. Hence, it is affirmed by this example that PEM-E-1 and PEM-I-1 can have a comparable solution in contrast to AMM-1 in the solution of the nonlinear problem. Notice that both AMM-1 and PEM-I-1 involve nonlinear iterations for each step while PEM-E-1 is non-iterative. An average iteration number is about 3.00 for AMM-1 and PEM-I-1 for $h = 0.001$. Whereas, it is about 3.02 for $h = 0.003$.

Meanwhile, an acceleration of $5\sin(t)$ is also imposed upon the building at its base with zero initial condition. The solution calculated from AMM-1 with a step size of $h = 0.001$ is considered as a reference solution. Both PEM-I-1 and PEM-E-1 in addition to AMM-1 are applied to compute the solutions. Calculated results are plotted in Fig. 8. It is revealed by the two plots of this figure that the forced vibration solutions calculated from PEM-E-1 and PEM-I-1 are almost the same as those computed from AMM-1 for

using the step sizes of $h = 0.05$ and 0.1. It is found in both plots that the result of PEM-I-1 overlaps together with that of AMM-I-1. This phenomenon is also discovered in Fig. 7, and this might be due to the same requirement of nonlinear iterations for each step. Besides, an average iteration number for each step for AMM-1 and PEM-I-1 is about 3.45 for $h = 0.05$ and 3.99 for $h = 0.1$. Since the slowest and fastest eigenvalues are imaginary and are $\left|\lambda_0^{\min}\right| = 12.06$ and $\left|\lambda_0^{\max}\right| = 353.21$, respectively, the system can be considered as a stiff system. Besides, the values of $\left|\Lambda_0^{\max}\right| = \left|\lambda_0^{\max}h\right|$ are found to be as large as 17.66 and 35.32 corresponding to $h = 0.05$ and 0.1. Consequently, it can be used to numerically affirm that the stability region of PEM-E-1 includes the imaginary axis as shown in Fig. 1. It is validated by this example that *explicit* PEM-E-1 can have roughly the same performance as *implicit* AMM-1 in the solution of stiff problems since it has a desired A-stability property and the second-order accuracy. Consequently, it might be very promising for solving stiff problems.

8.5 A dynamical system of nonlinear pendulum

A pendulum is generally made up of a weight attached by a light, inflexible rod to an axle. Thus, it can swing for larger angles. In this study, the magnitude of the friction force is assumed to be proportional to the velocity of the pendulum so that it can slow the pendulum to a halt. The mass and length of the pendulum are assumed to be 1kg and 1m, respectively. Besides, the coefficient of friction is 0.5. The oscillatory motion of the pendulum is controlled by the second-order equation of motion of

