INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING
Int. J. Numer. Meth. Engng 2009; **80**:565–595
Published online 1 September 2009 in Wiley InterScience (www.interscience.wiley.com). DOI: 10.1002/nme.2642

Asymptotic upper bounds for the errors of Richardson extrapolation with practical application in approximate computations

Aram Soroushian[1,*,†], Peter Wriggers[2] and Jamshid Farjoodi[3]

[1] *Structural Engineering Research Center, International Institute of Earthquake Engineering and Seismology, 19395 Tehran, Iran*
[2] *Institute of Mechanics and Computational Mechanics, University of Hannover Appelstrasse 9A, 30167 Hannover, Germany*
[3] *University College of Engineering, University of Tehran, 11365 Tehran, Iran*

SUMMARY

The results produced by Richardson extrapolation, though, in general, very accurate, are inexact. Numerical evaluation of this inexactness and implementation of the evaluation in practice are the objectives of this paper. First, considering linear changes of errors in the convergence plots, asymptotic upper bounds are proposed for the errors. Then, the achievement is extended to the results produced by Richardson extrapolation, and finally, an error-controlling procedure is proposed and successfully implemented in approximate computations originated in science and engineering. Copyright © 2009 John Wiley & Sons, Ltd.

Received 5 June 2008; Revised 17 March 2009; Accepted 2 April 2009

KEY WORDS: Richardson extrapolation; error upper-bound estimation; convergence plot; practical implementation; pseudo-convergence; time integration analysis

This paper is dedicated to the memory of the victims in the Tehran–Yerevan flight No. 7908, July 15, 2009

1. INTRODUCTION

In today's complicated world of engineering and science, many mathematical models cannot be analyzed analytically. In order to analyze these models and models with complicated analytical solutions approximately, applying numerical methods is indispensable. Two important issues in

*Correspondence to: Aram Soroushian, Structural Engineering Research Center, International Institute of Earthquake Engineering and Seismology, 19395 Tehran, Iran.
†E-mail: a.soroushian@iiees.ac.ir, Aram.Soroushian@Gmail.com

numerical methods are accuracy and computational cost, e.g. see [1–5]. Specifically, from the point of view of accuracy, a fundamental essentiality is convergence [6, 7], i.e.

$$\lim_{\lambda \to 0} U^a = U, \quad \lambda > 0 \tag{1}$$

In Equation (1), U^a and U, respectively, stand for the approximately computed and exact values of an arbitrary unknown, in the mathematical model, under consideration, and λ, known as the algorithmic parameter, has no specific physical (real) meaning, but a main role in the approximate computation [8]. Richardson extrapolation [9, 10] is a technique that, for approximately computed results, satisfying Equation (1) (also see [11]), accelerates the convergence, and hence, in many cases, can increase the accuracy. Because of the simple formulation and low computational cost associated with Richardson extrapolation, the implementation of this technique, in different practical problems, is considerable [12–16], and the study on its theoretical aspects is in continuous progress [17–19]. By estimating the errors of the results produced by Richardson extrapolation, we would achieve the capability to implement Richardson extrapolation in a more reliable manner. Arriving at this capability would be beneficial, specifically, for computations with high accuracy demand, when the computational facilities are limited or expensive. The report of a relevant research [20], also, talks about the errors of the results produced by Richardson extrapolation; nevertheless, this paper presents a slightly different formulation, leading to a practical accuracy-controlling procedure for computations, with one algorithmic parameter. In more detail, this paper is dedicated to the estimation of reliable asymptotic upper bounds for the errors of the results produced by Richardson extrapolation and the implementation of this estimation in real approximate computations. To arrive at these objectives: (1) convergence is assumed maintained; and (2) the algorithmic parameter is considered sufficiently small, not such that to cause the effects of round off dominate the errors; see the word *asymptotic* in the title of this paper. Equivalently, it is assumed that the convergence plots are as schematically displayed in Figure 1, and, being located at the section a in these plots, we are investigating the reliable upper-bound estimations for the errors of Richardson extrapolation, at values of the algorithmic parameter asymptotically larger than those causing considerable round off errors. In Figure 1, E represents the deviation of the approximately computed result U^a, from the exact result, U (see Equation (1)), i.e.

$$E = U^a - U \tag{2}$$

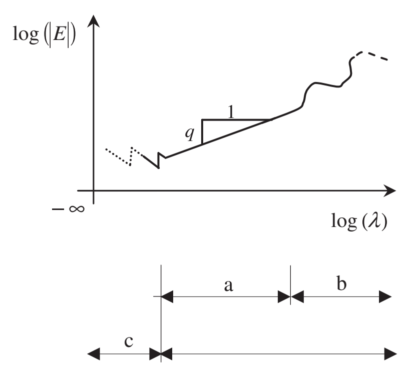

Figure 1. Schematic changes of converging errors with respect to the algorithmic parameters.

DOI: 10.1002/nme

($|E|$ implies the error [21]), $q \in Z^+ = \{1, 2, 3, \ldots\}$ denotes the rate of convergence (also see [5]), and λ stands for the algorithmic parameter. In view of these considerations, Section 2 presents an asymptotic upper-bound estimation for the errors of the results produced by Richardson extrapolation and displays the validity of the estimation via a simple example. Section 3 studies the reliability of the proposed upper-bound estimation, in an engineering computation, namely, time integration of semi-discretized equations of motion. Section 4 presents discussions on practical implementation of the proposed estimation, and concludes with a procedure for materializing more reliable, more accurate, and/or computationally less expensive approximate computations. Section 5 is dedicated to numerical validation of the proposed procedure; and, finally, in Section 6, the paper is closed with a brief set of the conclusions.

2. THE MAIN THEORY

2.1. Formulation

Approximate computations, e.g. computing the areas or volumes of miscellaneous 2D or 3D shapes, solving non-linear algebraic equations, and numerical integration, are associated with some additional variables/parameters. For instance, in approximate analysis of non-linear algebraic equations by the Newton–Raphson method [22], the number of iterations, the starting solution, and the analysis tolerance are additional parameters, affecting the approximately computed results, but not the exact results. More precisely, a result of an approximate computation is a function of the actual data (actual parameters), defining the characteristics of the problem, and some additional parameters [8], essential in the approximate computation. The actual parameters control the exact result, and the additional parameters, broadly known as the algorithmic parameters, control the approximation (without necessarily having real physical meanings).

Considering these, for approximate computations, with one algorithmic parameter (or when changes of the approximate results, with respect to one algorithmic parameter, are to be studied), the computation can be defined by

$$U^a = F(P_j, \lambda) \tag{3}$$

where U^a, P_j, and λ, respectively, denote the approximate result, the actual data (defining the problem), and the algorithmic parameter, and F is a representation of the approximate computation. Meanwhile, in view of the essentiality of convergence [5–8], the definition of the algorithmic parameter, λ, can be set in view of Equation (1) (see [6, 8]). Though, with such a definition, the algorithmic parameter is not necessarily a continuously changing parameter, it can simply be replaced with a generalized continuously changing parameter. As an example, when computing the surface between the x-axis and an arbitrary function $y = f(x)$, by the Simpson rule [21, 23, 24], the number of integration steps, though integer, and changing discontinuously, can be considered changing continuously by means of interpolation. With this consideration, Equation (1) implies that, in the vicinity of $\lambda = 0$, the F in Equation (3) and the U^a in Equations (1) and (2) are continuous functions [24] of λ. Shortly, assuming that, in the arbitrarily close vicinity of $\lambda = 0$, the derivatives of U^a and F with respect to λ exist, and denoting these derivatives by s_n,

$$s_n = \left. \frac{\partial^n F}{\partial \lambda^n} \right|_{\lambda \to 0}, \quad n = 1, 2, 3, \ldots \tag{4}$$

DOI: 10.1002/nme

we can implement the Taylor series [23, 24] and Equation (1) to expand the approximate result U^a about $\lambda=0$, i.e.

$$U^a = U + \sum_{n=1}^{\infty} \frac{s_n}{n!} \lambda^n \tag{5}$$

and, with attention to Equation (2), arrive at

$$\begin{aligned} E &= U^a - U = \sum_{n=1}^{N} \frac{s_n}{n!} \lambda^n \\ N &= \infty \end{aligned} \tag{6}$$

In view of Equations (4), the s_n in Equations (6) can be considered constant, with respect to λ (more discussion in this regard is presented later in this section). Furthermore, for converging results, it is an accepted practice to denote the speed, by which, the logarithms of errors decrease, with respect to the logarithm of the algorithmic parameter (q in Figure 1), as the rate of convergence [25]. In view of this definition and Equations (6), the rate of convergence, q, is a positive integer (also see [5]), such that

$$\begin{aligned} s_n &= 0, \quad n = 1, 2, 3, \ldots\; q-1 \\ s_n &\neq 0, \quad n = q, \quad q \in Z^+ \end{aligned} \tag{7}$$

Equations (6) and (7) simply result in

$$E = C_0 \lambda^q + C_1 \lambda^{q+1} + \cdots \qquad q \in Z^+ \tag{8a}$$

$$C_i = \frac{s_{q+i}}{(i+q)!}, \quad i = 0, 1, 2, 3, \ldots \tag{8b}$$

Regarding the existence of the derivatives in Equations (4), if we disregard the effects of round off, almost all approximate computations, producing results converging to exact results (see Equations (1) and (2)), are very well behaved near the exact solutions. This will not occur, if, for sufficiently small λ, the F in Equation (3) is not completely smooth [26], i.e. for converging results, the derivatives, of arbitrary order, of F, with respect to λ, need to be continuous [24], in the close vicinity of $\lambda=0$.

It is meanwhile worth noting, that, in view of Equation (5), the s_n in Equations (6) is constant, only when N goes to infinity. In other words, the validity of Equations (6) relies on the Taylor series in Equation (5), and by replacing the infinite N with a finite $N (N<\infty)$, we omit some terms from the right-hand side of Equations (6), with the sum $\sum_{n=N+1}^{\infty} (s_n/n!)\lambda^n$, obviously, depending on λ. As a result, for finite values of N, either, the s_n, in Equations (6), slightly depends on λ, or, the '$=$' sign should be replaced with the '$\cong$' sign. (A similar effect is predictable on Equations (8).)

Bearing in mind the above source of approximation, we can, based on Equations (1), (2), (3), and (8), arrive at the formulation of the Richardson extrapolation [9, 10, 12, 13, 17, 18], mainly a technique for accelerating convergence (faster decrease of errors, i.e. larger q in Figure 1). With two approximately computed results, Richardson extrapolation leads to [9, 12, 13]:

$$U^a_{R_{1,2}} = \frac{\lambda_1^q U_2^a - \lambda_2^q U_1^a}{\lambda_1^q - \lambda_2^q} \tag{9}$$

DOI: 10.1002/nme

where U_1^a and U_2^a stand for the approximate results, corresponding to $\lambda=\lambda_1$ and $\lambda=\lambda_2$ ($\lambda_1 \neq \lambda_2$), and, according to its typology, Equation (9) is valid, regardless of the relative sizes of λ_1 and λ_2, i.e. λ_1 can be smaller or larger than λ_2. From Equations (8) and (9), it is apparent that, sufficient smallness of λ_1 and λ_2 is the pre-requisite for the accuracy of the result obtained from Equation (9). This is considered provided, in view of the word *asymptotic* in the title of this paper and the two assumptions in Section 1. In more detail, neglecting round off, replacing the U in Equation (2), with $U^a_{R_{1,2}}$ (when considered for E_1 and E_2), and considering the first term in the right-hand side of Equation (8a), we can, in view of a recent research of the authors [27], and the section a in Figure 1, arrive at the Richardson extrapolation addressed in Equation (9). Therefore, for the closeness of the results produced by Richardson extrapolation to the exact results, λ_1 and λ_2 should be set, such that the contributions of the terms, after the first terms, in Equation (8a), can be considered negligible, and still, the effects of round off do not dominate the error. In such a case, i.e. when the assumptions, in Section 1, are satisfied, the results computed by Richardson extrapolation, i.e. $U^a_{R_{1,2}}$, would be much closer to the exact results, compared with the results leading to $U^a_{R_{1,2}}$, i.e. U_1^a and U_2^a. Consequently,

$$|E_i| = |U_i^a - U| \cong |U_i^a - U^a_{R_{1,2}}|, \quad i=1,2 \tag{10}$$

and by considering $\lambda_2 < \lambda_1$, and substituting $U^a_{R_{1,2}}$, from Equation (9), in Equation (10), we can arrive at

$$|E_2| = |U_2^a - U| \cong \frac{\lambda_2^q |U_1^a - U_2^a|}{\lambda_1^q - \lambda_2^q} \tag{11}$$

(Because of the role of Equation (11), in the discussions in this paper, the adequacy of Equation (11) is numerically studied, in the end of this section.)

