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Calculation of design sensitivity for large-size transient dynamic problems using Krylov subspace-based model order reduction†

Jeong Sam Han*
Department of Mechanical Design Engineering, Andong National University, Andong, 760-749, Korea

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Abstract

Nowadays, transient dynamic responses of a large-size finite element (FE) model can be solved within a reasonable computation time owing to rapid improvement in both numerical schemes and computing resources. However, increasing demands for accurate simulation and complicated modeling have led to larger and more complex finite element models, which consequently result in considerably high computational cost. In addition, when structural optimizations include transient responses such as displacement, velocity, and acceleration, the optimizations often do not end within a reasonable process time because the large-size simulation must be repeated many times. In order to reduce the computational cost in this respect, model order reduction (MOR) for the original full-order model (FOM) can be used for the transient response simulation. In this paper, a transient dynamic response analysis using Krylov subspace-based MOR and its design sensitivity analysis with respect to sizing design variables is suggested as an approach to the handling of large-size finite element models. Large-size finite element models can incur the problem of a long computation time in gradient-based optimization iterations because of the need for repeated simulation of transient responses. In the suggested method, the reduced order models (ROMs) generated from the original FOMs using implicit moment-matching via the Arnoldi process are used to calculate the transient response and its design sensitivity. As a result, the speed of numerical computation for the transient response and its design sensitivity is maximized. Newmark's time integration method is employed to calculate transient responses and their design sensitivities. In the case of the transient sensitivity analysis, we apply a temporal discretization scheme to the design sensitivity equation derived by directly differentiating the governing equation with respect to design variables. This methodology has been programmed on the MATLAB with the FE information extracted from the FE package ANSYS. Two application examples are provided to demonstrate the numerical accuracy and efficiency of the suggested approach. The relative errors of transient response and design sensitivity between the FOMs and ROMs are also compared according to the orders of the reduced model. Calculation of transient dynamic responses and their sensitivities using Krylov subspace-based MOR shows a sizeable reduction in computation time and a good agreement with those provided by the FOM.

Keywords: Model order reduction; Krylov subspace; Transient dynamic problem; Direct design sensitivity

1. Introduction

Transient structural optimization involves a process of repeated transient analysis by modifying the design variables to reach a design goal in which a time-dependent objective function is minimized, subjected to a set of time-varying constraints. In order to make the correct adjustment in gradient-based optimization, the rates of change in transient responses with respect to each design variable (i.e. transient design sensitivities), should be provided. When the transient responses of a large-scale FE model is involved in the gradient-based optimization iterations, the high computational cost necessary to calculate both response quantities and sensitivities as a function of time in the optimization often becomes a hindrance in practical applications. Therefore, the development of an efficient numerical method is especially desirable for the transient dynamic analysis and design sensitivity analysis in optimization iterations [1-3].

In the area of structural dynamic analysis, methods of model order reduction (MOR) such as the mode superposition method (MSM) [4], the modal acceleration method (MAM) [5], the load dependent Ritz vector (LDRV) method [6, 7], and the Lanczos algorithm [8, 9] have been studied to efficiently obtain transient responses. The MSM is a classical method and uses the subspace of undamped eigenvectors for projection because it has a clear physical meaning. It simultaneously diagonalizes both the mass and stiffness matrices of the system and preserves the system's undamped natural frequencies [4]. However, using the MSM may be cost-prohibitive for large-scale systems in terms of calculating the necessary eigenvectors with satisfactory accuracy. This draw-

*Corresponding author. Tel.: +82 54 820 6218, Fax.: +82 54 820 5167
E-mail address: jshan@anu.ac.kr
† Recommended by Associate Editor Maenghyo Cho

back can be overcome to some extent through the use of modal truncation schemes that reduce the number of retained eigenvectors. However, the truncated errors of transient responses from the MSM with a modal truncation scheme can sometimes be very large. Therefore, improved variants to the MSM, such as the MAM, have been suggested to compensate for the effect of neglected high-frequency modes [5]. In the LDRV method, a sequence of mass and stiffness orthogonal Ritz vectors is used to reduce the size of the system. LDRVs can be generated at a fraction of the cost required to calculate eigenvectors in the MSM since the LDRVs are generated from the externally applied load and are orthonormalized using the Gram-Schmidt orthogonalization procedure. The LDRV method has the same effect as MAM since its initial vector is static deflection for the structure due to the externally applied load [6]. It was reported that when some eigenvectors are already available, adding a few LDRVs to the basis is an easy way to increase the accuracy of transient analysis results [7]. The generation of LDRVs is identical to the Lanczos algorithm applied with full reorthogonalization if the same initial vector is used but the Lanczos algorithm originates from mathematics, whereas the LDRV method arises from engineering. In the Lanczos algorithm, orthogonalization is applied only with respect to the two preceding vectors, leading to a tridiagonal form of the dynamic equations that can be used to great advantage directly in time step integration [8, 9].