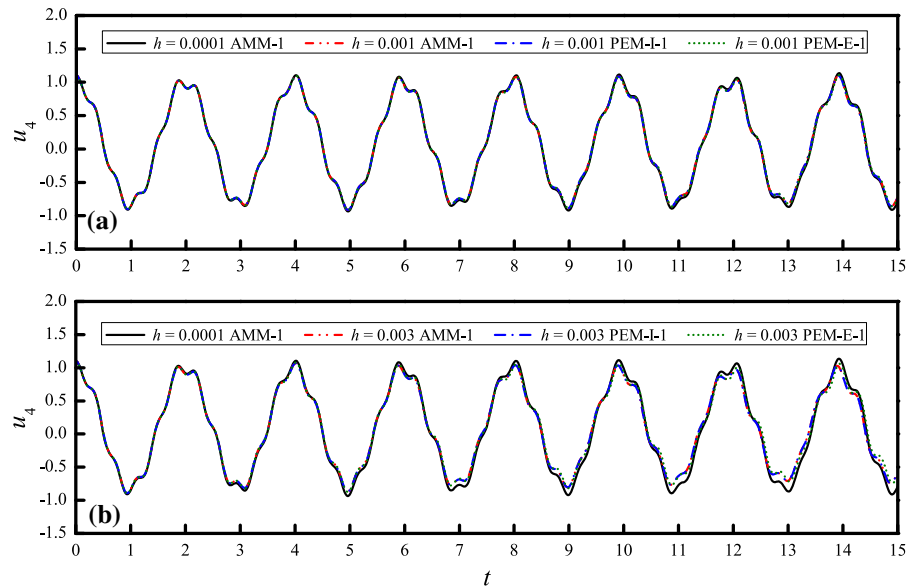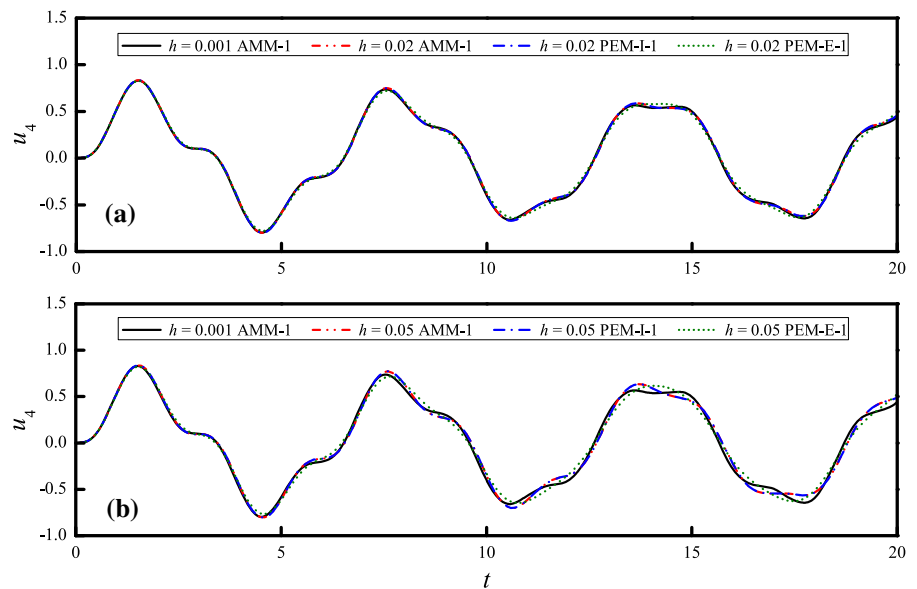**Fig. 7** Free vibration solutions for nonlinear four-story shear-frame

Fig. 8 Forced vibration solutions for nonlinear four-story shear-frame

$y'' + 0.5y' + 9.81\sin(y) = 0$. After setting $y_1 = y$ and $y_2 = y'_1 = y'$, one can have a set of first-order ODEs for the pendulum as:

$$\begin{Bmatrix} y'_1 \\ y'_2 \end{Bmatrix} = \begin{bmatrix} 0 & 1 \\ -\dfrac{9.81}{y_1}\sin y_1 & -0.5 \end{bmatrix} \begin{Bmatrix} y_1 \\ y_2 \end{Bmatrix} \qquad (42)$$

where y_1 is the angle of the pendulum from the vertical. A gravity acceleration of $9.81 \mathrm{m/sec^2}$ is taken. An initial condition of $y_1(0) = 0$ and $y_2(0) = 5$ is considered.

Since this is a nonlinear initial value problem, AMM-1 with a small step size of $h = 0.001$ is used to obtain a reference solution. In addition, AMM-1 and PEM-E-1 with a step size of $h = 0.01$ are also applied to calculate solutions. Numerical results are plotted in Fig. 9. The curve starts at the point $(y_1, y_2) = (0, 5)$ and subsequently it spirals clockwise toward the point $(0, 0)$. It is evident that the result calculated from AMM-1 with $h = 0.01$ almost coincides together with the reference solution while that calculated from

PEM-E-1 slightly deviates from the reference solution but can still provide a reliable solution. This is because that AMM-1 involves an iteration procedure and an average iteration number of 1.46 is found for each step while there are no nonlinear iterations for each step for PEM-E-1.

