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Enhanced composite time integration schemes for conservative nonlinear systems

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ABSTRACT

In this paper, two different composite time schemes are presented, and their numerical performances for conservative nonlinear systems are investigated. In the composite schemes, collocation and weighting parameters included in the time approximations are optimally determined by using the total energy of simple conservative nonlinear dynamic problems. Due to the unconventional optimization process of algorithmic parameters, enhanced total energy conserving capabilities are achieved without additional computational procedures. Linear and nonlinear benchmark problems are numerically solved by using the composite schemes, and numerical results are investigated to verify the enhanced total energy conserving capability of the composite schemes.

1. INTRODUCTION

Direct time integration schemes play critical roles in transient analyses of hyperbolic time-dependent problems. For this reason, numerous time integration methods have been developed based on various numerical techniques and theories to increase efficiencies and accuracies of transient analyses of complex engineering problems (Alamatian 2013, Kwon 2008, Rostami 2021). Recently, several implicit time schemes were developed based on the strategy of subdividing a complete time step into two sub-steps where different time schemes are employed. These schemes are often called the *composite scheme* (Baig 2005, Bathe 2005).

We can categorize two-stage implicit schemes into two different types depending on their computational structures. Both types have two sub-steps, but only one type requires the computation of the initial acceleration vector. If the initial acceleration vector

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is included in time approximations, it should be computed by using the equilibrium equation at $t = 0$, which also accompanies the factorization of the mass matrix. Many two-stage implicit time schemes, such as the Bathe method (Bathe 2005) and the Kim and Reddy method (Kim 2017), fall into this category. Interestingly, it can easily be shown that some of the recently developed two-stage implicit schemes (Kim 2017, Noh 2019) in this category are mathematically identical although they are developed based on different theories and techniques (Kim 2020).

In another type, on the other hand, the initial acceleration vector and the acceleration vector of the previous time step are not included in time approximations, and the computation of the initial acceleration vector at $t = 0$ is not required either. Sometimes, this type is called the *self-starting composite scheme* (Li 2019) whose computational structures are basically the same as those of the diagonally implicit two-stage Runge-Kutta method. Here, the meaning of 'self-starting' is that the scheme can be started by using pure mathematical initial conditions (i.e., the initial displacement and velocity vectors) without additional processes such as the computation of the initial acceleration vector or the integral of the external force vector. Advantages of this type have been explained in detail by Kim (2020).

In linear analyses, the absence of the initial acceleration vector (and the acceleration vector of the previous time step) in composite schemes can increase the computational efficiency because the factorization of the mass matrix can completely be omitted. In this case, two-stage schemes without the initial acceleration vector can achieve improved efficiency in linear analyses if effective coefficient matrices of the first and second sub-step are constructed to be identical to each other. If these two conditions (the absence of the initial acceleration vector and an identical effective coefficient matrix) are fully satisfied, only one factorization is required in linear analyses, which can reduce the computation time and effort. In this paper, we present a novel composite time scheme that can achieve the aforementioned computational advantages and improved accuracy simultaneously through unconventional parameter optimizations.

2. GENERAL FORMS WITHOUT INITIAL ACCELERATION VECTOR

According to Newton's second law of motion, various time dependent engineering problems are often described in the form of

$$\mathbf{M}\ddot{\mathbf{u}}(t) = \mathbf{f}(\mathbf{u}(t), \dot{\mathbf{u}}(t), t) \tag{1}$$

where t is the time, $\mathbf{M}$ is the mass matrix, $\mathbf{f}$ is the force vector, $\mathbf{u}$ is the displacement vector, and the single and double dots over the displacement vector denote the velocity and acceleration vectors, respectively. In linear structural dynamics, $\mathbf{f}$ is given by

$$\mathbf{f}(\mathbf{u}(t), \dot{\mathbf{u}}(t), t) = \mathbf{q}(t) - \mathbf{C}\dot{\mathbf{u}}(t) - \mathbf{K}\mathbf{u}(t) \tag{2}$$

Direct time integration schemes discretize Eq. (1) for the time interval $t_s \le t \le t_s + \Delta t$, where t_s is the starting point of the time interval, and Δt is the size of the time interval. It is noted that Δt is also called the time step. In the composite schemes without the initial acceleration vector, the equilibrium equation, velocity and displacement vectors of the first and second sub-steps are given, respectively, by

$$\mathbf{M}\,\ddot{\mathbf{u}}_{t_s+\tau_1\Delta t} = \mathbf{f}\left(\mathbf{u}_{t_s+\tau_1\Delta t},\ \dot{\mathbf{u}}_{t_s+\tau_1\Delta t},\ t_s+\tau_1\Delta t\right) \tag{3}$$

$$\dot{\mathbf{u}}_{t_s+\tau_1\Delta t} = \dot{\mathbf{u}}_{t_s} + (\tau_1\Delta t)\,\beta_{11}\,\ddot{\mathbf{u}}_{t_s+\tau_1\Delta t} \tag{4}$$

$$\mathbf{u}_{t_s+\tau_1\Delta t} = \mathbf{u}_{t_s} + (\tau_1\Delta t)\,\beta_{11}\,\dot{\mathbf{u}}_{t_s+\tau_1\Delta t} \tag{5}$$