The design sensitivity theory for the transient dynamic problems can be summarized according to the following three methods as described in Refs. [10, 11]. In the first approach, the direct method, the equations of motion are directly differentiated and solved using the time integration method [3, 11, 12]. In the second approach, the adjoint method [13], the sensitivity equations are revised in terms of a newly defined adjoint vector. This method has computational advantages for a design problem where the number of design variables is greater than the total number of objective and constraint functions. In the third method, the Green's function method [14], the derivatives are obtained in terms of the Green's function of the equations of motion. Even though the results from all three methods are theoretically identical, the relative computational efficiency depends on the relative numbers of design variables, degrees of freedom, and constraints [12]. It is noted that the direct differentiation method is more attractive for sensitivity analysis of transient dynamic response because it is not necessary to store the transient response of the system during forward integration and to use it during backward integration as in the adjoint variable method. As a different approach, from the late 1980s, a continuum-based design sensitivity analysis method [15] (in which sensitivity expression for the solid continuum prior to discretizing the system is written), has been used for transient dynamic response. In addition, the LDRVs and the MAM were utilized to further improve the accuracy and efficiency of both the transient analysis and sensitivity results in the continuum-based design sensitivity method [16]. From relatively recent interest in this area, substructuring-based model reductions have been developed to improve efficiency in transient analysis of large-scale systems [17].

In this paper, an efficient method that utilizes the Krylov subspace-based model order reduction (MOR) [1, 2, 18-22] is studied in order to calculate the approximation of both transient responses and their sensitivity with respect to sizing design variables as functions of time. The key idea herein is that equations of motion are reduced using a projection matrix generated from Krylov basis vectors instead of the traditional eigenvectors or Ritz vectors; then, direct transient and its sensitivity analyses are performed using the Newmark's time integration method [23]. The Krylov basis vectors are generated by the block-Arnoldi algorithm [18, 20] which comprises a series of static solutions; therefore, the computational costs are significantly lower compared to when normal eigenvectors are used. The Krylov vectors are numerically generated to be orthonormal and very similar to LDRVs, except for the mass orthonormality of LDRV. The Krylov subspace-based MOR originates from applied mathematics, whereas the LDRV method arises from engineering.

The remainder of the paper is organized as follows. In section 2, the conventional method for transient response and the design sensitivity analysis of a dynamic structural system are briefly reviewed and then extended to the proposed method in regard to Krylov-based MOR and Newmark's time integration scheme. In section 3, two application examples of a car body and a stiffened plate are provided to demonstrate the numerical accuracy and efficiency of the suggested approach. In terms of the accuracy of transient responses versus the orders or reduced-order model (ROM), the error indicator is employed and studied. Computational costs between the full-order model (FOM) and the ROMs are also compared and discussed. Finally, concluding remarks are given in section 4.

2. Transient response and its design sensitivity analysis

2.1 Sensitivity analysis of transient response

A structural dynamics problem in finite element (FE) matrix form is described by a second-order system of ordinary differential equations (ODEs)

$$\begin{aligned} \mathbf{M}\ddot{\mathbf{x}}(t) + \mathbf{C}\dot{\mathbf{x}}(t) + \mathbf{K}\mathbf{x}(t) &= \mathbf{F}(t) \\ \mathbf{y}(t) &= \mathbf{L}\mathbf{x}(t) \end{aligned} \tag{1}$$

where t is the time variable, $\mathbf{x}(t)\in\Re^N$ is a vector of state variables, and $\mathbf{y}(t)\in\Re^p$ is the output measurement vector. A set of initial conditions and is assumed on $\mathbf{x}(t)$. The matrices $\mathbf{M}$, $\mathbf{C}$, and $\mathbf{K}\in\Re^{N\times N}$ are the structural mass, damping, and stiffness matrices of the system, respectively. $\mathbf{F}\in\Re^N$ and $\mathbf{L}\in\Re^{p\times N}$ are a force vector and an output measurement matrix, respectively, for the observation at certain points. N is the dimension of the state variable vector $\mathbf{x}(t)$ and p is the number of output degrees of freedom of the system. In most practical cases, p is considerably smaller than N.

The sensitivity of the transient response of the dynamic system can be obtained by taking the first partial derivative of the governing equation with respect to a chosen design variable b_j (j = 1, 2, …, J):

$$\mathbf{M}\frac{\partial \ddot{\mathbf{x}}(t)}{\partial b_j}+\mathbf{C}\frac{\partial \dot{\mathbf{x}}(t)}{\partial b_j}+\mathbf{K}\frac{\partial \mathbf{x}(t)}{\partial b_j} = \frac{\partial \mathbf{F}(t)}{\partial b_j}-\left(\frac{\partial \mathbf{M}}{\partial b_j}\ddot{\mathbf{x}}(t)+\frac{\partial \mathbf{C}}{\partial b_j}\dot{\mathbf{x}}(t)+\frac{\partial \mathbf{K}}{\partial b_j}\mathbf{x}(t)\right) \quad (2)$$
$$\frac{\partial \mathbf{y}(t)}{\partial b_j}=\mathbf{L}\frac{\partial \mathbf{x}(t)}{\partial b_j}.$$

The initial conditions for the sensitivity equation, $\dot{\mathbf{x}}'_j(0)$ and $\mathbf{x}'_j(0)$ are assumed accordingly.

The solutions of Eqs. (1) and (2) can be obtained using a variety of temporal discretization schemes available in the Ref. [23]. Among the various methods, we employed Newmark's time integration method as described in the next section to calculate the transient response and its design sensitivity.