8.6 A series of mechanical systems

Since PEM-E-1 can simultaneously combine A-stability and explicit formulation, it might be computationally efficient for solving stiff problems. This can be validated by solving a stiff problem, which is intentionally designed. For this purpose, three prerequisites are required to design a stiff system: (1) it can be easily constructed; (2) an arbitrary number of equations can be formulated; and (3) it can have a large dispersion of eigenvalues. Thus, a large mechanical system is chosen for this study, where n boxcars are connected by n springs and the first spring is attached to a fixed wall. The boxcars are assumed to slide along a frictionless horizontal surface. The detailed structure of the mechanical system is depicted in Fig. 10, where $n = 125, 250$, and 500 are chosen to mimic the three systems governed by the equations of motion for $n = 125, n = 250$, and $n = 500$. A coupled governing equation of motion for each system can be formulated as shown in Eq. (39) except that $\mathbf{c} = 0$ is adopted. It is well recognized that a system of second-

order ODEs in n variables can be transformed into a system of first-order ODEs in $2n$ variables. After this transformation, three systems of first-order ODEs with $2n = 250$, $2n = 500$ and $2n = 1000$ can be simulated and can be also expressed as shown in Eq. (40) with $\mathbf{c} = 0$.

In the subsequent calculations, each mechanical system is subjected to a constant acceleration a_g at its base. Notice that the stiffness k_i will become nonlinear if $|u_i - u_{i-1}| \neq 0$. It is found that $\omega_0^{(k)} = \left|\pm\lambda_0^{(k)}\right|$, for $k = 1, 2, \ldots, n$, where $\omega_0^{(k)}$ is the initial natural frequency for the k-th mode and the initial eigenvalues are $\pm\lambda_0^{(k)}i$ correspondingly. The slowest and fastest initial eigenvalues and input constant acceleration for each system are summarized in Table 3. Clearly, each system may be considered as a stiff system since the slowest and fastest initial eigenvalues of each system are drastically different. In fact, $\left|\lambda_0^{\min}\right|$ is found to be 12.52, 6.27, and 3.14 for the systems of $2n = 250$, $2n = 500$, and $2n = 1000$, respectively. Whereas, $\left|\lambda_0^{\max}\right|$ is found to be as large as 2000.0 for all the three systems. AMM-1 and PEM-E-1 are adopted to solve such a stiff problem. In general, AMM-1 with $h = 0.001, 0.002$, and 0.004 is applied to calculate the solution for the systems $2n = 250$, $2n = 500$, and $2n = 1000$, respectively, and the result for each system is considered as a reference solution. Since AMM-1 and PEM-E-1 can have A-stability, there is no limitation on the