$$\mathbf{M}\,\ddot{\mathbf{u}}_{t_s+\tau_2\Delta t} = \mathbf{f}\left(\mathbf{u}_{t_s+\tau_2\Delta t},\ \dot{\mathbf{u}}_{t_s+\tau_2\Delta t},\ t_s+\tau_2\Delta t\right) \tag{6}$$

$$\dot{\mathbf{u}}_{t_s+\tau_2\Delta t} = \dot{\mathbf{u}}_{t_s} + (\tau_2\Delta t)\left(\beta_{21}\,\ddot{\mathbf{u}}_{t_s+\tau_1\Delta t} + \beta_{22}\,\ddot{\mathbf{u}}_{t_s+\tau_2\Delta t}\right) \tag{7}$$

$$\mathbf{u}_{t_s+\tau_2\Delta t} = \mathbf{u}_{t_s} + (\tau_2\Delta t)\left(\beta_{21}\,\dot{\mathbf{u}}_{t_s+\tau_1\Delta t} + \beta_{22}\,\dot{\mathbf{u}}_{t_s+\tau_2\Delta t}\right) \tag{8}$$

$$\dot{\mathbf{u}}_{t_s+\Delta t} = \dot{\mathbf{u}}_{t_s} + \Delta t\left(\beta_{31}\,\ddot{\mathbf{u}}_{t_s+\tau_1\Delta t} + \beta_{32}\,\ddot{\mathbf{u}}_{t_s+\tau_2\Delta t}\right) \tag{9}$$

$$\mathbf{u}_{t_s+\Delta t} = \mathbf{u}_{t_s} + \Delta t\left(\beta_{31}\,\dot{\mathbf{u}}_{t_s+\tau_1\Delta t} + \beta_{32}\,\dot{\mathbf{u}}_{t_s+\tau_2\Delta t}\right) \tag{10}$$

where the subscript $t_s + \tau_i\Delta t$ denotes the time point where the variable belongs, τ_1 and τ_2 are the collocation parameters that determine the location of the time point, and β_{11}, β_{21}, β_{22}, β_{31} and β_{32} are the weighting parameters.

3. UNCONVENTIONAL OPTIMIZATION OF ALGORITHMIC PARAMETERS

The algorithmic parameters in Eqs. (3)-(10) can be optimized differently for different purposes. Traditionally, the linear single degree of freedom (SDOF) problem and its exact solution were used to determine the algorithmic parameters. In traditional optimizations, the parameters of composite schemes are determined to achieve second-order accuracy, unconditional stability, and controllable numerical dissipation. As a result, most of the existing two-stage time implicit schemes have similar spectral characteristics. For example, the Kim and Reddy method (Kim 2017) and the Noh and Bathe method (Noh 2019) are spectrally identical, although they are represented by using different mathematical expressions. Hence, numerical solutions obtained from these two implicit schemes are completely the same. For details, see Kim (2020).

3.1 Enhance composite scheme with third-order energy conserving capability

Unlike traditional techniques for parameter optimizations, different conditions may be employed for different purposes. For example, additional mathematical conditions can also be obtained from the total energy of conservative nonlinear problems. In this study, additional conditions are used to enhance the total-energy conserving capability and computational efficiency of the newly proposed two-stage implicit time scheme.

For linear analyses, having an identical effective coefficient matrix in the first and second sub-steps of composite schemes can dramatically reduce overall computational time, because only one matrix factorization is required throughout the entire procedure. To have an identical effective coefficient matrix in the first and second sub-steps in linear analyses, we determine τ_1 as

$$\tau_1 = \frac{\tau_2\,\beta_{22}}{\beta_{11}} \tag{11}$$

The use of Eq. (11) makes the effective coefficient matrices of the first and second sub-steps exactly the same in linear analyses. Like the case of traditional parameter optimizations, β_{11}, β_{22}, β_{32}, and β_{31} can also be determined to ensure second-order accuracy as follows:

$$\beta_{11} = 1,\ \beta_{22} = 1-\beta_{21},\ \beta_{32} = 1-\beta_{31} \tag{12}$$

$$\beta_{31} = \frac{2\ \tau_2 - 1}{2\ \tau_2\ \beta_{21}} \tag{13}$$

At this point, β_{21} and τ_2 are undetermined parameters. Now, the total energy of conservative nonlinear systems may be used to determine β_{21}. To be specific, the total energy of the simple nonlinear pendulum or simple spring-mass system with hardening (or softening) nonlinear spring can be computed exactly by using the initial conditions. In conservative nonlinear problems, the total energy at arbitrary time points should be the same as the initial total energy. Hence, it is possible to state the exact total energy at arbitrary time points in terms of the initial conditions. Then, the difference between the exact total energy and the numerically computed total energy can be manipulated to determine β_{21}. In our case, the Taylor series of the difference of these two total energies can be expressed in the form of

$$|E_{\Delta t} - E_0| = O\left(\Delta t^{(h+1)}\right) \tag{14}$$

where $E_{\Delta t}$ is the numerically computed total energy by using the time scheme at $t = \Delta t$, E_0 is exactly computed total energy with the initial conditions, and h is the order of the convergence rate for the total energy of the nonlinear problem. It is noted that all existing composite scheme can give only second-order convergence rate (i.e., the case $h = 2$) for the total energy of conservative nonlinear problems. To have one higher-order convergence rate (i.e., the case $h = 3$), on the other hand, β_{21} can be determined as

$$\beta_{21} = \frac{2\left(3\ \tau_2{}^2 - 3\ \tau_2 + 1\right)}{3\ \tau_2\left(2\ \tau_2 - 1\right)} \tag{15}$$