2.2 Transient dynamic analysis using Newmark's integration method

The equilibrium equation of motion in Eq. (1) at time t + Δt can be considered as follows:

$$\mathbf{M}\ddot{\mathbf{x}}_{n+1}+\mathbf{C}\dot{\mathbf{x}}_{n+1}+\mathbf{K}\mathbf{x}_{n+1}=\mathbf{F}_{n+1} \quad (3)$$

where at time t + Δt, $\ddot{\mathbf{x}}_{n+1}$, $\dot{\mathbf{x}}_{n+1}$, $\mathbf{x}_{n+1}$, and $\mathbf{F}_{n+1}$ are the acceleration, velocity, displacement, and load, respectively. The Newmark integration method assumes that the relationship between displacement and velocity at time t + Δt from time t is given as

$$\dot{\mathbf{x}}_{n+1}=\dot{\mathbf{x}}_n+\left[(1-\delta)\ddot{\mathbf{x}}_n+\delta\ddot{\mathbf{x}}_{n+1}\right]\Delta t \quad (4)$$
$$\mathbf{x}_{n+1}=\mathbf{x}_n+\dot{\mathbf{x}}_n\Delta t+\left[(\tfrac{1}{2}-\alpha)\ddot{\mathbf{x}}_n+\alpha\ddot{\mathbf{x}}_{n+1}\right]\Delta t^2 \quad (5)$$

where α and δ are Newmark integration parameters that are determined to obtain integration accuracy and stability. The Newmark method is unconditionally stable for

$$\alpha \ge \frac{1}{4}\left(\frac{1}{2}+\delta\right)^2 \text{ and } \delta \ge \frac{1}{2}. \quad (6)$$

The values $\alpha=\frac{1}{4}\left(\frac{1}{2}+\delta\right)^2$ and δ = 0.505 are used in this paper.

The solution for the displacement at time t + Δt in Eq. (3) is obtained by first rearranging Eqs. (5) and (4) as follows:

$$\ddot{\mathbf{x}}_{n+1}=a_0(\mathbf{x}_{n+1}-\mathbf{x}_n)-a_2\dot{\mathbf{x}}_n-a_3\ddot{\mathbf{x}}_n \quad (7)$$
$$\dot{\mathbf{x}}_{n+1}=\dot{\mathbf{x}}_n+a_6\ddot{\mathbf{x}}_n+a_7\ddot{\mathbf{x}}_{n+1} \quad (8)$$

where $a_0=\frac{1}{\alpha\Delta t^2}$, $a_1=\frac{\delta}{\alpha\Delta t}$, $a_2=\frac{1}{\alpha\Delta t}$, $a_3=\frac{1}{2\alpha}-1$, $a_4=\frac{\delta}{\alpha}-1$, $a_5=\frac{\Delta t}{2}\left(\frac{\delta}{\alpha}-2\right)$, $a_6=\Delta t(1-\delta)$, and $a_7=\delta\Delta t$.

By substituting Eq. (7) into Eq. (8), we can express each equation for $\ddot{\mathbf{x}}_{n+1}$ and $\dot{\mathbf{x}}_{n+1}$ in terms of the single unknown $\mathbf{x}_{n+1}$ and the previously known responses at time t. These two equations for $\ddot{\mathbf{x}}_{n+1}$ and $\dot{\mathbf{x}}_{n+1}$ are then combined with Eq. (3) to solve for the unknown x_{n+1}:

$$\mathbf{K}^{eff}\mathbf{x}_{n+1}=\mathbf{F}^{eff}_{n+1} \quad (9)$$
$$\mathbf{K}^{eff}=a_0\mathbf{M}+a_1\mathbf{C}+\mathbf{K} \quad (10)$$

where

$$\mathbf{F}^{eff}_{n+1}=\mathbf{F}_{n+1}+\mathbf{M}\left(a_0\mathbf{x}_n+a_2\dot{\mathbf{x}}_n+a_3\ddot{\mathbf{x}}_n\right) +\mathbf{C}\left(a_1\mathbf{x}_n+a_4\dot{\mathbf{x}}_n+a_5\ddot{\mathbf{x}}_n\right). \quad (11)$$

The initial conditions $\dot{\mathbf{x}}(0)$ and $\mathbf{x}(0)$ in Eq. (1) are used to initialize $\mathbf{x}_0$, $\dot{\mathbf{x}}_0$, and $\ddot{\mathbf{x}}_0$. The solution process involves the LU decomposition of the effective stiffness matrix $\mathbf{K}^{eff}$ into lower and upper triangular matrices, $\mathbf{K}^{eff}=\mathbf{LU}$ and the calculation of the effective load at time t + Δt, $\mathbf{F}^{eff}_{n+1}$. Then, forward and back substitutions using **L** and **U** are carried out to compute the solution vector $\mathbf{x}_{n+1}$ in Eq. (9). When the displacement at time t + Δt, $\mathbf{x}_{n+1}$ has been obtained, $\ddot{\mathbf{x}}_{n+1}$ and $\dot{\mathbf{x}}_{n+1}$ can also be calculated using Eqs. (7) and (8).