Additionally, as it is implied in the literature, e.g. see [9, 10, 12], and obvious, from Equations (8a) and (9), for a series of approximate results $U_1^a, U_2^a, U_3^a, \ldots$ (respectively computed by implementing $\lambda_1, \lambda_2, \lambda_3, \ldots$ in an arbitrary computational procedure), converging to the exact result U, the results produced by Richardson extrapolation, i.e. $U^a_{R_{1,2}}, U^a_{R_{2,3}}, \ldots$, also, converge to U, with a rate q_R larger than q [9], i.e.

$$q_R > q \geqslant 1 \tag{12}$$

Therefore, for the series of approximate results, computed by Richardson extrapolation (see Equation (9)), considering a one-to-one relation between the values of the algorithmic parameter $\lambda_2, \lambda_3, \lambda_4, \ldots$ and the approximate results $U_{R_{1,2}}, U_{R_{2,3}}, U_{R_{3,4}}, \ldots$ and implementing Equation (11), we can first arrive at

$$|E_{R_{2,3}}| = |U^a_{R_{2,3}} - U| \cong \frac{\lambda_3^{q_R} |U^a_{R_{1,2}} - U^a_{R_{2,3}}|}{\lambda_2^{q_R} - \lambda_3^{q_R}} \tag{13}$$

(after presenting some different explanation, a formulation equivalent to Equation (13) is addressed in [20]) and then, in view of the definition in Equation (9), deduce

$$|E_{R_{2,3}}| = |U^a_{R_{2,3}} - U| \cong \frac{\lambda_3^{q_R} \left| \dfrac{\lambda_1^q U_2^a - \lambda_2^q U_1^a}{\lambda_1^q - \lambda_2^q} - \dfrac{\lambda_2^q U_3^a - \lambda_3^q U_2^a}{\lambda_2^q - \lambda_3^q} \right|}{\lambda_2^{q_R} - \lambda_3^{q_R}} \tag{14}$$

Moreover, it is reasonable to consider the changes of the algorithmic parameter according to

$$\frac{\lambda_1}{\lambda_2}=\frac{\lambda_2}{\lambda_3}=\frac{\lambda_3}{\lambda_4}=\cdots=r=\text{const.}>1 \tag{15}$$

and, for each $\lambda_1>0$ (see also Equation (3)), implement

$$0<\cdots<\lambda_{i+1}<\lambda_i=\frac{\lambda_1}{r^{i-1}}<\lambda_{i-1}<\cdots<\lambda_1, \quad i=2,3,4,\ldots \tag{16}$$

in Equation (14), to arrive at

$$|E_{R_{2,3}}|=|U^a_{R_{2,3}}-U|\cong\frac{|-r^q U^a_3+(r^q+1)U^a_2-U^a_1|}{(r^{q_R}-1)(r^q-1)} \tag{17}$$

and, then, from Equations (12) and (15) conclude

$$|E_{R_{2,3}}|<\frac{|-r^q U^a_3+(r^q+1)U^a_2-U^a_1|}{(r^q-1)^2} \tag{18}$$

In view of the formal definition of error [21], Equation (18) states an asymptotic upper-bound estimation for the errors associated with the Richardson extrapolations, addressed in Equation (9). This asymptotic upper bound, compared with Equation (13), suggested in [20], has two advantages: (1) while Equation (13) can be implemented, only when q_R is at hand, Equation (18) is independent of q_R, (2) with attention to the importance of reliability in error estimation, while Equation (13) has no claim about such a reliability, in view of Equations (12) and (15), the inequality sign in Equation (18) implies upper-estimating the errors of the results produced by Richardson extrapolation (specifically, when the errors are corresponding to the left part (not left end) of the section a in Figure 1). As a relation between the proposed upper-estimation and the exact error, we can, from Equations (17) and (18), define an upper-estimation (or reliability) index, I_r, as noted below:

$$I_r=\frac{r^{q_R}-1}{r^q-1}>\frac{r^{q_R}}{r^q}\geqslant r>1 \tag{19}$$

For Richardson extrapolations based on more than two approximate results (see [12, 13]), the formulations above should be rederived. For instance, with three approximately computed results, and C_0 and $C_j\,(j>0)$, as the coefficients of the first two nonzero terms in Equation (8a), Equations (9) and (18) change form to:

$$U^a_{R_{1,2,3}}=\frac{r^{2q+j}U^a_3-r^q(r^j+1)U^a_2+U^a_1}{r^{2q+j}-r^q(r^j+1)+1} \tag{20a}$$

$$|E_{R_{2,3,4}}|<\frac{|-r^{2q+j}U^a_4+(r^{2q+j}+r^{q+j}+r^q)U^a_3-(r^{q+j}+r^q+1)U^a_2+U^a_1|}{(r^q-1)(r^{2q+j}-r^q(r^j+1)+1)} \tag{20b}$$

Nevertheless, according to the definition of C_j above, the j in Equations (20) may be unknown, and besides, the number of the analysis repetitions is in practice finite and might be less than needed (compare Equations (20) with Equations (9) and (18)). Therefore, Richardson extrapolations based on two approximately computed results (Equations (9) and (18)) are in general of the most practical interest and hence under special consideration in this paper. Finally, bearing in mind that the

DOI: 10.1002/nme

proposed upper-estimation considers approximate computations, with one algorithmic parameter (the generalization is straightforward), we can claim materializing the first objective implied in the title of this paper and stated in Section 1, i.e. an asymptotic upper-bound estimation for the errors of Richardson extrapolation is achieved. This claim is numerically examined in the remainder of this section, and its practical implementation is discussed in Sections 3–5.

2.2. *Illustrative example*

The series in Equations (21),

$$\frac{\pi^2}{6}=\sum_{n=1}^{k}\frac{1}{n^2} \tag{21a}$$

$$\frac{\pi^2-8}{16}=\sum_{n=1}^{k}\frac{1}{(2n+1)^2(2n-1)^2} \tag{21b}$$

introduce two methods for approximating π; and, for both methods, we can consider $1/k$ as the algorithmic parameter (see Equation (1)). Deviations of the approximate results from the exact result are expressed as,

$$E_k=\left(6\sum_{n=1}^{k}\frac{1}{n^2}\right)^{1/2}-\pi \tag{22a}$$

$$E_k=\left(8+16\sum_{n=1}^{k}\frac{1}{(2n+1)^2(2n-1)^2}\right)^{1/2}-\pi \tag{22b}$$

To study whether the requirements essential for the validity of Equation (18) are provided, the convergence plots corresponding to Equations (21) and (22) are depicted in Figure 2 (as apparent in Figure 2(b), the effect of round off dominates the error, at $\lambda<2\times10^{-4}$). According to these plots, the convergence rates, for the two series, q, are one and three, and the convergence rates for the corresponding results produced by Richardson extrapolation, q_R, are two and four, respectively. Considering $k=1,4,16,64,\ldots$ in Equations (21) (and causing Equation (15) to be satisfied with $r=4$), the validity of Equation (18) is studied in Tables I and II. Apparently, Equation (18)

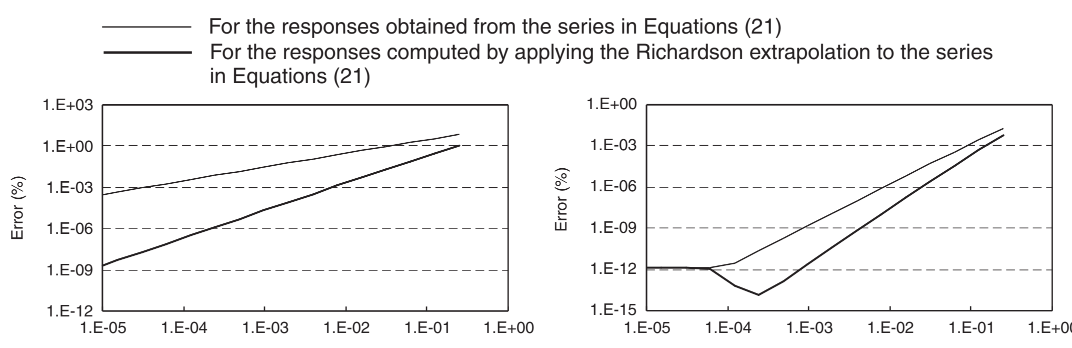

Figure 2. Convergence plots corresponding to the series in Equations (21) (for computing π): (a) corresponding to the series in Equation (21a) and (b) corresponding to the series in Equation (21b).

Table I. The validity of Equations (18) and (11) for the series in Equations (21a) ($q=1$).

			Adequacy of Equation (18)		
$\lambda(\frac{1}{k})$	U^a	U_R^a	Left-hand side of Equation (18) ($\lvert E_{R_{2,3}}\rvert=\lvert U_R^a-\pi\rvert$)	Right-hand side of Equation (18)	Errors in satisfying Equation (11) (%)
1	2.4494949	—	—	—	—
$\frac{1}{4}$	2.9226130	3.0803207	—	—	—
$\frac{1}{16}$	3.0831930	3.1367197	0.004872955	0.018799655	8.34
$\frac{1}{64}$	3.1267528	3.1412727	0.000319941	0.001517672	2.16
$\frac{1}{256}$	3.1378675	3.1415724	0.000020214	0.000999089	0.54
$\frac{1}{1024}$	3.1406604	3.1415914	0.000001267	0.000006316	0.136
$\frac{1}{4096}$	3.1413595	3.1415926	0.000000079	0.000000396	0.034
$\frac{1}{16384}$	3.1415344	3.1415926	0.000000005	0.000000025	0.008

Table II. The validity of Equations (18) and (11) for the series in Equations (21b) ($q=3$).

			Adequacy of Equation (18)		
$\lambda(\frac{1}{k})$	U^a	U_R^a	Left-hand side of Equation (18) ($\lvert E_{R_{2,3}}\rvert=\lvert U_R^a-\pi\rvert$)	Right-hand side of Equation (18)	Error in satisfying Equation (11) (%)
1	3.1269438	—	—	—	—
$\frac{1}{4}$	3.1410160	3.1412393	—	—	—
$\frac{1}{16}$	3.1415809	3.1415898	2.8E−6	5.6E−6	24.0
$\frac{1}{64}$	3.1415925	3.1415926	1.4E−8	4.5E−8	6.83
$\frac{1}{256}$	3.1415927	3.1415927	5.6E−11	2.1E−10	1.77
$\frac{1}{1024}$	3.1415927	3.1415927	2.2E−13	8.8E−13	0.44
$\leqslant\frac{1}{4096}$	Round off dominates the error (see Figure 2(b))				

upper-estimates the errors of the results produced by Richardson extrapolation, with the reliability addressed in Equation (19). (In addition, the validity of Equation (11) in the linear sections of the convergence plots is studied in the last columns of Tables I and II.)

3. ENGINEERING APPLICATION (TIME INTEGRATION ANALYSIS)

3.1. Brief introduction and adaptation

Considering the simplicity of the numerical study presented in the previous section, prior to the implementation of the proposed estimation in a practical error (accuracy)-controlling procedure, we would rather apply the estimation to more complicated computations. In this regard, attention is paid to time integration analysis. Time integration is one of the most versatile tools for structural dynamic analysis [28, 29], specifically, when the forcing functions are complicated and available as digitized

DOI: 10.1002/nme

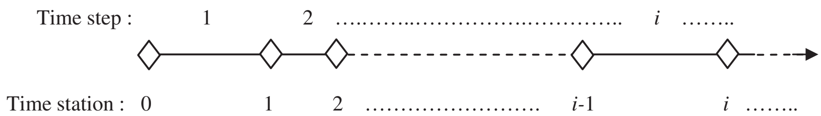

Figure 3. Typical arrangement of time steps and time stations in time integration analyses.

records [30], some of the natural frequencies are very close, the damping is nonclassical, and/or the existing nonlinearities are not negligible, e.g. analysis of building structural systems subjected to ground strong motions [5, 29, 31, 32]. Therefore, the study of time integration analyses, from different theoretical and practical points of view, e.g. convergence, accuracy, and computational cost, started years ago [33, 34], continued in the last decades [35–42], and is still being dealt with [5, 43–46]. To briefly review the general process of time integration analysis, in view of Figure 3, sizes of time steps or a criterion for adaptive time stepping, e.g. see [47], should be set, first. Then, the main analysis starts from the initial conditions (if needed, after applying a starting procedure [46]); and with marching along the time axis, approximate responses are being determined at discrete time stations, consecutively, based on the formulation of the integration method, and, if needed, some nonlinearity considerations.

The results, i.e. responses, generated by time integration are in general inexact [29, 32], and hence, should converge to the exact results [6, 7]. Therefore, the achievements in the previous section should hold. Considering a specific time integration analysis, and, the integration step size, as the algorithmic parameter (see Equation (1) and [5, 8]), in order to make an idea about the errors, it is broadly accepted to repeat the analyses with half steps, and, study the accuracies by comparing the results [31, 48, 49]. (The validity of this approach can be explained by Equation (11), and the column criteria in the literature; see [20].) In view of these repetitions (recommended for practical analyses [31]) and Equations (15) and (16), it is reasonable to apply the Richardson extrapolation to the already computed consecutive responses, each corresponding to a different value of the algorithmic parameter. This is carried out for time integration analyses; see [13, 48]; and hence, we can consider time integration analysis as an appropriate real engineering computational case, for checking the validity of the upper-bound estimation proposed in Section 2. Consequently, the objective, in this section, is to demonstrate that the proposed upper-estimation can successfully be applied to time integration analyses. In order to achieve this objective, if we interpret the U in the previous section, as an arbitrary unknown (or an arbitrary combination of unknowns), in the equation of motion below [50, 51]:

$$\begin{aligned} &\mathbf{M}\ddot{\mathbf{u}}(t)+\mathbf{f}_{\mathrm{int}}(t)=\mathbf{f}(t), \quad 0\leqslant t<t_{\mathrm{end}} \\ &\text{Initial Conditions:} \left| \begin{array}{l} \mathbf{u}(t=0)=\mathbf{u}_0 \\ \dot{\mathbf{u}}(t=0)=\dot{\mathbf{u}}_0 \\ \mathbf{f}_{\mathrm{int}}(t=0)=\mathbf{f}_{\mathrm{int}_0} \end{array} \right. \\ &\text{Additional Constraints: } \mathbf{Q} \end{aligned} \tag{23}$$

Richardson extrapolation, and the upper-bound estimation proposed in Section 2, can directly be applied to the results of time integration analyses, and we would be able to study the validity of the proposed upper-estimation. In Equations (23), t and t_{end} imply the time and the duration of the transient behavior, $\mathbf{M}$ is the mass matrix, $\mathbf{f}_{\mathrm{int}}$ and $\mathbf{f}(t)$ stand for the vectors of internal force and excitation, $\mathbf{u}(t), \dot{\mathbf{u}}(t)$, and $\ddot{\mathbf{u}}(t)$ denote the unknown vectors of displacement, velocity, and acceleration, $\mathbf{u}_0, \dot{\mathbf{u}}_0$, and $\mathbf{f}_{\text{int}_0}$ define the initial status of the mathematical model (regarding the essentiality of considering $\mathbf{f}_{\text{int}_0}$ in Equations (23), also see [52]), and finally, $\mathbf{Q}$ represents some restricting conditions, e.g. additional constraints in problems involved in impact or elastic–plastic behavior [53, 54], all in view of the degrees of freedom set for the mathematical model [50, 51].