The last undetermined parameter τ_2 is stated in terms of the ultimate spectral radius ρ_∞ as

$$\tau_2 = \frac{2\ \sqrt{2\ \rho_\infty + 2} + 1}{3\ \sqrt{2\ \rho_\infty + 2}} \tag{16}$$

where $\rho_\infty \in [0, 1]$. In this study, we will investigate the case of $\rho_\infty = 1$ and 0. By determining β_{21} and τ_2 according to Eqs. (15)-(16), the effective coefficient matrices of the first and second sub-steps become identical to each other in linear analyses, and the scheme can give one higher-order total energy convergence for conservative nonlinear problems. It should be emphasized that these improvements are purely due to the optimized set of algorithmic parameters, which does not accompany additional computational effort when compare with the existing composite schemes. It is noted that the two-stage scheme with the algorithmic parameters given in Eqs. (11)-(16) is unconditionally stable for linear problems.

3.2 Enhance composite scheme with fourth-order energy conserving capability

In nonlinear analyses, the effective coefficient system matrices of the first and second sub-steps cannot be constructed identically even if the condition given in Eq. (11) is used. Considering this particular aspect of nonlinear analyses, we may determine all algorithmic parameters to secure fourth-order total energy convergence rate (i.e., the case $h = 4$). In this case, the algorithmic parameters are determined as

$$\beta_{11} = 1, \quad \beta_{21} = \frac{3}{2} - \frac{\sqrt{3}}{2}, \quad \beta_{21} = -\frac{1}{2} + \frac{\sqrt{3}}{2}, \quad \beta_{31} = \beta_{32} = \frac{1}{2} \tag{17}$$

and

$$\tau_1 = \frac{1}{2} - \frac{\sqrt{3}}{6}, \quad \tau_2 = \frac{1}{2} + \frac{\sqrt{3}}{6} \tag{18}$$

It is noted that the second case cannot adjust the level of numerical dissipation in the high-frequency range. It is also noted that the second case has been developed by using a different approach by Kim (2021). Interestingly, the algorithmic parameters presented in Eqs. (17)-(18) can be determined solely based on the total energy convergence condition of conservative simple nonlinear problems without considering the traditional accuracy and stability conditions derived from the linear single-degree-of-freedom problem.

3.3 Major operations in linear analyses

The numbers of major matrix and vector operations required in linear analyses are summarized in Table 1 by assuming that the existing schemes have identical effective coefficient matrices for the first and second sub-steps. As shown in Table 1, the existing composite schemes require two factorizations of system matrices (i.e., the effective coefficient and mass matrices) and the numbers of other operations are the same for all cases. It is noted that the second case (the scheme with fourth-order energy conserving capability) also requires two factorizations because two different effective coefficient matrices should be factorized.

Operations	Existing	Proposed (1^{st})	Proposed (2^{nd})
$\mathbf{A}^{-1}$ (inverse)	2	1	2
$\mathbf{Ab}$ (matrix times vector)	6	6	6
$\mathbf{A}_1 + \mathbf{A}_2$ (matrix addition)	2	2	2
$\mathbf{b}_1 + \mathbf{b}_2$ (vector addition)	8	8	8

Table 1 Comparison of major matrix and vector operations in composite schemes.

We also note that the discussion regarding the improved efficiency of the scheme is limited to only linear analyses. In nonlinear analyses, it is impossible to construct the effective coefficient matrices of the first and second sub-steps to be the same, and several times of reconstructions and factorizations of effective coefficient matrices are also required in each time step. Hence, factorization of the mass matrix at $t = 0$ is not a significant factor in nonlinear analyses.

4. NUMERICAL VERIFICATIONS

4.1 Damped and forced two degree of freedom problem

Simple linear problems are frequently used to test time schemes because numerical solutions can directly be compared with exact solutions. Here, we solve the two degree of freedom problem given by

$$\mathbf{M}\ddot{\mathbf{u}}(t) + \mathbf{C}\dot{\mathbf{u}}(t) + \mathbf{K}\mathbf{u}(t) = \mathbf{q}(t), \quad \dot{\mathbf{u}}(t) = \mathbf{0}, \quad \mathbf{u}(t) = \mathbf{0} \tag{19}$$

where

$$\mathbf{M} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \mathbf{C} = \frac{1}{25}\begin{bmatrix} 14 & -2 \\ -2 & 6 \end{bmatrix}, \quad \mathbf{K} = \begin{bmatrix} 6 & -2 \\ -2 & 2 \end{bmatrix}, \quad \mathbf{u}(\mathbf{t}) = \begin{Bmatrix} u_1(t) \\ u_2(t) \end{Bmatrix}$$

$$\mathbf{q}(t) = \begin{Bmatrix} 12\sin(2\pi t) + 4\cos(t) + 20\,\mathrm{e}^{-t} \\ 0 \end{Bmatrix} \tag{20}$$