For the sensitivity analysis of the dynamic transient response, the following two approaches yield the same sensitivity equations. The first approach involves applying a temporal discretization scheme to Eq. (2), which has been derived by directly differentiating Eq. (1). Alternatively, the temporally discretized equation in Eq. (9) can be differentiated with respect to design variables. The differentiation of Eq. (9) yields the following sensitivity equation:

$$\begin{aligned}&\left(a_0\mathbf{M}+a_1\mathbf{C}+\mathbf{K}\right)\frac{\partial \mathbf{x}_{n+1}}{\partial b_j}\\ &=\frac{\partial \mathbf{F}_{n+1}}{\partial b_j}-\left(\frac{\partial \mathbf{M}}{\partial b_j}\ddot{\mathbf{x}}_{n+1}+\frac{\partial \mathbf{C}}{\partial b_j}\dot{\mathbf{x}}_{n+1}+\frac{\partial \mathbf{K}}{\partial b_j}\mathbf{x}_{n+1}\right)\\ &+\mathbf{M}\left(a_0\frac{\partial \mathbf{x}_n}{\partial b_j}+a_2\frac{\partial \dot{\mathbf{x}}_n}{\partial b_j}+a_3\frac{\partial \ddot{\mathbf{x}}_n}{\partial b_j}\right)\\ &+\mathbf{C}\left(a_1\frac{\partial \mathbf{x}_n}{\partial b_j}+a_4\frac{\partial \dot{\mathbf{x}}_n}{\partial b_j}+a_5\frac{\partial \ddot{\mathbf{x}}_n}{\partial b_j}\right).\end{aligned} \quad (12)$$

Note that the derivation of Eq. (12) assumes that the time interval does not depend on the design variables. The sensitivity equation is solved with a set of initial conditions, $\frac{\partial \mathbf{x}_0}{\partial b_j}$, $\frac{\partial \dot{\mathbf{x}}_0}{\partial b_j}$, and $\frac{\partial \ddot{\mathbf{x}}_0}{\partial b_j}$.

Differentiation of Eqs. (7) and (8) gives sensitivity equations of the acceleration and velocity vectors, respectively, at time t + Δt.

$$\frac{\partial \ddot{\mathbf{x}}_{n+1}}{\partial b_j} = a_0\left(\frac{\partial \mathbf{x}_{n+1}}{\partial b_j} - \frac{\partial \mathbf{x}_n}{\partial b_j}\right) - a_2\frac{\partial \dot{\mathbf{x}}_n}{\partial b_j} - a_3\frac{\partial \ddot{\mathbf{x}}_n}{\partial b_j} \quad (13)$$

$$\frac{\partial \dot{\mathbf{x}}_{n+1}}{\partial b_j} = \frac{\partial \dot{\mathbf{x}}_n}{\partial b_j} + a_6\frac{\partial \ddot{\mathbf{x}}_n}{\partial b_j} + a_7\frac{\partial \ddot{\mathbf{x}}_{n+1}}{\partial b_j}. \quad (14)$$

Therefore, the value of the displacement sensitivity calculated by solving Eq. (12) can be substituted into the above two sensitivity equations to obtain the derivatives of the acceleration and velocity vectors in a manner similar to Eqs. (7) and (8).

2.3 Design sensitivity analysis of transient response using model order reduction

The basic aim of model order reduction based on the Krylov subspace is to find a low-dimensional subspace $\mathbf{V}^{N\times n}$ of

$$\mathbf{x}(t) \cong \mathbf{V}\mathbf{z}(t) \quad \text{where} \quad \mathbf{z}(t) \in \Re^n,\ n << N \quad (15)$$

such that the trajectory of the original high-dimensional state vector $\mathbf{x}$(t) in Eq. (1) can be well approximated by the projection matrix $\mathbf{V}$ in relation to a considerably reduced vector $\mathbf{z}$(t) of order n. From this relation, the velocity and acceleration are expressed as

$$\dot{\mathbf{x}}(t) = \mathbf{V}\dot{\mathbf{z}}(t), \quad \ddot{\mathbf{x}}(t) = \mathbf{V}\ddot{\mathbf{z}}(t). \quad (16)$$

Provided that the subspace $\mathbf{V}$ is found, the original Eq. (1) is projected onto $\mathbf{V}$. Multiplying the obtained result by $\mathbf{V}^T$ yields the reduced system as follows:

$$\begin{gathered}\underbrace{\mathbf{V}^T\mathbf{M}\mathbf{V}}_{\mathbf{M}_r}\ddot{\mathbf{z}}(t) + \underbrace{\mathbf{V}^T\mathbf{C}\mathbf{V}}_{\mathbf{C}_r}\dot{\mathbf{z}}(t) + \underbrace{\mathbf{V}^T\mathbf{K}\mathbf{V}}_{\mathbf{K}_r}\mathbf{z}(t) = \underbrace{\mathbf{V}^T\mathbf{F}}_{\mathbf{F}_r}(t) \\ \mathbf{y}(t) = \underbrace{\mathbf{L}\mathbf{V}}_{\mathbf{L}_r}\mathbf{z}(t)\end{gathered} \quad (17)$$

with the following initial conditions

$$\mathbf{z}(0) = \mathbf{V}^T\mathbf{x}(0), \quad \dot{\mathbf{z}}(0) = \mathbf{V}^T\dot{\mathbf{x}}(0). \quad (18)$$