3.2. Numerical study

3.2.1. Preliminary notes. First, we should point out that the two examples, in this section, are set such that, the closed-form solutions exist, and, we can depict the convergence plots (see Figure 1), to be implemented in the study of the upper-bound estimations proposed. (This restriction is omitted in the remainder of this paper.) The first example considers a simple single degree of freedom (SDOF) system, by studying which, the main concept is examined; and, in the second example, the adequacy of the proposed upper-bound estimation is studied, via a complicated multi degree of freedom (MDOF) system.

3.2.2. Simple SDOF system. Almost the simplest motion can be defined by the equations below:

$$\begin{aligned} &\ddot{u}(t)+u(t)=0 \\ &\text{Initial Conditions:} \left| \begin{aligned} &u(t=0)=1 \\ &\dot{u}(t=0)=0 \end{aligned} \right. \end{aligned} \tag{24}$$

The exact solution is as stated in Equation (25),

$$u(t)=\cos(t) \tag{25}$$

In view of Equation (25), studying Equations (24) in the time interval $0\leqslant t<20$, with the average acceleration time integration method [34], several times, each time, with steps half in its previous analysis ($r=2$, in Equations (15) and (16)), leads to the error changes, reported, as the solid graphs, in Figure 4. With attention to these figures, for the carried out analyses, the rate of convergence is 2, i.e. $q=2$. Repeating the errors study, for the responses obtained by applying the Richardson extrapolation to the responses of time integration analyses results in the solid graphs in Figure 5. In order to check the adequacy of the proposed formulations, i.e. Equations (11) and (18), the consequences of implementing these formulations (the right-hand side for Equation (18)) are reported, as the dashed graphs, respectively, in Figures 4 and 5. In addition, the results of applying the existing estimation for the errors of Richardson extrapolation [20] (see Equation (13)) are depicted, as the dotted graphs, in Figure 5. As expected, in the linear section of the solid graphs in Figure 4, the dashed and solid graphs (see Equation (11)) pictorially coincide, and, in the linear section of the solid graphs in Figure 5 (see Equation (18)), the dashed graphs upper-estimate the solid graphs, while the dotted graphs (see Equation (13)), though estimate the solid graph more accurately, are less reliable upper-estimations. (Furthermore, in view of Figures 4 and 5, $q=2$ and $q_R=4$, and as expected (see Equation (19)), the reliability of the upper-estimation in Figure 5, is about $(r^{q_R}-1)/(r^q-1)\cong 5$.) Consequently, in the analysis of Equations (24) by the average acceleration method [34], the upper-bound error estimation proposed for the results produced by Richardson extrapolation is completely reliable in the vicinity of zero steps, asymptotically, not affected by round off. The adequacy of the upper-bound error estimation based on three approximate results (Equation (20b)) is also successfully examined in Figure 6.

DOI: 10.1002/nme

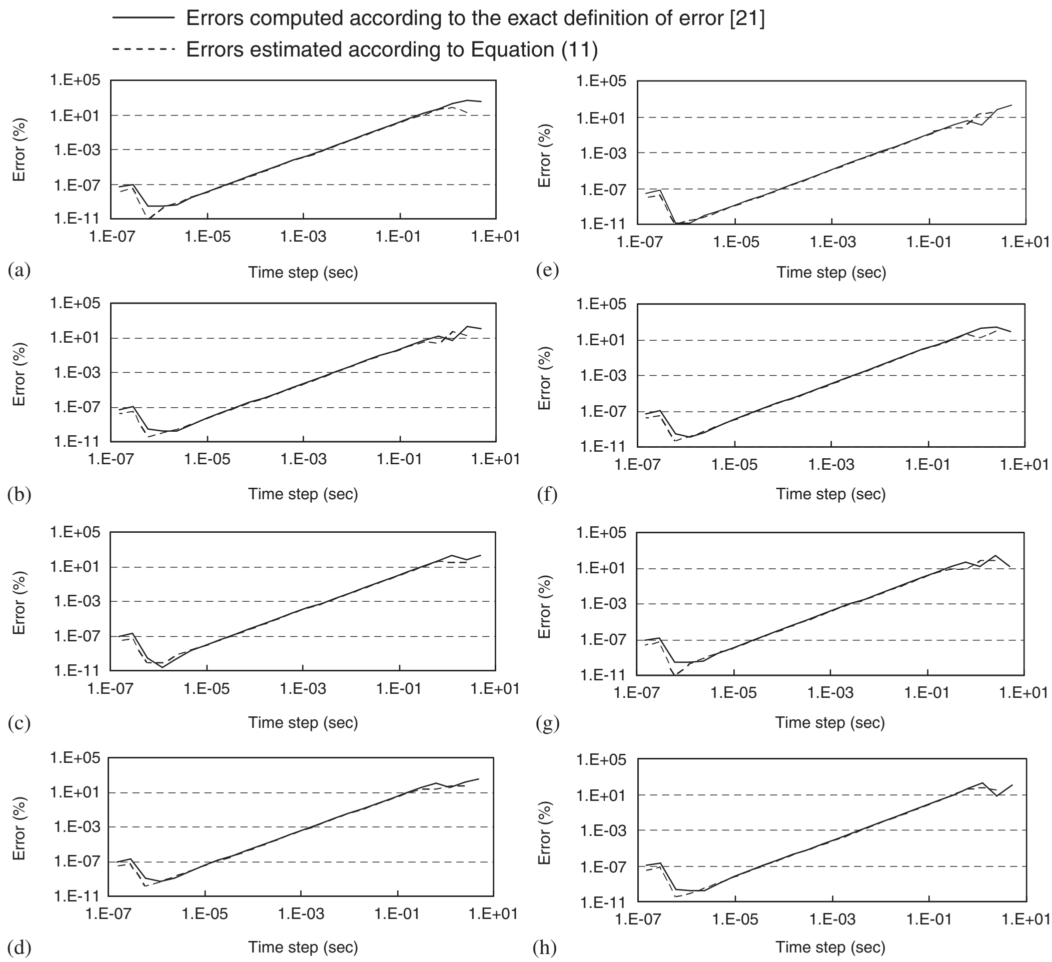

Figure 4. Convergence plots for the results of Equations (24) computed by the average acceleration method [34]: (a) displacement at $t=5$ s; (b) displacement at $t=10$ s; (c) displacement at $t=15$ s; (d) displacement at $t=20$ s; (e) velocity at $t=5$ s; (f) velocity at $t=10$ s; (g) velocity at $t=15$ s; and (h) velocity at $t=20$ s.

3.2.3. Complicated MDOF system. As a more complicated example, consider the system, defined in Equations (26) and Figure 7:

$$\mathbf{M}\ddot{\mathbf{u}}+\mathbf{K}\mathbf{u}=\mathbf{f}, \quad 0\leqslant t<6.0$$

$$t=0: \left| \begin{array}{l} \mathbf{u}=\{1\ \ 1\ \ 1\ \ 1\ \ 1\}^{\mathrm{T}} \\ \dot{\mathbf{u}}=\bar{\mathrm{O}} \end{array} \right.$$

$$\mathbf{M}=10\begin{bmatrix} 20 & 0 & 0 & 0 & 0 \\ 0 & 17 & 0 & 0 & 0 \\ 0 & 0 & 15 & 0 & 0 \\ 0 & 0 & 0 & 12 & 0 \\ 0 & 0 & 0 & 0 & 10 \end{bmatrix}, \quad \mathbf{K}=1000\begin{bmatrix} 9 & -4 & 0 & 0 & 0 \\ -4 & 7 & -3 & 0 & 0 \\ 0 & -3 & 5 & -2 & 0 \\ 0 & 0 & -2 & 3 & -1 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix} \tag{26}$$

DOI: 10.1002/nme

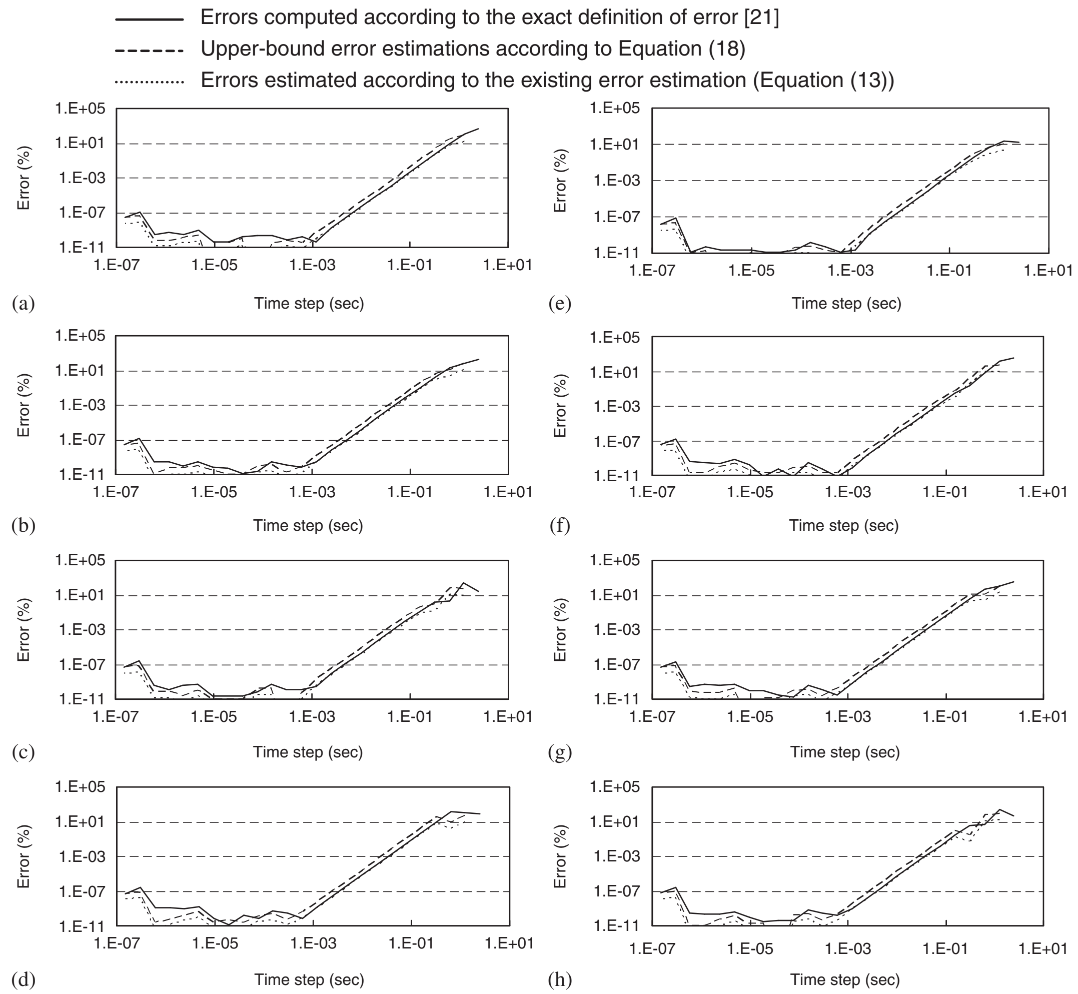

Figure 5. Convergence plots for the results of Equations (24) computed by the average acceleration method [34] and enhanced by the Richardson extrapolation (Equation (9)): (a) displacement at $t=5$ s; (b) displacement at $t=10$ s; (c) displacement at $t=15$ s; (d) displacement at $t=20$ s; (e) velocity at $t=5$ s; (f) velocity at $t=10$ s; (g) velocity at $t=15$ s; and (h) velocity at $t=20$ s.

$$\mathbf{f}=\begin{Bmatrix} f_1\\ f_2\\ f_3\\ f_4\\ f_5 \end{Bmatrix} \quad \begin{array}{l} f_1=8999.21875\cos\left(\dfrac{t}{16}\right)-4000\cos\left(\dfrac{t}{4}\right)\\ f_2=-4000\cos\left(\dfrac{t}{16}\right)+6989.375\cos\left(\dfrac{t}{4}\right)-3000\cos(t)\\ f_3=-3000\cos\left(\dfrac{t}{4}\right)+4850\cos(t)-2000\cos(4t)\\ f_4=-2000\cos(t)+1080\cos(4t)-1000\cos(16t)\\ f_5=-1000\cos(4t)-24600\cos(16t) \end{array}$$