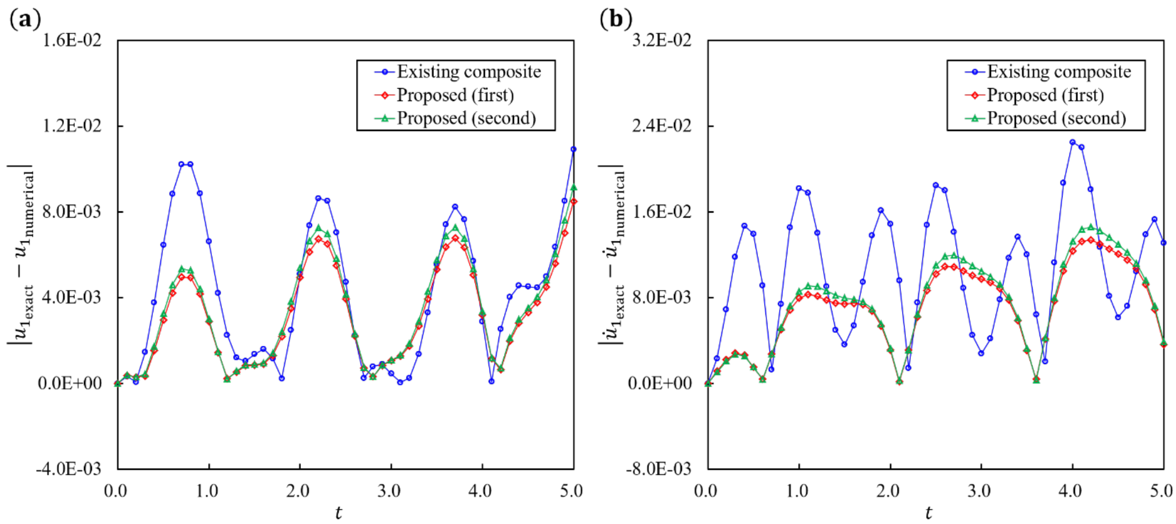

Fig. 1 Errors with $\Delta t = 0.1$. (a) Displacement. (b) Velocity.

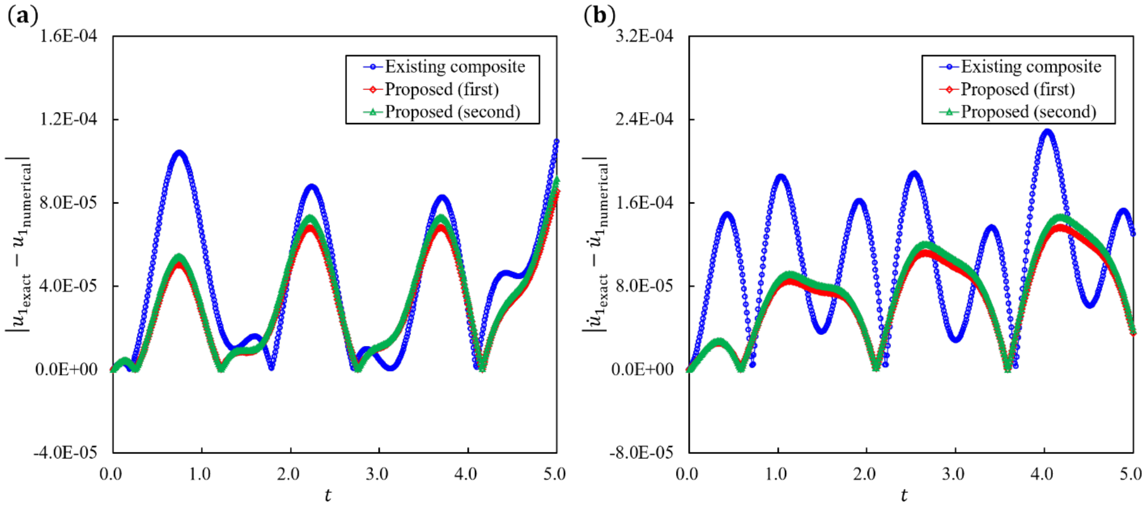

Fig. 2 Errors with $\Delta t = 0.01$. (a) Displacement. (b) Velocity.

In our numerical test, we compare numerical solutions obtained from various two-stage implicit schemes with $\Delta t = 0.1$ and 0.01. It is noted that the numerical solutions obtained from the Newmark scheme (i.e., the trapezoidal rule) with a half time step are the same as those obtained from the non-dissipative cases of the existing composite schemes such as the collocation composite scheme (Kim 2017), the generalized composite time integration algorithm (Kim 2018), and the ρ_∞-Bathe methods (Noh 2019). As shown in Figs. 1 and 2, errors of the newly proposed scheme is slightly smaller than those of the non-dissipative case of the existing composite scheme.