The system matrices in the reduced system are denoted as $\mathbf{M}_r = \mathbf{V}^T\mathbf{M}\mathbf{V}$, $\mathbf{C}_r = \mathbf{V}^T\mathbf{C}\mathbf{V}$, $\mathbf{K}_r = \mathbf{V}^T\mathbf{K}\mathbf{V}$, $\mathbf{F}_r = \mathbf{V}^T\mathbf{F}$, and $\mathbf{L}_r = \mathbf{L}\mathbf{V}$. The most efficient way to compute a reasonably accurate basis for the Krylov subspace is implicit moment matching through the Arnoldi process [18-20]. In terms of the moment-matching method for a second-order dynamical system, it is shown that the reduced system in Eq. (17) matches the first n moments of the full-order system in Eq. (1) if the projection matrix $\mathbf{V}_n$ is chosen from the nth Krylov subspace $\mathcal{K}_n$ given as

$$\begin{aligned} &colspan\{\mathbf{V}_n\} = \mathcal{K}_n(\mathbf{K}^{-1}\mathbf{M}, \mathbf{K}^{-1}\mathbf{F}) \\ &= \text{span}\{\mathbf{K}^{-1}\mathbf{F}, (\mathbf{K}^{-1}\mathbf{M})\mathbf{K}^{-1}\mathbf{F}, \cdots, (\mathbf{K}^{-1}\mathbf{M})^{n-1}\mathbf{K}^{-1}\mathbf{F}\}. \end{aligned} \quad (19)$$

Numerically, the Arnoldi process generates the projection matrix $\mathbf{V}_n$ to be orthonormal. Thus, $\mathbf{V}^T\mathbf{V} = \mathbf{I}_n$. The initial conditions on $\mathbf{z}$(t) in Eq. (18) are obtained using Eq. (16) and the orthonormality of $\mathbf{V}_n$.

Note that the reduction of the dimension of the systems to n << N is achieved in Eq. (17) while the output vector $\mathbf{y}$(t) retains the same size as that in Eq. (1), with the result that transient dynamics responses can be very efficiently calculated from Eq. (17).

By assuming that the projection matrix $\mathbf{V}$ in Eq. (15) can be treated as constant with respect to the perturbation of a design variable, i.e., $\partial\mathbf{V}/\partial b_j = \mathbf{0}$, the first derivative of Eq. (15) becomes

$$\frac{\partial \mathbf{x}(t)}{\partial b_j} = \frac{\partial \mathbf{V}}{\partial b_j}\mathbf{z}(t) + \mathbf{V}\frac{\partial \mathbf{z}(t)}{\partial b_j} \quad \rightarrow \quad \frac{\partial \mathbf{x}(t)}{\partial b_j} = \mathbf{V}\frac{\partial \mathbf{z}(t)}{\partial b_j}. \quad (20)$$

Consequently, the velocity and acceleration derivatives in Eq. (16) become

$$\begin{aligned}\frac{\partial \dot{\mathbf{x}}(t)}{\partial b_j} &= \mathbf{V}\frac{\partial \dot{\mathbf{z}}(t)}{\partial b_j} \\ \frac{\partial \ddot{\mathbf{x}}(t)}{\partial b_j} &= \mathbf{V}\frac{\partial \ddot{\mathbf{z}}(t)}{\partial b_j}.\end{aligned} \quad (21)$$

Applying these three derivatives and Eqs. (15) and (16) to Eq. (2) and multiplying by $\mathbf{V}^T$ on both sides yields the transient sensitivity equation for the reduced system as follows:

$$\begin{gathered}\underbrace{\mathbf{V}^T\mathbf{M}\mathbf{V}}_{\mathbf{M}_r}\frac{\partial \ddot{\mathbf{z}}(t)}{\partial b_j} + \underbrace{\mathbf{V}^T\mathbf{C}\mathbf{V}}_{\mathbf{C}_r}\frac{\partial \dot{\mathbf{z}}(t)}{\partial b_j} + \underbrace{\mathbf{V}^T\mathbf{K}\mathbf{V}}_{\mathbf{K}_r}\frac{\partial \mathbf{z}(t)}{\partial b_j} = \mathbf{V}^T\frac{\partial \mathbf{F}(t)}{\partial b_j} \\ -\left(\mathbf{V}^T\frac{\partial \mathbf{M}}{\partial b_j}\mathbf{V}\ddot{\mathbf{z}}(t) + \mathbf{V}^T\frac{\partial \mathbf{C}}{\partial b_j}\mathbf{V}\dot{\mathbf{z}}(t) + \mathbf{V}^T\frac{\partial \mathbf{K}}{\partial b_j}\mathbf{V}\mathbf{z}(t)\right) \\ \frac{\partial \mathbf{y}(t)}{\partial b_j} = \underbrace{\mathbf{L}\mathbf{V}}_{\mathbf{L}_r}\frac{\partial \mathbf{z}(t)}{\partial b_j}\end{gathered} \quad (22)$$

with initial conditions

$$\mathbf{z}'_j(0) = \mathbf{V}^T\mathbf{x}'_j(0), \quad \dot{\mathbf{z}}'_j(0) = \mathbf{V}^T\dot{\mathbf{x}}'_j(0). \quad (23)$$

Note that through Eqs. (17) and (22), the transient responses and their design sensitivities are efficiently calculated as a result of achieving reduction in the dimension of the systems to n << N.