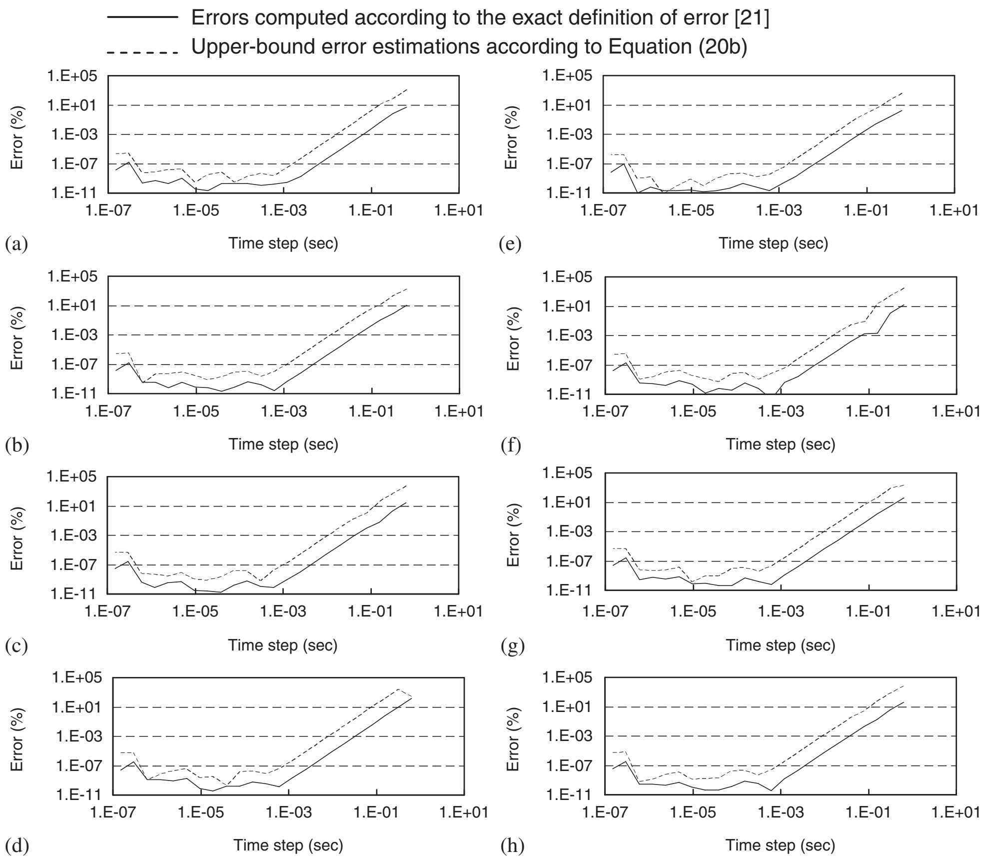

Figure 6. Convergence plots for the results of Equations (24) computed by the average acceleration method [34] and enhanced by the Richardson extrapolation (Equation (20a)): (a) displacement at $t=5$ s; (b) displacement at $t=10$ s; (c) displacement at $t=15$ s; (d) displacement at $t=20$ s; (e) velocity at $t=5$ s; (f) velocity at $t=10$ s; (g) velocity at $t=15$ s; and (h) velocity at $t=20$ s.

(where, the right-hand side superscript 'T' implies matrix transposition). In view of the analytical closed-form solution, i.e.

$$\begin{aligned}\mathbf{u} &= \{u_1 \;\; u_2 \;\; u_3 \;\; u_4 \;\; u_5\}^{\mathrm{T}} \\ &= \left\{\cos\left(\frac{t}{16}\right) \;\; \cos\left(\frac{t}{4}\right) \;\; \cos(t) \;\; \cos(4t) \;\; \cos(16t)\right\}^{\mathrm{T}}\end{aligned} \tag{27}$$

Equations (26) define a moderately stiff mathematical model [2, 55, 56]. Time integrating the problem, with the Houbolt [33, 46, 57], central difference [58], and HHT ($\alpha=-0.1, \beta=0.3025, \gamma=0.6$) [37, 59] methods, results in approximate responses, which, after implementing the

DOI: 10.1002/nme

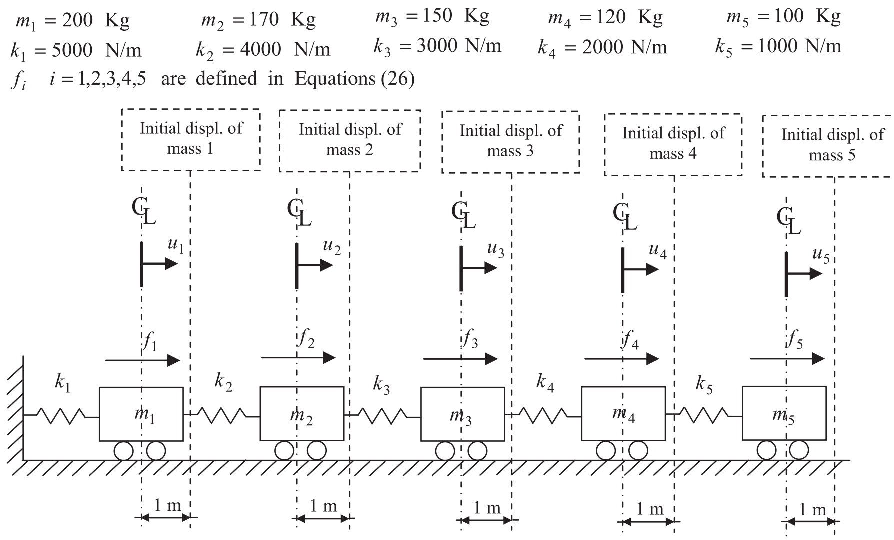

Figure 7. The spring-mass-dashpot model of the system defined in Equations (26).

Richardson extrapolation, and taking into account different error norms [60], brings about the error reports in Figures 8–10. Apparently, all the plots evidence the validity of Equation (18). It is also worth noting that, because of the definition of **f** in Equations (26) and the second-order of accuracy [61], of the above-mentioned integration methods, for all analyses, $q=1$; see [5, 38, 52].

4. PRACTICAL IMPLEMENTATION

4.1. Preliminary notes

Section 2 presented an upper-bound estimation for the errors, associated with Richardson extrapolation, and studied the validity of the estimation, via simple examples. Section 3 studied the adequacy of the proposed estimation, when applied to time integration analysis. This section intends to implement the achievements, in reliably estimating the errors and proposing a practical accuracy-controlling procedure.

A starting question is, while the proposed upper-estimation is reliable, only at the linear sections of the convergence plots, how we can implement it, in approximate analyses, in general, without exact solutions (and hence without convergence plots and any information about the linear sections of the convergence plots). In other words, as also implied in the examples in Section 3, without the exact solutions and checking whether we are at the section a in Figure 1, implementing the proposed estimation, loses its reliability. Considering these, it is reasonable to implement a recent achievement [52] (also see [27]), according to which, when: (1) round off is negligible, (2) time integration, with sufficiently small steps, can model the mathematical model in Equations (23), with desired accuracy, and (3) in absence of nonlinearity, errors properly converge to zero, the

DOI: 10.1002/nme

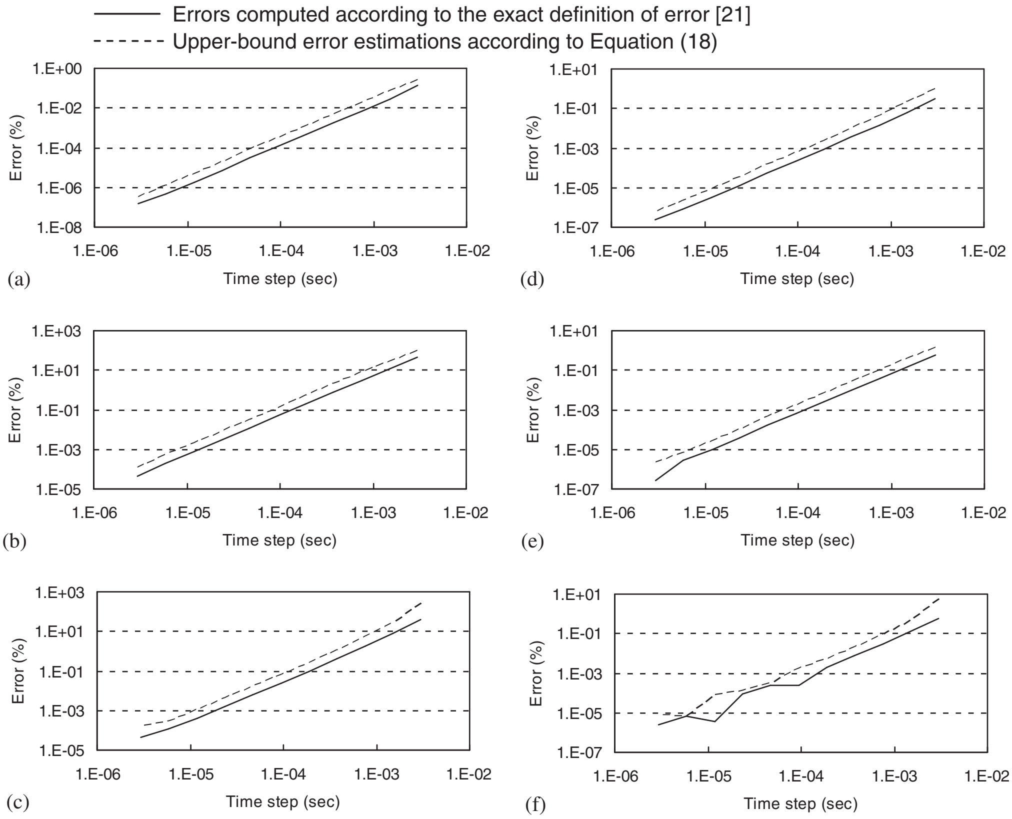

Figure 8. Convergence plots for the responses of Equations (26) computed by the Houbolt method [33, 46, 57] and enhanced by the Richardson extrapolation (Equation (9)): (a) u_1 (with the L_∞ norm); (b) u_3 (with the L_∞ norm); (c) u_5 (with the L_∞ norm); (d) displacement at $t=3.0\,\text{s}$ (with the L_2 norm); (e) displacement at $t=4.5\,\text{s}$ (with the L_2 norm); and (f) displacement at $t=6.0\,\text{s}$ (with the L_2 norm).

equivalence stated in Figure 11 is valid, for time integration analyses. In Figure 11, D_j represents the difference between two consecutively computed (see Equation (15)) results, i.e.

$$D_j = U_j^a - U_{j-1}^a \tag{28}$$

In view of the fact that the equivalence in Figure 11 is explained based on the concept of convergence [52] (and in many approximate computations, the three assumptions above can be guaranteed by considering the associated algorithmic parameter and satisfying the assumptions in Section 1), it seems meaningful to extend the idea, addressed above, to general approximate computations, all to satisfy the requirements of convergence [6, 7]. In more detail, regardless of the approximate computation, under consideration, if we can provide the requirements of convergence, the linearity of the changes of D (or $-D$), with respect to the algorithmic parameter, in a log–log diagram,

DOI: 10.1002/nme

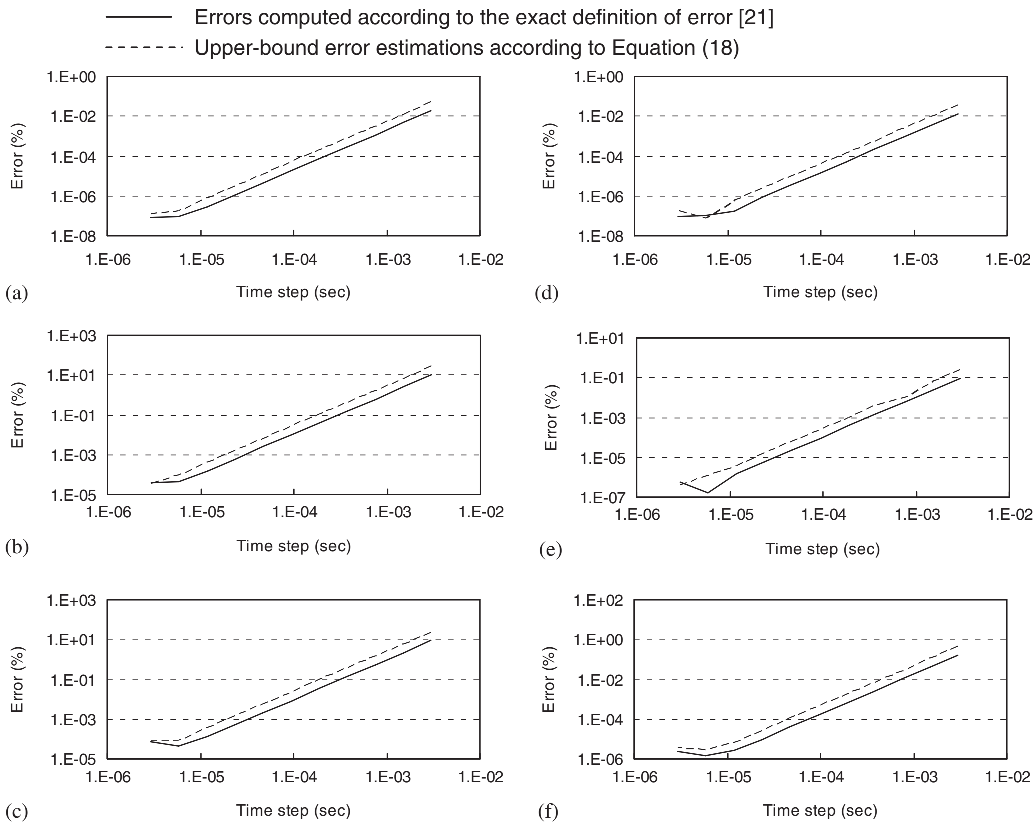

Figure 9. Convergence plots for the responses of Equations (26) computed by the central difference method [58] and enhanced by the Richardson extrapolation (Equation (9)): (a) u_1 (with the L_∞ norm); (b) u_3 (with the L_∞ norm); (c) u_5 (with the L_∞ norm); (d) displacement at $t=3.0$ s (with the L_2 norm); (e) displacement at $t=4.5$ s (with the L_2 norm); and (f) displacement at $t=6.0$ s (with the L_2 norm).