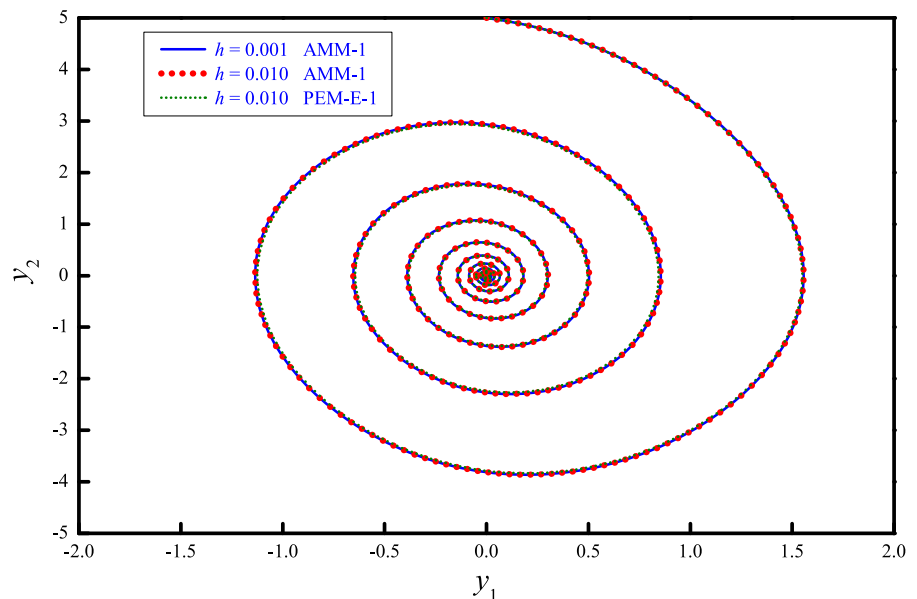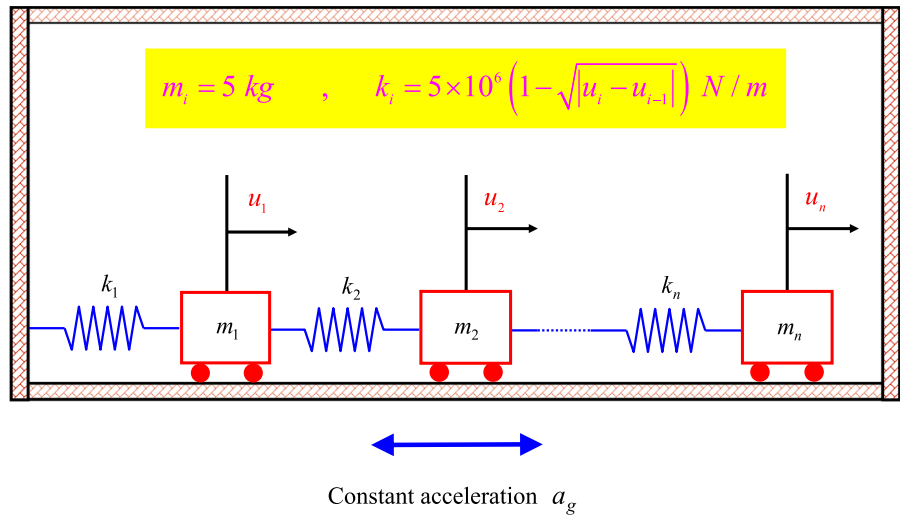Fig. 9 Numerical results for oscillatory motion of pendulum

Fig. 10 A large, nonlinear mechanical system under constant acceleration

step size. As a result, a step size can be chosen by an accuracy consideration only and a total number of $N = 250$ steps is conducted for each system. Hence, a time history of $t_d = 250h$ will be achieved for each analysis. The step size h, response history t_d and total number of steps N for each system are also listed in Table 3.

It seems that the step size of $h = 0.01, 0.02,$ and 0.04 are the maximum allowable step sizes to obtain reliable results for the systems of $2n = 250, 2n = 500,$ and $2n = 1000$, respectively. The calculated results of the three systems are shown in Fig. 11. The solutions obtained from PEM-E-1 almost overlap together with those obtained from AMM-1 for each system; thus, it is substantiated that PEM-E-1 can have a comparable accuracy with AMM-1. A-stability of PEM-E-1 is indicated by this example. This is because that $\left|\lambda_0^{\min}\right|$ and $\left|\lambda_0^{\max}\right|$ are widely separated for each system and the value of $\left|\lambda_0^{(n)}h\right|$ for the initial fastest eigenvalue of each system is found to be as large as 20, 40 and 80

Table 3 The slowest and fastest initial eigenvalues and loading data

n	$\min\left|\lambda_0^{(k)}\right|$	$\max\left|\lambda_0^{(k)}\right|$	$a_g\,(\text{m/sec}^2)$	$t_d(\text{sec})$
250	12.52	2000.00	100	2.5
500	6.27	2000.00	25	5
1000	3.14	2000.00	6.25	10

corresponding to the systems of $2n = 250, 2n = 500,$ and $2n = 1000$. For the presence of the fastest eigenmode, it is generally required to use a very small step size to maintain stability for a numerical method that has no A-stability.