To numerically calculate the transient response and its design sensitivity, the same Newmark time integration procedure is employed. If the reduced vector $\mathbf{z}$(t) and its first and second time derivatives at time t + Δt are denoted as $\mathbf{z}_{n+1}$, $\dot{\mathbf{z}}_{n+1}$, and $\ddot{\mathbf{z}}_{n+1}$, respectively, then Newmark's integration method yields the governing equation for the unknown $\mathbf{z}_{n+1}$ as follows:

$$\hat{\mathbf{K}}^{eff}\mathbf{z}_{n+1} = \hat{\mathbf{F}}^{eff}_{n+1} \quad (24)$$

$$\hat{\mathbf{K}}^{eff} = a_0\mathbf{M}_r + a_1\mathbf{C}_r + \mathbf{K}_r \quad (25)$$

where

$$\begin{aligned}\hat{\mathbf{F}}^{eff}_{n+1} &= \mathbf{V}^T\mathbf{F}_{n+1} + \mathbf{M}_r\left(a_0\mathbf{z}_n + a_2\dot{\mathbf{z}}_n + a_3\ddot{\mathbf{z}}_n\right) \\ &+\mathbf{C}_r\left(a_1\mathbf{z}_n + a_4\dot{\mathbf{z}}_n + a_5\ddot{\mathbf{z}}_n\right).\end{aligned} \quad (26)$$

The initial conditions $\dot{\mathbf{z}}(0)$ and $\mathbf{z}(0)$ in Eq. (18) are used to initialize $\mathbf{z}_0$, $\dot{\mathbf{z}}_0$, and $\ddot{\mathbf{z}}_0$. When the reduced vector at time t + Δt, $\mathbf{z}_{n+1}$ has been obtained, $\ddot{\mathbf{z}}_{n+1}$ and $\dot{\mathbf{z}}_{n+1}$ are calculated using the following relations:

$$\ddot{\mathbf{z}}_{n+1} = a_0(\mathbf{z}_{n+1} - \mathbf{z}_n) - a_2\dot{\mathbf{z}}_n - a_3\ddot{\mathbf{z}}_n \quad (27)$$

$$\dot{\mathbf{z}}_{n+1} = \dot{\mathbf{z}}_n + a_6\ddot{\mathbf{z}}_n + a_7\ddot{\mathbf{z}}_{n+1}. \quad (28)$$

We can calculate the design sensitivity of the transient response using the reduced order model (ROM) by applying the sensitivity analysis formulation derived for Eq. (1) directly to Eq. (17). The temporally discretized equation in Eq. (24) can be differentiated with respect to design variables and can be expressed as

$$\begin{aligned}&\left(a_0\mathbf{M}_r + a_1\mathbf{C}_r + \mathbf{K}_r\right)\frac{\partial \mathbf{z}_{n+1}}{\partial b_j} = \mathbf{V}^T\frac{\partial \mathbf{F}_{n+1}}{\partial b_j} \\ &-\left(\mathbf{V}^T\frac{\partial \mathbf{M}}{\partial b_j}\mathbf{V}\ddot{\mathbf{z}}_{n+1} + \mathbf{V}^T\frac{\partial \mathbf{C}}{\partial b_j}\mathbf{V}\dot{\mathbf{z}}_{n+1} + \mathbf{V}^T\frac{\partial \mathbf{K}}{\partial b_j}\mathbf{V}\mathbf{z}_{n+1}\right) \\ &+\mathbf{M}_r\left(a_0\frac{\partial \mathbf{z}_n}{\partial b_j} + a_2\frac{\partial \dot{\mathbf{z}}_n}{\partial b_j} + a_3\frac{\partial \ddot{\mathbf{z}}_n}{\partial b_j}\right) \\ &+\mathbf{C}_r\left(a_1\frac{\partial \mathbf{z}_n}{\partial b_j} + a_4\frac{\partial \dot{\mathbf{z}}_n}{\partial b_j} + a_5\frac{\partial \ddot{\mathbf{z}}_n}{\partial b_j}\right).\end{aligned} \quad (29)$$

The sensitivity equation using the MOR is solved with a set of initial conditions, $\frac{\partial \mathbf{z}_0}{\partial b_j}$, $\frac{\partial \dot{\mathbf{z}}_0}{\partial b_j}$, and $\frac{\partial \ddot{\mathbf{z}}_0}{\partial b_j}$, which are assumed from Eq. (23).

The accuracy of the design sensitivities for the transient responses depends on the quality of the Krylov basis vectors **V**. It has been reported that the assumption that the Krylov basis vectors are treated as constant with respect to the perturbation of a design variable is apparently feasible for the sensitivity analysis of frequency response (FR) problems, and the accuracy of FR sensitivities calculated from ROMs was fairly good compared to the case in which a FOM is used [2].

In order to obtain the derivatives of the acceleration and velocity vectors in a ROM, the displacement sensitivity calculated by solving Eq. (29) can be substituted into sensitivity equations for the acceleration and velocity vectors in a way similar to Eqs. (13) and (14).

$$\frac{\partial \ddot{\mathbf{z}}_{n+1}}{\partial \mathrm{b}_j} = a_0\left(\frac{\partial \mathbf{z}_{n+1}}{\partial \mathrm{b}_j} - \frac{\partial \mathbf{z}_n}{\partial \mathrm{b}_j}\right) - a_2\frac{\partial \dot{\mathbf{z}}_n}{\partial \mathrm{b}_j} - a_3\frac{\partial \ddot{\mathbf{z}}_n}{\partial \mathrm{b}_j} \quad (30)$$

$$\frac{\partial \dot{\mathbf{z}}_{n+1}}{\partial b_j} = \frac{\partial \dot{\mathbf{z}}_n}{\partial b_j} + a_6\frac{\partial \ddot{\mathbf{z}}_n}{\partial b_j} + a_7\frac{\partial \ddot{\mathbf{z}}_{n+1}}{\partial b_j}. \quad (31)$$