would imply the same trend, for the changes of $|E|$, and vice versa, i.e.

$$\begin{cases} \text{Changes of } D \text{ or} -D \text{ are acceptable (linear)} \Leftrightarrow \text{Changes of } |E| \text{ are acceptable (linear)} \\ \text{(both with respect to } \lambda, \text{in a log–log diagram, when not affected by round off)} \end{cases} \tag{29}$$

Consequently, for an arbitrary approximate computation, when round off is negligible, in order to determine the range of values of the algorithmic parameter, for which, the upper-estimation is valid, instead of $|E|$, we can consider the changes of $|D|$ (also see [27]). Apparently, in talking about the errors of Richardson extrapolation, the changes, addressed in Equation (29), are associated with the results obtained by applying the Richardson extrapolation to consecutive analyses, and hence, in view of Equations (9) and (20a), D_j can be computed, only after at least three approximate analyses. Though the validity of Equation (29) is also demonstrated in the literature [52], for further reliability, the special case of the last example, studied in Figures 8–10, is restudied in

DOI: 10.1002/nme

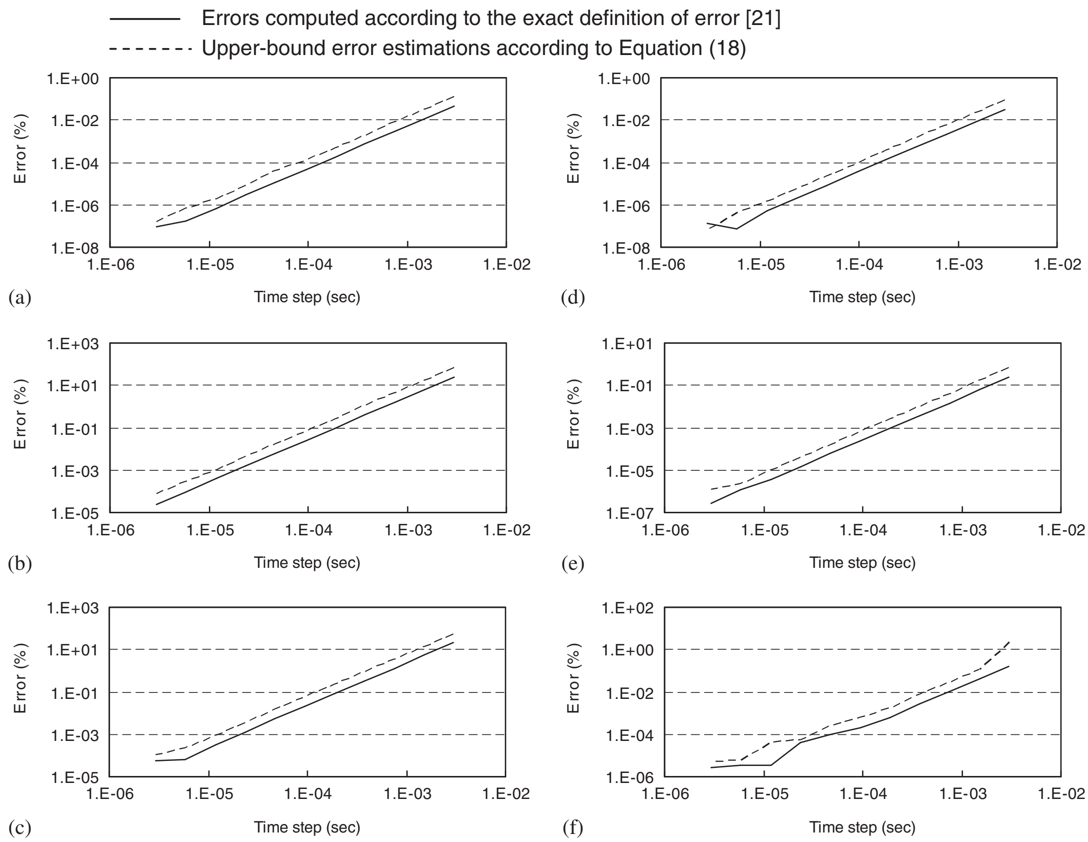

Figure 10. Convergence plots for the responses of Equations (26) computed by the HHT ($\alpha=-0.1, \beta=0.3025, \gamma=0.6$) method [37, 59] and enhanced by the Richardson extrapolation (Equation (9)): (a) u_1 (with the L_∞ norm); (b) u_3 (with the L_∞ norm); (c) u_5 (with the L_∞ norm); (d) displacement at $t=3.0$ s (with the L_2 norm); (e) displacement at $t=4.5$ s (with the L_2 norm); and (f) displacement at $t=6.0$ s (with the L_2 norm).

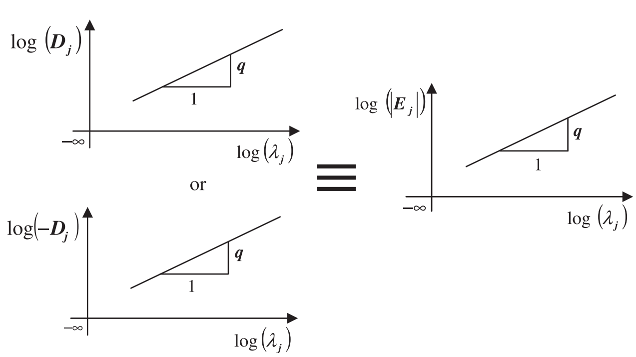

Figure 11. A relation between the deviations D, obtained from Equation (28), and the errors $|E|$.

DOI: 10.1002/nme

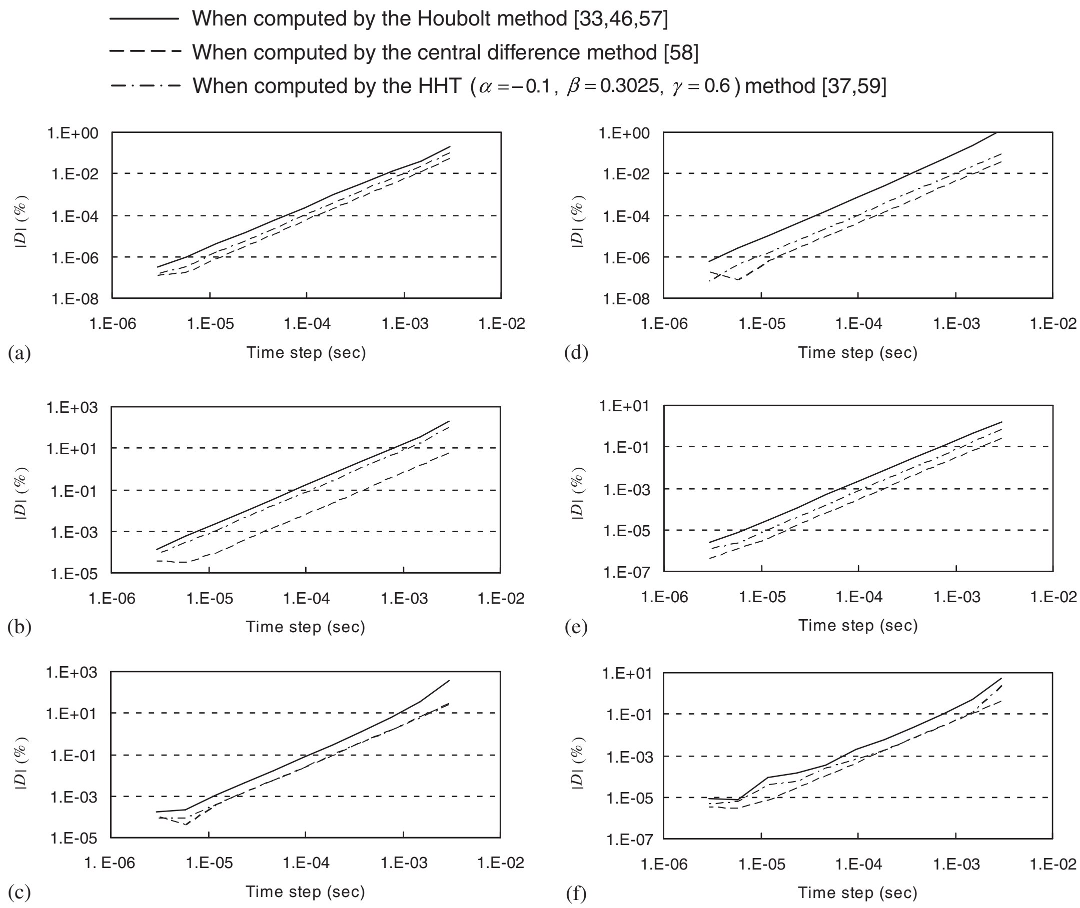

Figure 12. The study of the convergence plots, corresponding to Figures 8–10, with no attention to the exact solutions: (a) u_1 (with the L_∞ norm); (b) u_3 (with the L_∞ norm); (c) u_5 (with the L_∞ norm); (d) displacement at $t = 3.0$ s (with the L_2 norm); (e) displacement at $t = 4.5$ s (with the L_2 norm); and (f) displacement at $t = 6.0$ s (with the L_2 norm).

Figure 12. Comparing the range of the linear trends of the plots in Figure 12 with the trends of the solid graphs in Figures 8–10 clearly reveals the adequacy of Equation (29). With this introduction, in the remainder of this section, the existing error-controlling practice is reviewed, and, enhanced to a new procedure, applicable to general approximate computations with one algorithmic parameter.

4.2. Accuracy-controlling computation

4.2.1. The existing practice. Considering an arbitrary specific approximate computation, the approach, broadly accepted in practice, for arriving at a desired accuracy, is to carry out the approximate computation, with two different values of the algorithmic parameter, and compare

DOI: 10.1002/nme

the results. The procedure is as noted below:

1. Considering convergence, accuracy, and computational cost, as the main concerns in approximate computations, select a value for the algorithmic parameter (generally with some assumptions on the unknown result).
2. Carry out the approximate computation.
3. Appropriately change the value set for the algorithmic parameter and repeat the computation.
4. Compare the results obtained from the last two computations, paying attention to the rate of convergence, the change of the algorithmic parameter, and the accuracy, we are interested in (for sufficiently small values of the algorithmic parameter, not under the effect of dominating round off, we can halve the algorithmic parameter and consider the difference of the two results as an upper-bound estimation of the error; see [48]); if the accuracy is sufficient, stop; otherwise, return to stage 3.

(As some simple applications of the above procedure, we can refer to: (a) repeating time integration analyses with smaller steps [31, 48, 49], (b) practical application of numerical integration methods, e.g. Simpson's rule [23, 24] and repeating the integration with smaller steps after the main integration, (c) finite or boundary element analysis with finer spatial meshes, after the first analysis [22, 62].) The above procedure is not reliable (see [48, 63]), and in addition, procedures in need of consecutive analyses are inherently computationally expensive. Therefore, in order to arrive at more efficient approximate computations (consider the second objective implied in the title of this paper), a new procedure, leading to reliable further accuracies, and/or less computational costs, is presented in Section 4.2.2.