In general, the computing time for each analysis can be applied to evaluate the computational efficiency of a solution method. Thus, the CPU time for each analysis is recorded for AMM-1 and PEM-E-1 and is listed in Table 4. PEM-E-1 consumes much less CPU time in contrast to AMM-1 after comparing the third column to the second column. This is because that implicit AMM-1 involves nonlinear iterations for each step while there is no involvement of nonlinear iterations for explicit PEM-E-1. A ratio of R is defined as the CPU time consumed by PEM-E-1 over that by AMM-1. It is manifested from the last column of Table 4 that R decreases with an increasing number of the equations. Hence, the saving of the CPU demand for PEM-E-1 in contrast to a conventional implicit method, such as AMM-1 will increase as the number of $2n$ increases. In fact, the ratio R as shown in the last column is 1.6% for the system of $2n = 500$ and it becomes as small as 0.93% for the system of $2n = 1000$.

The Newton–Raphson method is often involved as an iteration procedure is adopted to solve nonlinear equations. A direct elimination method is chosen to solve a system of linear equations for each iteration, where a triangulation, a substitution, and a stiffness matrix update are involved. Thus, a total number of triangulations, substitutions, and stiffness matrix

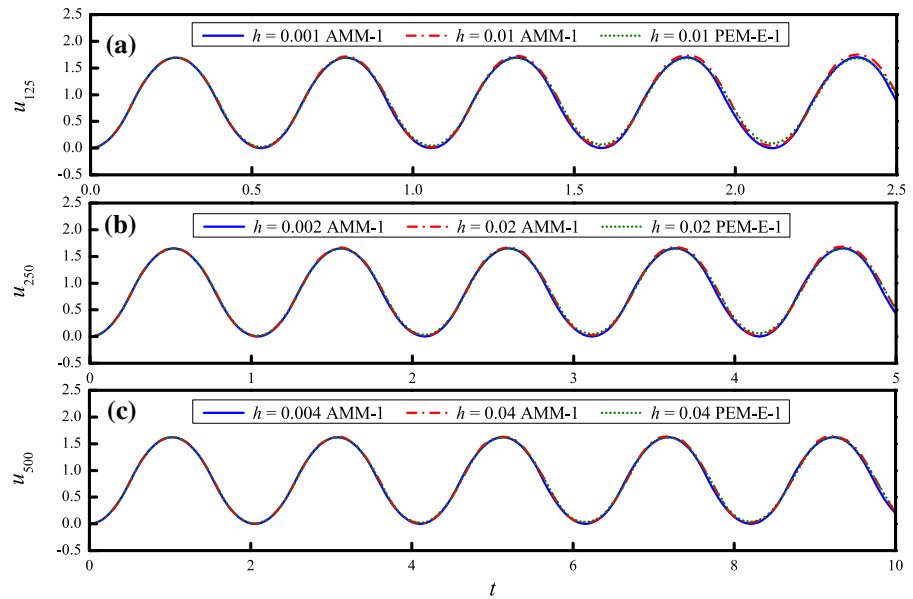**Fig. 11** Numerical solutions for large nonlinear mass-spring systems

Table 4 Comparison of CPU time

n	h(sec)	N (total steps)	AMM-1	PEM-E-1	$R = \frac{\text{PEM-E-1}}{\text{AMM-1}}$
250	0.01	250	65.55	1.02	0.016
500	0.02	250	505.02	4.91	0.0097
1000	0.04	250	3822.06	35.53	0.0093

updates is identical to the total number of nonlinear iterations for each step in a whole solution procedure. No nonlinear iterations are involved for an explicitly implemented problem-dependent method, such as PEM-E-1. In fact, it only requires a triangulation at the start of the solution procedure. Subsequently, only a substitution and a stiffness matrix update are needed for each step. The computational effort for conducting a substitution is much less than that for a triangulation for a large system.