Finally, the values of transient sensitivity at the selected observation points are recovered by the following relations.

$$\frac{\partial \mathbf{y}(t)}{\partial b_j} = \underbrace{\mathbf{LV}}_{\mathbf{L}_r}\frac{\partial \mathbf{z}(t)}{\partial b_j} \quad (32)$$

$$\frac{\partial \dot{\mathbf{y}}(t)}{\partial b_j} = \underbrace{\mathbf{LV}}_{\mathbf{L}_r}\frac{\partial \dot{\mathbf{z}}(t)}{\partial b_j} \quad (33)$$

$$\frac{\partial \ddot{\mathbf{y}}(t)}{\partial b_j} = \underbrace{\mathbf{LV}}_{\mathbf{L}_r}\frac{\partial \ddot{\mathbf{z}}(t)}{\partial b_j}. \quad (34)$$

This methodology has been programmed on the MATLAB [24] with the FE information extracted from the FE package ANSYS [25].

3. Numerical examples

3.1 Stiffened plate

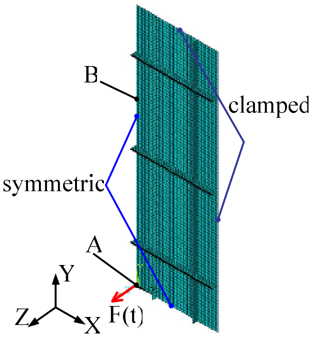
A stiffened plate structure of 500 × 1,500 mm^2 is considered to show the numerical efficiency and accuracy of the suggested method (see Fig. 1). One quarter of the structure is modeled because the structure is symmetric about both the X- and Y-axis, and all the outer edges are clamped as a boundary condition. The Young's modulus E = 73 GPa, mass density ρ = 7,850 kg/m^3, and Poisson's ratio ν = 0.33 are used for the structure. The full-order ANSYS finite element model consists of 5,280 shell elements and its total degrees of freedom (DOF) is up to 31,051.

3.1.1 Transient responses

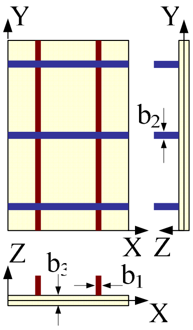
A step force of 1 kN is applied to the middle point (A) in the Z-direction. The transient dynamic responses are observed at points A and B as shown in Fig. 1. As a damping for the system, Rayleigh damping with α = 0 and β = 0.1 ms is assumed. The transient responses are calculated until t = 0.1 s with a time step of 1/2,000 s.

The transient responses using the FOM such as displacement, velocity, and acceleration at the points A and B are compared with those using ROMs of order n = 10 as shown in Fig. 2. The displacement and velocity from ROM (n = 10) are indiscernible in the time range of interest (see Fig. 2). The approximate acceleration from ROM is extremely accurate at B while it is less accurate at A and not able to perfectly trace the high-frequency oscillations as shown in Fig. 2(c). However, the acceleration calculated using the ROM of order 30 gives a perfect match with that using the FOM.

In order to evaluate the accuracy of the approximate transient responses from ROMs, relative errors defined as Eqs. (35) and (36) are plotted in Fig. 3. The true relative error of



(a) Finite element model



(b) Definition of design variables

Fig. 1. Finite element model of a stiffened plate and the definition of design variables.

the root mean square (RMS) is defined as:

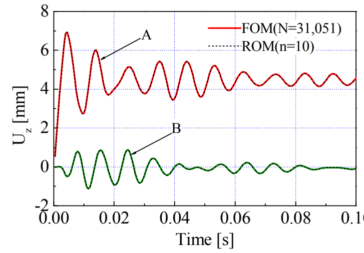
$$E(n) = \frac{1}{N_t}\sqrt{\sum_{t_i=0}^{N_t \cdot \Delta t}\left(\frac{\mathbf{y}_n(t_i) - \mathbf{y}(t_i)}{\mathbf{y}(t_i)}\right)^2} \tag{35}$$

where $\mathbf{y}_n(t_i)$ and $\mathbf{y}(t_i)$ refer to the transient responses calculated from a ROM of order n and the FOM in N_t time points with a time step of Δt, respectively. In this study, displacements at points A and B are used for the evaluation. Because the computational cost for calculation of $\mathbf{y}(t_i)$ in Eq. (35) is too expensive to use in many cases, we adopt the error indicator which is expressed with responses from two successive ROMs as follows:

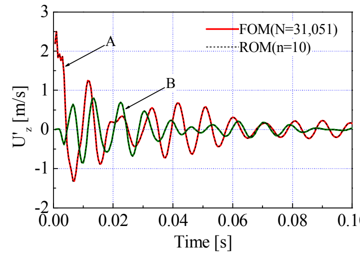
$$e(n) = \frac{1}{N_t}\sqrt{\sum_{t_i=0}^{N_t \cdot \Delta t}\left(\frac{\mathbf{y}_n(t_i) - \mathbf{y}_{n+1}(t_i)}{\mathbf{y}_{n+1}(t_i)}\right)^2} \ . \tag{36}$$

The relation $E(n) \approx e(n)$ was observed for some electro-thermal MEMS models in Ref. [21]. As shown in Fig. 3, this problem has the same tendency. Therefore, it can be said that even for structural dynamic models, the relation $E(n) \approx e(n)$ is valid and can be used to select the optimal order of ROM.