4.2.2. The new procedure. Based on the capability, provided in upper-estimating the errors of the results produced by Richardson extrapolation, and considering q, as the rate of the convergence, the existing error-controlling practice can be enhanced to the procedure below:

1. Select a value for the algorithmic parameter $\lambda=\lambda_1$; select a value for the r in Equations (15) and (16), e.g. $r=2$ is appropriate for time integration analyses (see [31]); select the maximum computational error acceptable, namely *Tol*.
2. Compute λ_2, λ_3, and λ_4, considering Equations (15) or (16), and the value set for r.
3. Compute U_1^a and U_2^a (corresponding to λ_1 and λ_2), by implementing the procedure of the computational method; if $|U_1^a - U_2^a|$ is smaller than *Tol*, accept U_2^a, as the result, with sufficient accuracy; stop.
4. Compute U_3^a (corresponding to λ_3), by implementing the procedure of the computational method; if $|U_1^a - U_2^a|$ is about r^q times larger than $|U_2^a - U_3^a|$ and $(|U_2^a - U_3^a|)/(r^q - 1)$ is smaller than *Tol*, accept U_3^a, as the result, with sufficient accuracy; stop.
5. Compute U_4^a, corresponding to λ_4, by implementing the procedure of the computational method.
6. In view of the expected convergence rate q (e.g. see [5, 25, 38, 64]), obtain $U_{R_{1,2}}^a, U_{R_{2,3}}^a, U_{R_{3,4}}^a$, from (see Equation (9))

$$U_{R_{i,i+1}}^a = \frac{\lambda_i^q U_{i+1}^a - \lambda_{i+1}^q U_i^a}{\lambda_i^q - \lambda_{i+1}^q} = \frac{r^q U_{i+1}^a - U_i^a}{r^q - 1}, \quad i=1,2,3,4 \tag{30}$$

DOI: 10.1002/nme

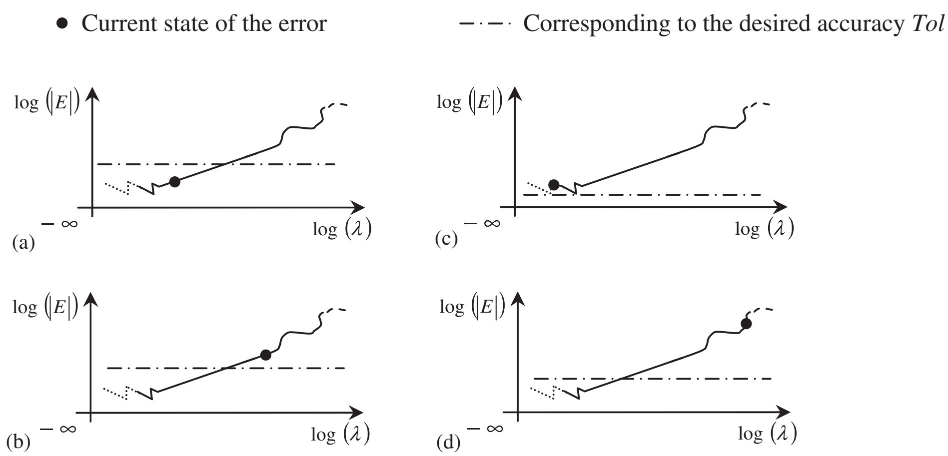

Figure 13. Schematic correspondence between the convergence plots and the cases studied in the proposed procedure: (a) stage 9; (b) stage 10; (c) stage 11; and (d) stage 12.

7. Obtain the values of D_3, D_4, corresponding to the values computed in stage 6, from (see Equation (28))

$$\begin{aligned} D_3 &= U^a_{R_{2,3}} - U^a_{R_{1,2}} \\ D_4 &= U^a_{R_{3,4}} - U^a_{R_{2,3}} \\ D_5 &= U^a_{R_{4,5}} - U^a_{R_{3,4}} \end{aligned} \tag{31}$$

8. Based on the values of U^a_2, U^a_3, U^a_4, determine the maximum of $|E_{R_{3,4}}|$, with attention to (see Equation (18)),

$$|E_{R_{3,4}}|_{\max} = \frac{|-r^q U^a_4 + (r^q+1)U^a_3 - U^a_2|}{(r^q-1)^2} \tag{32}$$

9. If, based on the latest values obtained from Equation (31), the log–log changes of $|D_i|$, with respect to λ_i, are pictorially linear and inclined with an integer-valued slope about and greater than q, and, in view of the *Tol*, set in stage 1, $|E_{R_{3,4}}|_{\max}$ is sufficiently small, we can rely on the sufficiency of the obtained accuracy (see Figure 13(a)); accept $U^a_{R_{3,4}}$, as the approximate result, with sufficient accuracy; stop.
10. If, based on the latest values obtained from Equation (31), the log–log changes of $|D_i|$, with respect λ_i, are pictorially linear and inclined with an integer-valued slope about and greater than q, but, in view of the *Tol*, set in stage 1, $|E_{R_{3,4}}|_{\max}$ is not sufficiently small, the obtained accuracy is not sufficient (see Figure 13(b)); determine λ_5, considering stages 1 and 2; and obtaining $U^a_5, U^a_{R_{4,5}}$, and D_5, respectively, from the computational method,

DOI: 10.1002/nme

Equation (30), and Equation (31), implement

$$\begin{aligned} U_1^a &= U_2^a, \quad U_2^a = U_3^a, \quad U_3^a = U_4^a, \quad U_4^a = U_5^a \\ U_{R_{1,2}}^a &= U_{R_{2,3}}^a, \quad U_{R_{2,3}}^a = U_{R_{3,4}}^a, \quad U_{R_{3,4}}^a = U_{R_{4,5}}^a \\ D_2 &= D_3, \quad D_3 = D_4, \quad D_4 = D_5 \\ \lambda_1 &= \lambda_2, \quad \lambda_2 = \lambda_3, \quad \lambda_3 = \lambda_4, \quad \lambda_4 = \lambda_5 \end{aligned} \tag{33}$$

and return to stage 8.

11. If, based on the latest values obtained from Equation (31), the log–log changes of $|D_i|$, with respect to λ_i, are not pictorially linear, with an integer-valued slope about and greater than q, and in view the already computed values, for the Richardson extrapolation, we are in the round off dominated region of the convergence plot (e.g. when we have already been in the linear section of the plot with insufficient accuracy and now neither the accuracy is sufficient nor the log-log changes of $|D_i|$ with respect to λ_i is linear), the desired accuracy is not obtainable, with the available computational facility, and the values set, in stage 1 (see Figure 13(c)); stop.
12. Considering the most general case, not studied in stages 9–11, i.e. when the log–log changes of $|D_i|$, with respect to λ_i, is not pictorially linear, with an integer-valued slope about and greater than q, and we are not in the round off dominated region of the convergence plot (see Figure 13(d)), compute λ_5, with attention to stages 1 and 2; obtain $U_5^a, U_{R_{4,5}}^a$, and D_5, respectively, from the computational method, Equation (30), and Equation (31); implement Equations (33), and return to stage 8.

(Extending the procedure above to Richardson extrapolations, based on more than two results, is straightforward.) Consequently, the second objective, addressed in Section 1 and the title of this paper, is materialized, and by means of the procedure above, we can implement the upper-bound estimation, proposed in Section 2, in controlling the accuracies, of many approximate computations. Section 5 examines the efficiency of the new procedure.

5. NUMERICAL VALIDATION OF THE PROPOSED PROCEDURE

5.1. Preliminary notes

With the aim of displaying the adequacy of the proposed procedure, this section studies two examples, from different scientific/engineering origins. The main attention in the first example is to the basic concepts, and the second example concentrates on a more complicated problem. Both examples are first studied for accuracies, obtainable after specific numbers of consecutive computations, and are then interpreted from the viewpoint of computational cost. Regarding the computational cost, as implied in the explanations in Sections 2, 3, and 4, the computational costs needed for implementing the Richardson extrapolation and checking the corresponding convergence trends (of D) are in general small. Besides, extending the existing accuracy-controlling practice (see Section 4.2.1), to the procedure, proposed in Section 4.2.2, has small effect on the computational storage (depending on the r in Equation (15), less than 15%). Therefore, for the sake of simplicity, the total time spent, for approximate computations, on one computer, is considered as an appropriate measure for the computational cost; see also [5, 55].

DOI: 10.1002/nme

5.2. *Integration by the trapezoidal rule*

The trapezoidal integration method [21, 23, 24] is implemented in numerical computation of the I, introduced below:

$$I = \int_0^1 \frac{4}{1+x^2}\, dx \tag{34}$$

Obviously, the inverse of the number of divisions throughout the integration interval (herein, equal to the integration step size) is an appropriately set algorithmic parameter. After the first analysis, sequentially, repeating the integration with smaller steps, where the r, in Equation (15), is considered equal to 5, results in Table III. The changes of $|D|$, with respect to the algorithmic parameter, are depicted in Figure 14 ($q=2, q_R=6$). Based on this information, the existing and proposed accuracy-controlling procedures are applied to the computation of I. The computational costs, and accuracies, are reported in Tables IV and V (having π as the exact solution, the errors and the reliabilities are evaluated; the exact values are not used in the procedures), for a range of values

Table III. Results computed for the I in Equation (34) by the Trapezoidal rule [21, 23, 24].

Total number of the previous computations	λ (integration step size)	Computed result	Computational cost (s)
0	1	3.0000000000000	0.023744125
1	0.2	3.1349261138110	0.022736375
2	0.04	3.1413259869313	0.021989875
3	0.008	3.1415819869231	0.022551625
4	0.0016	3.1415922269231	0.025416375
5	0.00032	3.1415926365231	0.029339500
6	0.000064	3.1415926529071	0.091136125
7	0.0000128	3.1415926535625	0.404692290
8	0.00000256	3.1415926535887	1.95360
9	0.000000512	3.1415926535897	9.78267
10	0.0000001024	3.1415926535896	48.5195
11	0.00000002048	3.1415926535909	243.4245
12	0.000000004096	3.1415926535891	1225.1615
13	0.0000000008192	3.1415926535926	6116.2595

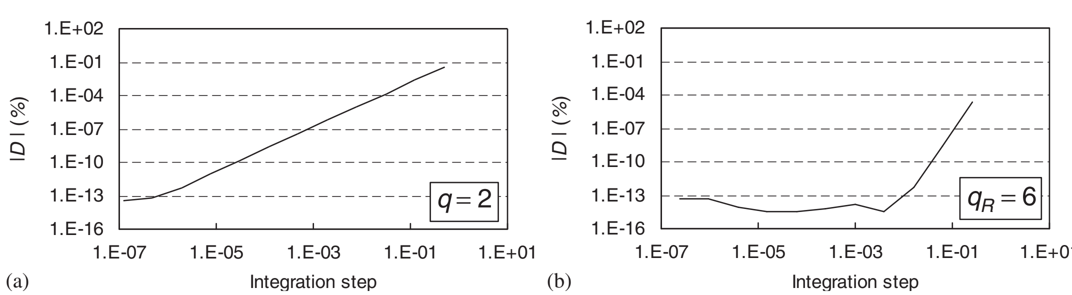

Figure 14. Changes of $|D|$ in the analysis of Equation (34) by the Trapezoidal rule [21, 23, 24], corresponding to the results of: (a) the main computation and (b) the main computation enhanced by the Richardson extrapolation.

Table IV. Accuracies, reliabilities, and computational costs, when implementing the existing practice to the results reported in Table III.

	Total number of the previous computations	Results of the Trapezoidal rule (equal to results of the procedure)	Error (%)		Computational cost (s)
			Estimated	Exact	
	0	3.0000000000000			
	1	3.1349261138110	4.303964716	0.212202552	0.046
	2	3.1413259869313	0.203731582	0.008488263	0.068
	3	3.1415819869231	0.008148760	0.000339531	0.091
	4	3.1415922269231	0.000325949	1.35812E−05	0.116
	5	3.1415926365231	1.30380E−05	5.43250E−07	0.146
	6	3.1415926529071	5.21519E−07	2.17308E−08	0.237
	7	3.1415926535625	2.08620E−08	8.68772E−10	0.642
	8	3.1415926535887	8.33984E−10	3.47882E−11	2.595
	9	3.1415926535897	3.18197E−11	2.96852E−12	12.378
Unreliable ↓	10	3.1415926535896	3.18055E−12	6.14907E−12	60.897
	11	3.1415926535909	4.13755E−11	3.52264E−11	304.322
	12	3.1415926535891	5.72924E−11	2.20660E−11	1529.483
	13	3.1415926535926	1.11418E−10	8.93524E−11	7645.743

Table V. Accuracies, reliabilities, and computational costs, when implementing the proposed procedure to the results reported in Table III.

	Total number of the previous computations	Results of the Trapezoidal rule	Results of the procedure	Error (%)		Computational cost (s)
				Estimated	Exact	
	0	3.0000000000000				
	1	3.1349261138110	3.1349261138110	4.303964716	0.212202552	0.046
	2	3.1413259869313	3.14159264831131	0.13855E−02	1.68019E−07	0.068
	3	3.1415819869231	3.14159265358943	7.00031E−09	1.17186E−11	0.091
	4	3.1415922269231	3.14159265358977	4.52763E−13	2.66454E−14	0.116
Unreliable ↓	5	3.1415926365231	3.14159265358977	1.20000E−15	2.62013E−14	0.146
	6	3.1415926529071	3.14159265358977	4.90826E−16	2.66454E−14	0.237
	7	3.1415926535625	3.14159265358981	5.49726E−14	1.55431E−14	0.642
	8	3.1415926535887	3.14159265358979	2.15964E−14	1.33227E−15	2.595
	9	3.1415926535897	3.14159265358974	6.66297E−14	5.15143E−14	12.378
	10	3.1415926535896	3.14159265358960	1.93312E−13	1.97176E−13	60.897
	11	3.1415926535909	3.14159265359095	1.80168E−12	1.16129E−12	304.322
	12	3.1415926535891	3.14159265358902	2.55846E−12	7.68718E−13	1529.483
	13	3.1415926535926	3.14159265359275	4.93546E−12	2.95275E−12	7645.743

DOI: 10.1002/nme

of the algorithmic parameter, ending with the domination of round off, where the estimations are unreliable (see also Figure 14). In view of these results, the computational costs essential to arrive at some specific accuracies, with the existing and proposed procedures are compared in Table VI. In order to display that the accuracies, provided by the proposed procedure, are reliable, in the linear section of the pseudo (based on $|D|$)-convergence plot, the computed errors are compared with the exact errors in Figure 15, where also the exact and pseudo-convergence plots are depicted. Apparently, the two plots are linear in an almost common interval of the algorithmic parameter, and in that interval, the estimated errors are more than the exact errors, i.e. the proposed procedure is reliable, and can correctly predict this reliability. (The study carried out for this example is repeated, with the Simpson integration rule [21], and conceptually similar results are obtained, not reported here, for the sake of brevity.)