4.2 Simple nonlinear pendulum

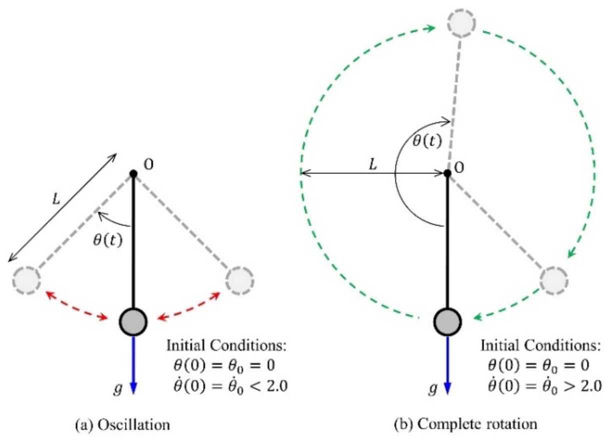

Fig. 3. Description of the simple nonlinear pendulum problem (Kim 2017, 2019)

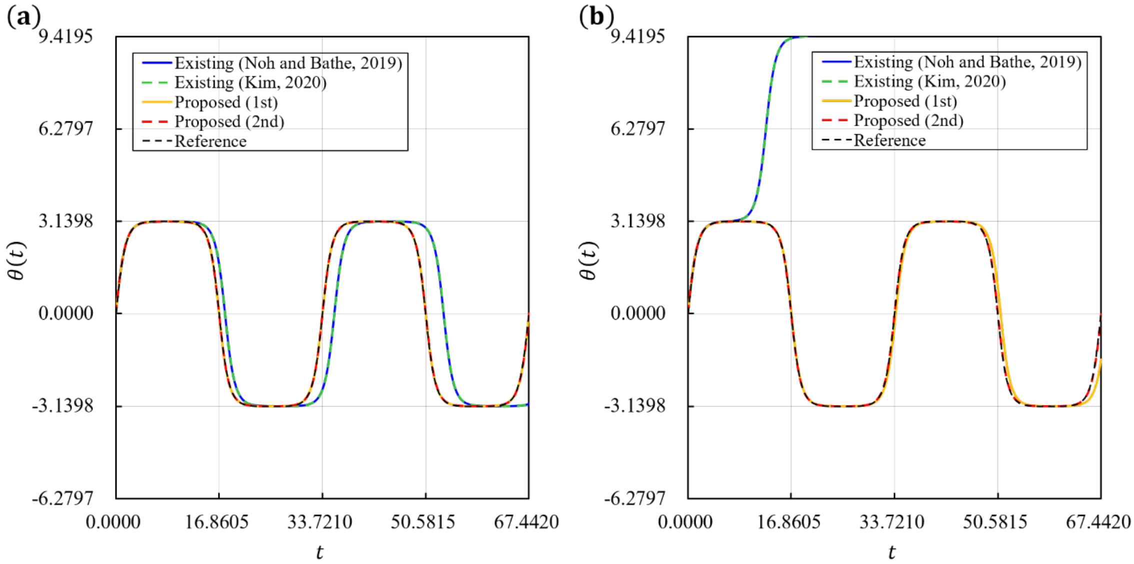

Fig. 4 Case of $\dot{\theta}_0 = 1.999999238456499$ (a) $\Delta t = T/10000$. (b) $\Delta t = T/1000$

Here, the simple nonlinear pendulum problem and a special set of initial conditions is used for the test of the time scheme. The governing equation is given by

$$\ddot{\theta}(t)+\omega^2\sin(\theta(\mathrm{t})) = 0, \quad \theta(0) = \theta_0, \quad \dot{\theta}(0) = \dot{\theta}_0 \tag{21}$$

where $\omega = \sqrt{g/L}$. It should be noted that two special sets of initial conditions were considered by Kim (2017). With the initial conditions proposed by Kim and Reddy, the simple pendulum problem given in Fig. 3 can be used as benchmark test problems. As given in Kim (2017, 2019), the case of $\dot{\theta}_0 = 1.999999238456499$ is also used to synthesize two highly nonlinear cases that give clear physical insights. The minimum total energy required for the pendulum to make a complete rotation about the pivot point is $E_0 = 1.0$. With $\dot{\theta}_0 = 1.999999238456499$, the total energy of the first case becomes about $E_0 = 0.999998476913288$. With this particular set of initial conditions, the pendulum cannot make a complete rotation, but instead, the pendulum oscillates between two peak points with the period $T = 33.7210$.