The total number of triangulations, substitutions, and stiffness matrix updates for both AMM-1 and PEM-E-1 are shown in Table 5 for comparison. It is revealed by column 5 that the total number of triangulations for AMM-1 is 1003, 866, and 788 for the systems of $2n = 250$, $2n = 500$, and $2n = 1000$, where a convergent solution can be achieved after an average iteration number of 4.01, 3.46, and 3.15 for each step for the three systems correspondingly. Whereas, only a triangulation is needed for PEM-E-1. Besides, the total number of substitutions and stiffness updates for AMM-1 is 1003, 866, and 788 for

the three systems while it is only 250 for PEM-E-1 for each system. The difference in the total number of the triangulations leads to the drastic difference in CPU time. It is also found that the total number of substitutions or stiffness updates for PEM-E-1 is only about one-fourth to one-third of that required by AMM-1. Consequently, PEM-E-1 can have much better computational efficiency in contrast to conventional implicit methods, such as AMM-1, for solving a subclass of stiff problems.

9 Conclusions

A new series of linear multi-step formulas is proposed in this work. In contrast to conventional linear multi-step formulas, its coefficients are no longer limited to be scalar constants but can be a function of the eigenvalues of the problem under analysis or a function of the physical properties for defining the problem. This series of formulas is derived from an eigen-based theory since the eigenvalues and

Table 5 Comparison of major consumed CPU time between AMM-1 and PEM-E-1

N-DOF	AMM-1					PEM-E-1			
	Total number of steps	Average iteration number	Total number of iterations	Total number of triangulations	Total number of substitutions	Total number of stiffness updates	Total number of steps	Total number of triangulations	Total number of substitutions	Total number of stiffness updates
250	250	4.01	1003	1003	1003	1003	250	1	250	250
500	250	3.46	866	866	866	866	250	1	250	250
1000	250	3.15	788	788	788	788	250	1	250	250

corresponding eigenvectors of the system of the coupled first-order ODEs will play a key role in the development of this type of formulas for solving a system of coupled first-order ODEs. The profile of this development is to decompose a system of coupled first-order ODEs into a series of uncoupled first-order ODEs. Then, an eigen-dependent formula is developed to solve each uncoupled first-order ODE. Finally, all the eigen-dependent formulas are combined to formulate a problem-dependent formula by applying a reverse procedure of an eigen-decomposition technique. This conversion from all the eigen-dependent formulas to a problem-dependent formula can avoid an eigen-analysis and a superposition of each eigen-mode solution for each step. Hence, this series of solution methods has a characteristic of eigen dependency and problem dependency. In addition, its problem-dependent coefficients are not scalar constants but constant matrices with the same size of the system of the first-order ODEs under analysis.

A successful development of an eigen-dependent formula to solve each uncoupled first-order ODE is a prerequisite to develop a problem-dependent formula. Some assumptions regarding to the formulation of the difference formulas and polynomial fractions of eigen-dependent coefficients are also very important to develop an eigen-dependent formula. These assumptions in conjunction with the previously described profile for developing a problem-dependent method can be used to form a typical procedure for developing a problem-dependent method for solving first-order ODEs. This series of problem-dependent methods can be explicitly or implicitly implemented. A combination of A-stability and explicit formulation can be very computationally efficient for solving a subclass of first-order stiff ODEs, such as problems in vibrations and chemical kinetics, the analysis of control systems and the study of dynamical systems. Although only a series of the problem-dependent methods are developed in this work, it seems this methodology to develop the problem-dependent methods can be also applied to develop other problem-dependent formulas for solving systems of coupled first-order ODEs.

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