Table VI. Computational costs essential for arriving at specific precisions in the analysis of Equation (34) by the Trapezoidal rule.

Precisions requested (%) (errors acceptable)	20	5	1	1×10^{-1}	1×10^{-3}	1×10^{-5}	1×10^{-8}	1×10^{-12}
Computational cost (s)								
Existing practice	0.046481	0.046481	0.068470	0.091022	0.116438	0.236914	2.595206	>7645.7
Proposed procedure	0.046481	0.046481	0.068470	0.091022	0.091022	0.091022	0.091022	0.116438
Reduction of the computational cost (%)	0	0	0	0	21.83	61.58	96.49	>99.99

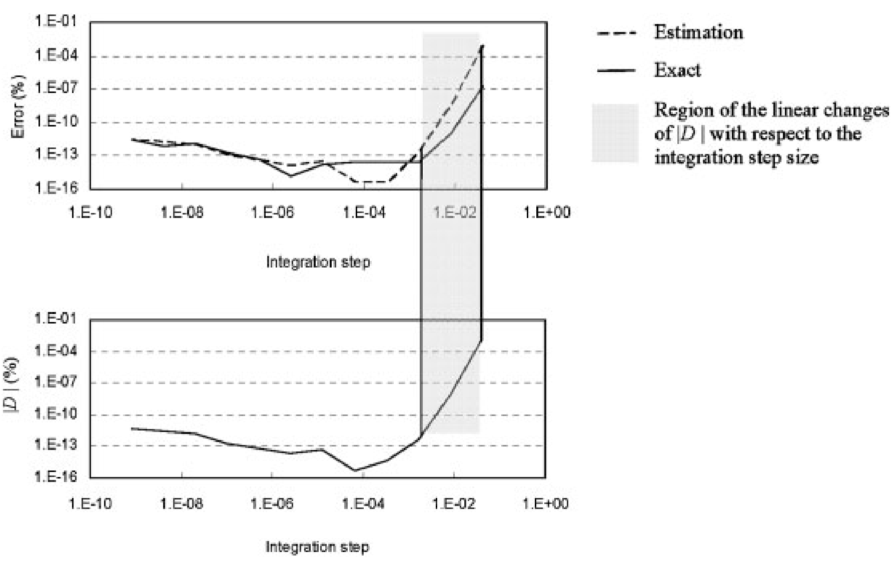

Figure 15. The reliability of the proposed procedure in the linear section of the pseudo-convergence plot, when applied to the Trapezoidal integration of Equation (34).

DOI: 10.1002/nme

5.3. Seismic analysis of a shear building

As implied in Section 3.1, time integration analyses are approximate computations, to which, we can apply the procedure, proposed in Section 4. This section examines the consequence, by studying the time integration analysis of the shear building [29, 31, 32], introduced in Figure 16 and Table VII. Considering the top displacement and base shear, as the responses under consideration, the histories of the exact responses are depicted in Figure 17. The system is analyzed, by the Generalized-α

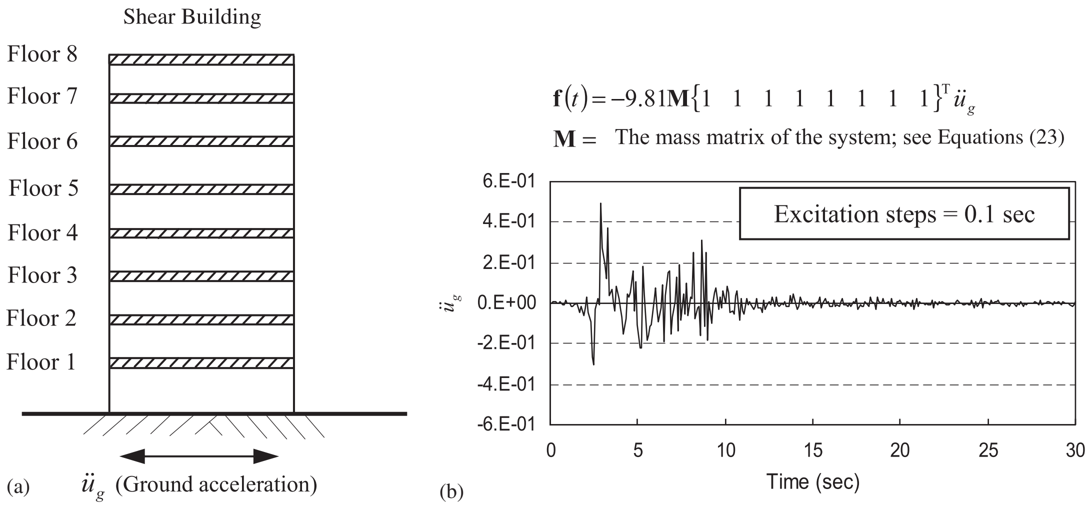

Figure 16. The structural system under consideration as the second example: (a) structural system and (b) excitation.

Table VII. The structural properties for the system schematically introduced in Figure 16.

Floor	1	2	3	4	5	6	7	8
Mass $\times 10^{-3}$ (Kg)	2072	2068	2064	2060	2056	2052	2048	2044
Stiffness $\times 10^{-6}$ (N/m)	86	84	82	70	68	66	64	62
Damping (N s/m)	Negligible (considered zero)							

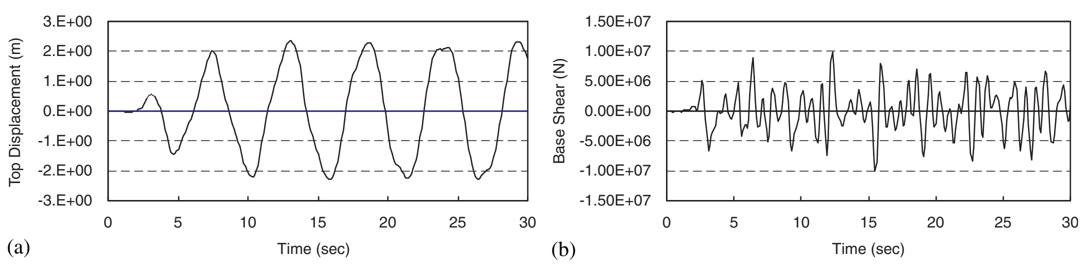

Figure 17. Two exact responses histories for the system defined in Figure 16 and Table VII: (a) top displacement and (b) base shear.

DOI: 10.1002/nme

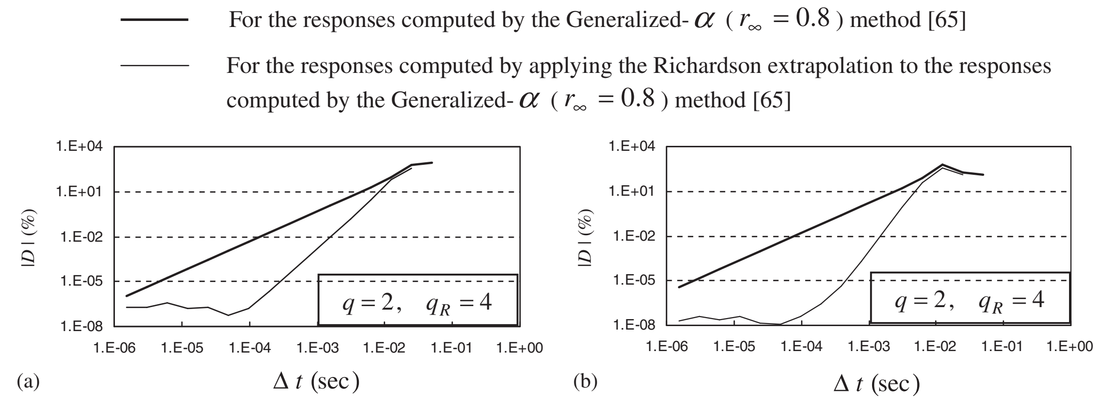

Figure 18. Pseudo-convergence plots for the system defined in Figure 16 and Table VII analyzed by the Generalized-α $(r_\infty = 0.8)$ method [65]: (a) top displacement with the L_2 norm and (b) final base shear.

$(r_\infty = 0.8)$ method [65], with steps, all equal to $\Delta t = 0.1$ s (for the existing comments regarding the size of Δt, see [5, 31, 66, 67]), and the analysis is repeated, several times, while implementing $r = 2$ (see Equation (15)). The changes of responses absolute deviations, computed for the top displacement (with the L_2 norm [60]) and final base shear, along with the corresponding changes of the results, enhanced by the Richardson extrapolation, are reported in Figure 18. Considering these, the existing and proposed accuracy-controlling procedures have resulted in Tables VIII and IX (where, in view of the explanation in Section 5.1, the computational cost is studied by considering the total number of integration steps, N'). In view of the estimated errors, reported in Tables VIII and IX, the computational costs, essential to arrive at specific accuracies, are compared in Figure 19. (The coincidence of the range of integration steps, for which the proposed procedure is reliable, with the range of steps, for which the changes of $|D|$, with respect to step sizes, is linear, in the log–log diagram, is apparent, with a thorough attention to Tables VIII, IX and Figure 18.)

6. CONCLUSION

Considering the everyday need for more accurate and less computationally expensive numerical methods, this paper has first discussed the errors associated with the Richardson extrapolation, resulting in an asymptotic upper-bound estimation for the errors. The upper-bound estimation is then implemented in proposing an error-controlling computational procedure, applicable to general approximate computations, with one algorithmic parameter (see Equation (3)). We summarize the most important achievements as follows:

1. For sufficiently small algorithmic parameters, causing linear convergence trends and not still under the dominating effect of round off, an asymptotic upper-bound estimation is proposed for the errors associated with the Richardson extrapolation.

DOI: 10.1002/nme

Table VIII. Accuracies, reliabilities, and computational costs, when implementing the existing accuracy-controlling practice to the responses computed by the Generalized-α ($r_\infty = 0.8$) method [65] for the problem defined in Figure 16 and Table VII.

	Total number of the previous analyses/ smallest Δt (s)	Errors (%) Estimated for top displacement (with the L_2 norm) / Estimated for final base shear	Errors (%) Exact for top displacement (with the L_2 norm) / Exact for final base shear	Computational cost (N')
	0/0.1E−0			
Unreliable ↑	1/0.5E−1	0.8596E3 0.1384E3	0.3242E3 0.7461E0	900
Unreliable ↑	2/0.25E−1	0.6018E3 0.1932E3	0.9813E2 0.2080E3	2100
	3/0.125E−1	0.8547E2 0.6561E3	0.2510E2 0.8057E2	4500
	4/0.625E−2	0.1952E2 0.7548E2	0.6294E1 0.2075E2	9300
	5/0.3125E−2	0.4763E1 0.1641E2	0.1575E1 0.5198E1	18 900
	6/0.15625E−2	0.1184E1 0.3950E1	0.3937E0 0.1300E1	38 100
	7/0.78125E−3	0.2955E0 0.9779E0	0.9844E-1 0.3249E0	76 500
	8/0.390625E−3	0.7384E−1 0.2439E0	0.2461E−1 0.8120E−1	153 300
	9/0.1953125E−3	0.1846E−1 0.6093E−1	0.6152E−2 0.2030E−1	306 900
	10/0.9765625E−4	0.4614E−2 0.1523E−1	0.1538E−2 0.5080E−2	614 100
	11/0.48828125E−4	0.1154E−2 0.3808E−2	0.3845E−3 0.1270E−2	1 228 500
	12/0.24414063E−4	0.2884E−3 0.9519E−3	0.9609E−4 0.3170E−3	2 457 300
	13/0.12207031E−4	0.7207E−4 0.2380E−3	0.2402E−4 0.7930E−4	4 914 900
	14/0.61035156E−5	0.1789E−4 0.5951E−4	0.6134E−5 0.1983E−4	9 830 100

DOI: 10.1002/nme

Table IX. Accuracies, reliabilities, and computational costs, when implementing the proposed accuracy-controlling procedure to the responses computed by the Generalized-α ($r_\infty = 0.8$) method [65] for the problem defined in Figure 16 and Table VII.