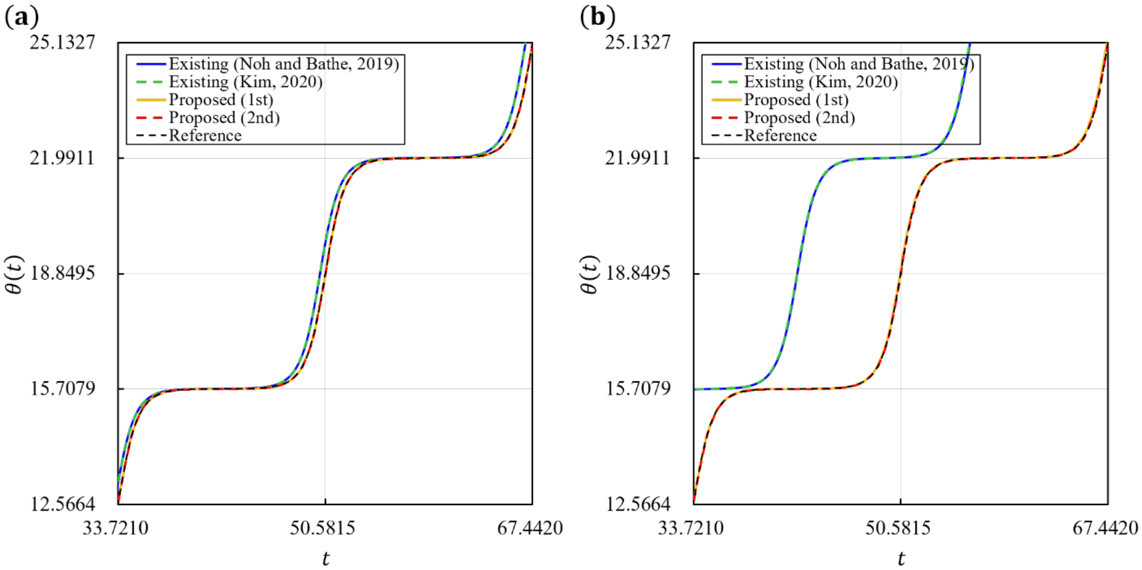

Fig. 5 (a) Case of $\dot{\theta}_0 = 2.000000761543501$ (a) $\Delta t = T/10000$ (b) $\Delta t = T/1000$

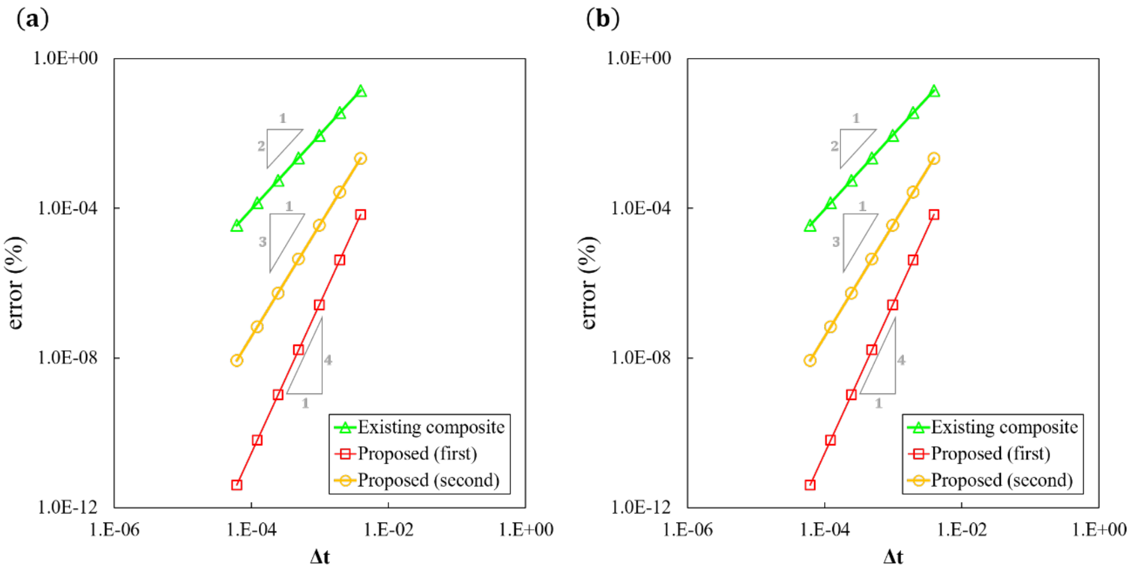

Fig. 6 Convergence rate of total energies (a) Displacement (b) Velocity

With $\dot{\theta}_0 = 2.000000761543501$, the total energy of the second case becomes about $E_0 = 1.0000001523087292$, and the pendulum passes the peak points slowly. For this case, the period becomes about $T = 16.8605$. As shown in this particular problem, the proposed time schemes give more accurate predictions mainly due to the enhanced total energy conserving capability. Regarding the enhanced total energy conserving capability, Fig. 6 shows that the improved convergence rates of two cases are in a good agreement with the mathematical conditions used in the optimization of the algorithmic parameters.

4.3 Excitation of an elastic bar

Here, the most dissipative case (i.e., $\rho_\infty = 0$) of the first case (the scheme with third-order energy conserving capability) is tested by using the excitation of an elastic bar problem. This particular problem has been used to test high-frequency filtering capabilities of various time schemes. The problem is described in Fig. 7. In the spatial discretization, one thousand uniform linear elements are used.

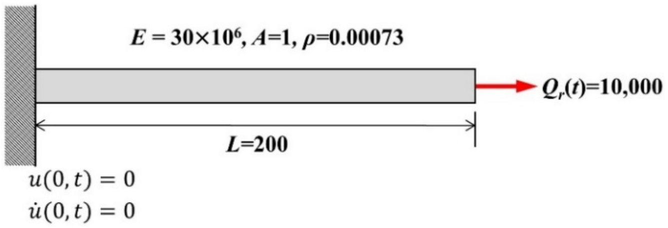

Fig. 7. Description of the excitation of an elastic bar problem (Malakiyeh 2019)

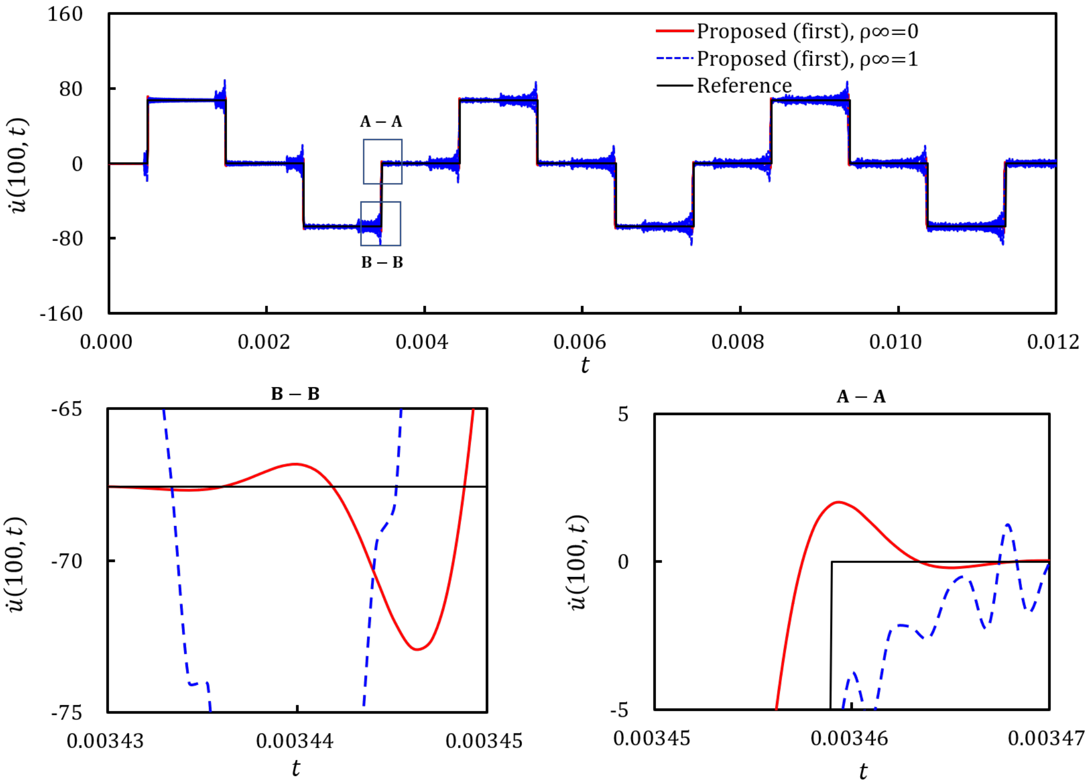

Fig. 8 High-frequency filtering capability of the first case for $\rho_\infty = 0$ and 1.