	Total number of the previous analyses/ smallest Δt (s)	Errors (%): Estimated for top displacement (with the L_2 norm) / Estimated for final base shear	Errors (%): Exact for top displacement (with the L_2 norm) / Exact for final base shear	Computational cost (N')
	0/ 0.1E0			
Unreliable ↑	1/0.5E−1			
Unreliable ↑	2/0.25E−1	0.1145E3 0.4351E2	0.6248E2 0.2776E3	2100
	3/0.125E−1	0.2035E2 0.1290E3	0.2907E1 0.3808E2	4500
	4/0.625E−2	0.9204E0 0.1252E2	0.1527E0 0.8137E0	9300
	5/0.3125E−2	0.4784E−1 0.2669E0	0.9250E−2 0.1300E−1	18 900
	6/0.15625E−2	0.2889E−2 0.4248E−2	0.5810E−3 0.2090E−3	38 100
	7/0.78125E−3	0.1813E−3 0.6799E−4	0.3730E−4 0.4760E−5	76 500
	8/0.390625E−3	0.1161E−4 0.1486E−5	0.2470E−5 0.3050E−6	153 300
	9/0.1953125E−3	0.7643E−6 0.9256E−7	0.1950E−6 0.2770E−7	306 900
Unreliable ↓	⩾10/ ⩽0.976563E−4	Round off dominates the error (see Figure 18)		⩾614 100

2. Compared with the existing error estimation (see [20]), the proposed estimation is not only independent of the results (those obtained from Richardson extrapolation) rate of convergence q_R, but also is more reliable.
3. Based on the proposed upper-bound estimation, the existing accuracy-controlling practice is enhanced to a new accuracy-controlling procedure. The new procedure can decrease the computational costs essential for arriving at requested accuracies (and evaluates the reliabilities of the obtained accuracies), and is efficient, specifically, when higher accuracies

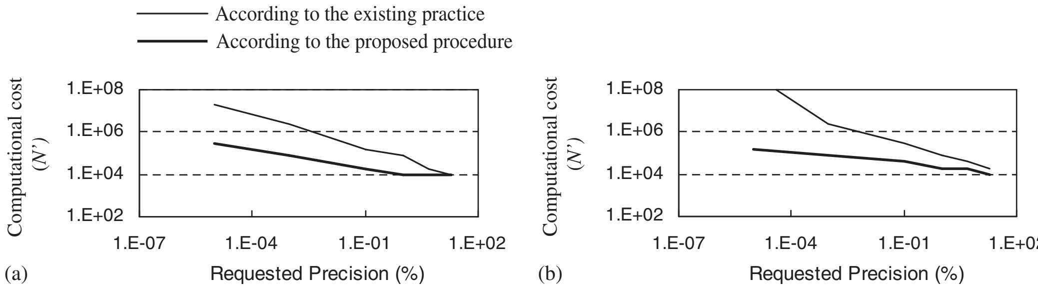

Figure 19. The relation between the precision provided and the computational cost spent, in time integration of the problem in Figure 16 and Table VII, with the Generalized-α ($r_\infty = 0.8$) method [65]: (a) top displacement with the L_2 norm and (b) final base shear.

(corresponding to the lower parts of the linear sections in the pseudo-convergence plots) are to be provided.

4. The proposed accuracy-controlling procedure is theoretically set for arbitrary approximate computations, and, examined, by considering the Trapezoidal integration rule [21, 23, 24], and direct time integration analysis, by the Generalized-α ($r_\infty = 0.8$) method [65].

ACKNOWLEDGEMENTS

The first author is very thankful to Miss Sharis Minasian and Dr Amir Kayvan Ghorbani-Tanha for their kind assistance in finding some essential documents from the literature. The reviewers' kindness in reviewing this long paper is sincerely appreciated. Finally, the first author appreciates the comments of Prof. F. Arbabi on the English of the paper.

REFERENCES

1. Golub GH, Ortega JM. *Scientific Computing and Differential Equations*. Academic Press: New York, U.S.A., 1992.
2. Quateroni A, Sacco R, Saleri F. *Numerical Mathematics*. Springer: New York, 2000.
3. Zhou X, Tamma KK, Sha D. Design spaces, measures and metrics for evaluating quality of time operators and consequences leading to improved algorithms by design—illustration to structural dynamics. *International Journal for Numerical Methods in Engineering* 2005; **64**:1841–1870.
4. Fung TC, Chen ZL. Krylov precise time-step integration method. *International Journal for Numerical Methods in Engineering* 2006; **68**:1115–1136.
5. Soroushian A. A technique for time integration with steps larger than the excitation steps. *Communications in Numerical Methods in Engineering* 2008; **24**:2087–2111.
6. Henrici P. *Discrete Variable Methods in Ordinary Differential Equations*. Wiley: New York, 1962.
7. Strikwerda JC. *Finite Difference Schemes and Partial Differential Equations*. Wadsworth & Books/Cole: U.S.A., 1989.
8. Gear CW. *Numerical Initial Value Problems in Ordinary Differential Equations*. Prentice-Hall: Englewood Cliffs, 1971.
9. Richardson LF, Gaunt JA. The deferred approach to the limit. *Philosophical Transactions of the Royal Society of London* 1927; **226**:299–361.
10. Richardson LF. The approximate arithmetical solution by finite differences of physical problems including differential equations, with an application to the stresses in a masonry dam. *Philosophical Transactions of the Royal Society of London* 1910; **210**:307–357.

DOI: 10.1002/nme

11. Soroushian A, Wriggers P, Farjoodi J. On practical integration of semi-discretized nonlinear equations of motion. Part 1: reasons for probable instability and improper convergence. *Journal of Sound and Vibration* 2005; **284**:705–731.
12. Brezenski C, Redivo Zagalia M. *Extrapolation Methods*: *Theory and Practice*. North-Holland: Amsterdam, 1991.
13. Bismarck-Nasr MN, De Oliveira AM. On enhancement of accuracy in direct time integration dynamic response problems. *Earthquake Engineering and Structural Dynamics* 1991; **20**:699–703.
14. Orduña-Bustamante F. Accurate finite difference calculation of the natural frequencies of Euler–Bernoulli beams using Richardson extrapolation. *Journal of Sound and Vibration* 1993; **162**:361–367.
15. Lima PM. Richardson extrapolation in boundary value problems for differential equations with nonregular right-hand side. *Journal of Computational and Applied Mathematics* 1994; **50**:385–400.
16. Kpegba KW, Ottavy N, Souchet R. Improvement of stress intensity factors computed from path-independent integrals by Richardson's extrapolation. *Communications in Numerical Methods in Engineering* 1998; **14**:289–304.
17. Richards SA. Completed Richardson extrapolation in space and time. *Communications in Numerical Methods in Engineering* 1997; **13**:573–582.
18. Sidi A. New convergence results on the generalized Richardson extrapolation process $\mathrm{GREP}^{(1)}$ for logarithmic sequences. *Mathematics of Computation* 2002; **71**:1569–1596.
19. Celik IB, Li J, Hu G, Shaffer C. Limitations of Richardson extrapolation and some possible remedies. *Journal of Fluids Engineering—Transactions of the ASME* 2005; **127**:795–805.
20. Ström T. Practical error estimates for repeated Richardson extrapolation schemes. *BIT Numerical Mathematics* 1973; **13**:196–205.
21. Ralston A, Rabinowitz P. *A First Course in Numerical Analysis*. McGraw-Hill: New York, 1983.
22. Cook RD, Malkus DS, Plesha ME, Witt RJ. *Concepts and Applications of Finite Element Analysis*. Wiley-Interscience: U.S.A., 2002.
23. Spiegel MR. *Advanced Mathematics for Engineers and Scientists*. McGraw-Hill: U.S.A., 1971.
24. Apostol TM. *Calculus*, *Vol. I*. Wiley: New York, 1967.
25. Wood WL. *Practical Time Stepping Schemes*. Oxford: U.S.A., 1990.
26. Brown JW, Churchill R. *Fourier Series and Boundary Value Problems*. McGraw-Hill: Singapore, 1993.
27. Soroushian A, Wriggers P, Farjoodi J. A statement for the convergence of approximate responses and its application in structural dynamics. *The Proceedings of the 2nd International Conference* '*From Scientific Computing to Computational Engineering*', *2nd IC-SCCE*, Athens, July 2006.
28. Chung J, Hulbert GM. A family of single-step Houbolt time integration algorithms for structural dynamics. *Computer Methods in Applied Mechanics and Engineering* 1994; **118**:1–11.
29. Chopra AK. *Dynamics of Structures*: *Theory and Application to Earthquake Engineering*. Prentice-Hall: U.S.A., 1995.
30. Havskov J, Alguacil G. *Instrumentation in Earthquake Seismology* (*Modern Approaches in Geophysics*). Springer: Netherlands, 2005.
31. Clough RW, Penzien J. *Dynamics of Structures*. McGraw-Hill: New York, 1993.
32. Gupta AK. *Response Spectrum Method*: *In Seismic Analysis and Design of Structures*. CRC: U.S.A., 1992.
33. Houbolt JC. A recurrence matrix solution for the dynamic response of elastic aircraft. *Journal of the Aeronautical Sciences* 1950; **17**:540–550.
34. Newmark NM. A method of computation for structural dynamics. *Journal of Engineering Mechanics* (ASCE) 1959; **85**:67–94.
35. Bathe KJ, Wilson EL. Stability and accuracy analysis of direct integration methods. *Earthquake Engineering and Structural Dynamics* 1973; **1**:283–291.
36. Park KC. An improved stiffly stable method for direct integration of nonlinear structural dynamics equations. *Journal of Applied Mechanics* 1975; **42**:464–470.
37. Hilber HM, Hughes TJR, Taylor RL. Improved numerical dissipation for time integration algorithms in structural dynamics. *Earthquake Engineering and Structural Dynamics* 1977; **5**:283–292.
38. Penry SN, Wood WL. Comparison of some single-step methods for the numerical solution of the structural dynamic equation. *International Journal of Numerical Methods in Engineering* 1985; **21**:1941–1955.
39. Hoff C, Pahl PJ. Development of an implicit method with numerical dissipation for time integration algorithms in structural dynamics. *Computer Methods in Applied mechanics and Engineering* 1987; **67**:367–385.
40. Chung J, Lee JM. A new family of explicit time integration methods for linear and non-linear structural dynamics. *International Journal for Numerical Methods in Engineering* 1994; **37**:3961–3976.
41. Smolinski P, Wu Y-S. An implicit multi-time step integration method for structural dynamics problems. *Computational Mechanics* 1998; **22**:337–343.

42. Haitian Y, Qing G, Xinglin G, Chengwei W. A new algorithm of time stepping in the non-linear dynamic analysis. *Communications in Numerical Methods in Engineering* 2001; **17**:597–611.
43. Bui QV. Modifed Newmark family for non-linear dynamic analysis. *International Journal for Numerical Methods in Engineering* 2004; **61**:1390–1420.
44. Hauret P, Le Tallec P. Energy-controlling time integration methods for nonlinear elastodynamics and low velocity impact. *Computer Methods in Applied Mechanics and Engineering* 2006; **195**:4890–4916.
45. Chang S-Y. Investigation of WBZ-α method for solving nonlinear systems. *Engineering Computations* 2007; **24**:384–406.
46. Soroushian A, Farjoodi J. A unified starting procedure for the Houbolt method. *Communications in Numerical Methods in Engineering* 2008; **24**:1–13.
47. Zeng LF, Wiberg N-E, Li XD. A posteriori local error estimation and adaptive time-stepping for Newmark integration in dynamic analysis. *Earthquake Engineering and Structural Dynamics* 1992; **21**:555–571.
48. Soroushian A, Farjoodi J. More reliable responses for time integration analyses. *Structural Engineering and Mechanics* 2003; **16**:219–240.
49. Ruge P. A priori local error estimation with adaptive time-stepping. *Communications in Numerical Methods in Engineering* 1999; **15**:479–491.
50. Henrych J. *Finite Models and Methods of Dynamics in Structures*. Elsevier: Netherlands, 1990.
51. Argyris J, Mlejnek JP. *Dynamics of Structures*. Elsevier: Netherlands, 1991.
52. Soroushian A. New methods to maintain responses' convergence and control responses' errors in the analysis of nonlinear dynamic models of structural systems. *Ph.D. Thesis*, University of Tehran, 2003 (in Persian).
53. Wriggers P. *Computational Contact Mechanics*. Wiley: U.S.A., 2002.
54. Hughes TJR, Pister KS, Taylor RL. Implicit–explicit finite elements in nonlinear transient analysis. *Computer Methods in Applied Mechanics and Engineering* 1979; **17/18**:159–182.
55. Zhou KK, Tamma KK. A new unified theory underlying time dependent first-order systems: a prelude to algorithms by design. *International Journal for Numerical Methods in Engineering* 2004; **60**:1699–1740.
56. Hairer E, Wanner G. *Solving Ordinary Differential Equations II*: *Stiff and Differential-Algebraic Problems*. Springer: U.S.A., 1996.
57. Katona MG, Zienkiewicz OC. A unified set of single step algorithms part 3: the beta-m method, a generalization of the Newmark scheme. *International Journal for Numerical Methods in Engineering* 1985; **21**:1345–1359.
58. Clough RW. *Numerical Integration of Equations of Motion*, Lectures on Finite Element Methods in Continuum Mechanics. University of Alabama: Huntsville, 1973; 525–533.
59. Hughes TJR. *The Finite Element Method*: *Linear Static and Dynamic Finite Element Analysis*. Prentice-Hall: U.S.A., 1987.
60. Noble B, Daniel JW. *Applied Linear Algebra*. Prentice-Hall: Englewood Cliffs, NJ, 1977.
61. Lambert JD. *Computational Methods in Ordinary Differential Equations*. Wiley: U.K., 1973.
62. Zienkiewicz OC, Taylor RL. *Finite Element Method*. McGraw-Hill: U.S.A., 1991.
63. Soroushian A. On analyses conventional error control for buildings structural systems subjected to earthquake-included poundings. *The Proceedings of the 5th International Conference on Seismology and Earthquake Engineering*, *SEE5*, Tehran, May 2007.
64. Belytschko T, Hughes TJR. *Computational Methods for Transient Analysis*. Elsevier: Netherlands, 1983.
65. Chung J, Hulbert GM. A time integration algorithm for structural dynamics with improved numerical dissipation: the generalized-α method. *Journal of Applied Mechanics* (ASME) 1993; **60**:371–375.
66. Bathe KJ. *Finite Element Procedures*. Prentice-Hall: Englewood Cliffs, NJ, 1996.
67. McNamara JF. Solution schemes for problems of nonlinear structural dynamics. *Journal of Pressure Vessels* 1974; **96**:147–155.