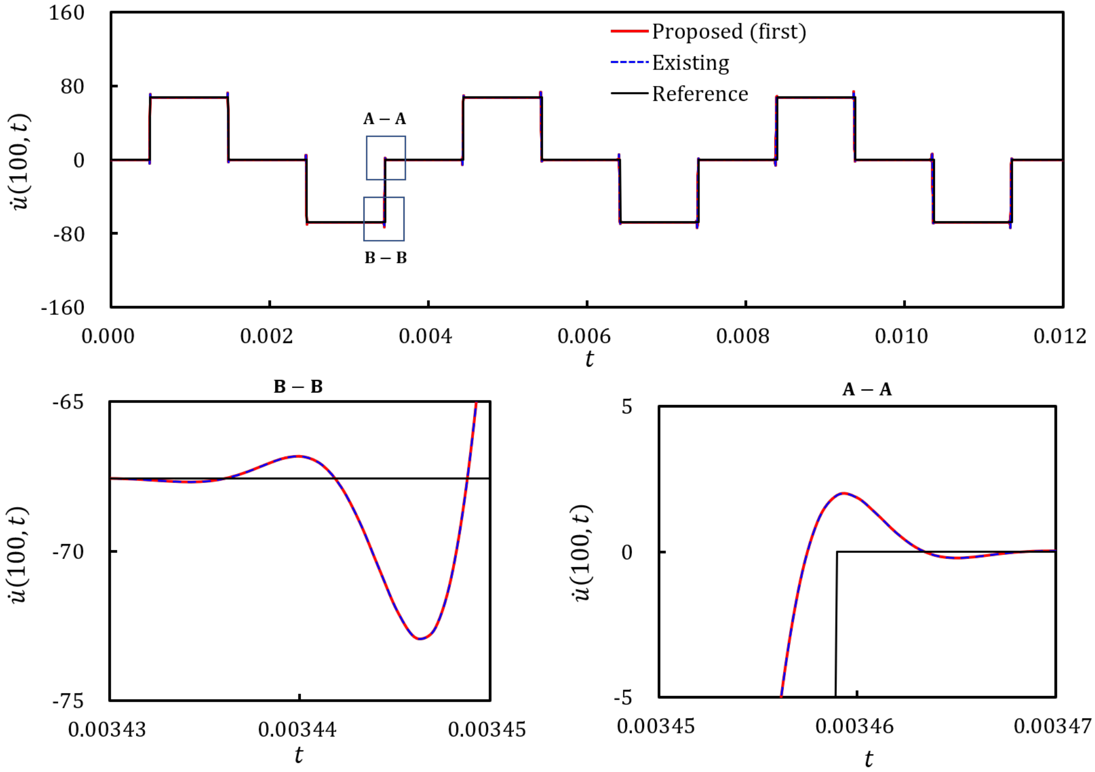

Fig. 9 Comparison of solutions of the first case and the existing schemes for $\rho_\infty = 0$.

As shown in Fig. 8, the numerical dissipation in the most dissipative case can improve the quality of numerical solutions when compared with the non-dissipative case. The spurious oscillations around the wave front disappear in the most dissipative case if Δt is chosen as 9.86577×10^{-7}s according to CFL=1.0. This case shows that the dissipation control capability and numerical dissipation of the proposed scheme can improve qualities of numerical solutions in some situations where the spurious high-frequency mode should be eliminated. In addition, this process does not increase the computational effort at all. Fig. 9 shows that the most dissipative case of the proposed case can give equivalently improved numerical solutions for the impact and wave propagation problems when compared with the existing composite schemes. However, the level of numerical dissipation should be minimized for general cases where the high-frequency filtering is unnecessary. In general analyses, such as analyses of conservative systems, the use of $\rho_\infty = 1$ is recommended.

5. CONCLUSION

In this paper, the algorithmic parameters of the implicit schemes have been determined to minimize the total energy error of simple conservative nonlinear dynamic systems. As a result, improved dissipation properties were obtained in the implicit schemes. As aforementioned, the use of the optimized algorithmic parameters does not increase computational costs. Hence, the computational effort in each scheme is equivalent to that of the existing composite schemes. The newly proposed case presented in this paper noticeably improved numerical performances when compared to the existing composite schemes as shown in the numerical examples.

REFERENCES

Alamatian, J. (2013), “New implicit higher order time integration for dynamic analysis”, *Struct. Eng. Mech.*, **48**(5), 711-736.

Baig, M. M. I. and Bathe, K. J. (2005), “On direct time integration in large deformation dynamic analysis”, In 3rd MIT conference on computational fluid and solid mechanics.

Bathe, K. J. and Baig, M. M. I. (2005), “On a composite implicit time integration procedure for nonlinear dynamics”, *Comput. Struct.*, **83**(31-32), 2513-2524.

Kim, W. and Reddy, J. N. (2017), “A new family of higher-order time integration algorithms for the analysis of structural dynamics”, *J. Appl. Mech.*, **84**(7), 071008.

Kim, W. and Reddy, J. N. (2017), “An improved time integration algorithm: A collocation time finite element approach”, *Int. J. Struct. Stab. Dyn.*, **17**(02), 1750024.

Kim, W. and Choi, S. Y. (2018), “An improved implicit time integration algorithm: The generalized composite time integration algorithm”, *Comput. Struct.*, **196**, 341-354.

Kim, W. (2019), “An accurate two-stage explicit time integration scheme for structural dynamics and various dynamic problems”, *Int. J. Numer. Methods Eng.*, **120**(1), 1-28.

Kim, W. (2020), “An improved implicit method with dissipation control capability: The simple generalized composite time integration algorithm”, *Appl. Math. Model.*, **81**, 910-930.

Kim, W. and Reddy, J. N. (2020), “A comparative study of implicit and explicit composite time integration schemes”, *Int. J. Struct. Stab. Dyn.*, **20**(13), 2041003.

Kim, W. and Reddy, J. N. (2021), “A critical assessment of two-stage composite time integration schemes with a unified set of time approximations”, *Lat. Am. J. Solids Struct.*, **18**.

Kwon, O. S., Elnashai, A. S. and Spencer, B. F. (2008), “A framework for distributed analytical and hybrid simulations”, *Struct. Eng. Mech.*, **30**(3), 331-350.

Li, J. and Yu, K. (2019), “An alternative to the Bathe algorithm”, *Appl. Math. Model.*, **69**, 255-272.

Malakiyeh, M. M., Shojaee, S. and Bathe, K. J. (2019), “The Bathe time integration method revisited for prescribing desired numerical dissipation”, *Comput. Struct.*, **212**, 289-298.

Noh, G. and Bathe, K. J. (2019), “The Bathe time integration method with controllable spectral radius: The ρ_∞-Bathe method”, *Comput. Struct.*, **212**, 299-310.

Rostami, S., Hooshmand, B., Shojaee, S. and Hamzehei-Javaran, S. (2021), “Survey of cubic B-spline implicit time integration method in computational wave propagation” *Struct. Eng. Mech.*, **79**(4), 473-485.