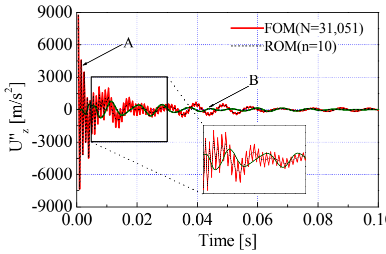
When the order of ROM is 10, the relative error E(10) is about 10^{-5} and the ROM gives fairly accurate approximations of displacement and velocity but less accurate acceleration.



(a) Displacement in the Z-direction



(b) Velocity in the Z-direction



(c) Acceleration in the Z-direction

Fig. 2. Transient responses at points A and B (FOM and ROM (n = 10)).

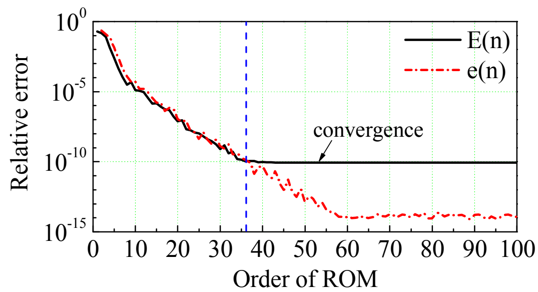


Fig. 3. Relative error and error indicator for transient responses of the stiffened plate model.

For n = 30, E(30) is around 10^{-9} and all the approximate transient responses match perfectly with those from the FOM. It should be noted that one needs to increase the order of ROM further if the accuracy level of approximate displacement is necessary for approximate acceleration.

The convergence of the relative error occurs after the order of ROM reaches 35 (see Fig. 3). This is due to the limited numerical precision when the time integration is performed in MATLAB, where floating-point numbers have a finite precision of roughly 16 significant digits [24].

3.1.2 Sensitivity analysis of transient responses

The thicknesses of three parts of the stiffened plate are selected as design variables for the transient sensitivity analysis. They are the thickness of the vertical (b_1), horizontal (b_2) stiffeners, and plate (b_3) (see Fig. 1(b)). In the initial design, the design variables are b_1 = 2 mm, b_2 = 2 mm, and b_3 = 5 mm, respectively. The design sensitivities of transient responses expressed by Eqs. (2) and (22) are compared in Figs. 4-9 according to the order of the ROMs. For numerical calculation, Eqs. (12) and (29) are used. The derivatives of system matrices in the sensitivity equations are approximated by the semi-analytical approach using the forward difference method with 0.1% design perturbations.

For simplicity, only the transient responses in the Z-direction are considered. In terms of the transient responses, the design variable b_2 has the largest sensitivities of displacement and velocity. The accuracy of approximate sensitivities using the ROM of order 10 is fairly good compared to that of the FOM. For the responses at A, the approximate transient sensitivities perfectly match those obtained from FOM, except for the acceleration sensitivities with respect to b_3 (see Fig. 6(c)). In the case of responses at B, the approximate sensitivities using the ROM (n = 10) are relatively accurate compared to those using the FOM, but there are slight discrepancies at initial time ranges and at some peaks. However, the computed transient sensitivities from the ROM of order 30 perfectly match all the sensitivities from FOM. Compared to Eq. (24), Eq. (29) has more terms on the right side that need to be approximated to calculate their derivatives; consequently, the accuracy of the transient sensitivities slightly decreases compared to that of the transient responses only.

3.2 Car body

The second numerical example is a car body [2] as shown in Fig. 10. The finite element model of the car body is discretized into 91,525 shell elements, 4,017 weld spots, and 362 mass elements through the commercial FE package, ANSYS. It has 93,349 nodes and the total number of DOF of the FOM is as high as 535,992. The Young's modulus E = 207 GPa, mass density ρ = 7,800 kg/m^3, and Poisson's ratio ν = 0.28 are used for the shell elements. The various colors in Fig. 10 refer to the varying thickness of each part. In this case, the car body consists of 111 panels with thickness varying between 0.7 and 4 mm.

3.2.1 Transient responses

A step force of F_Z = 1 kN is applied in the Z-direction to a mass element (point A of Fig. 10) which represents the engine of the car. Four points at the bottom of the car body are fixed as a boundary condition as shown in Fig. 9. Structural damping with Rayleigh damping constants α = 0 and β = 1 ms is assumed for the transient analysis. The transient analysis is performed up to t = 2 s with a time step of 1/1,000 s. The transient responses are observed at points A and B as shown in Fig. 10. The latter point is located on the floor of the car body under the driver's seat.

The transient responses using the FOM at points A and B are compared with those using ROM of the order n = 20 as shown in Fig. 11. The approximated displacement, velocity, and acceleration by ROM (n = 20) are visually almost indistinguishable up to t = 2 s from the exact transient responses using the FOM (see Fig. 11).

In order to evaluate the accuracy of the approximate transient responses from ROMs, relative errors are plotted in Fig. 12. In this example, displacements at points A and B are used for the evaluation. As shown in Fig. 12, this example has the same trend as the first example and the relation $E(n) \approx e(n)$ is also observed. When the order of ROM is 20, the relative error E(20) is about 10^{-5} and the ROM gives fairly accurate approximations of transient responses. The convergence of the relative error occurs after the order of ROM reaches 60 (see Fig. 12).

3.2.2 Sensitivity analysis of transient responses

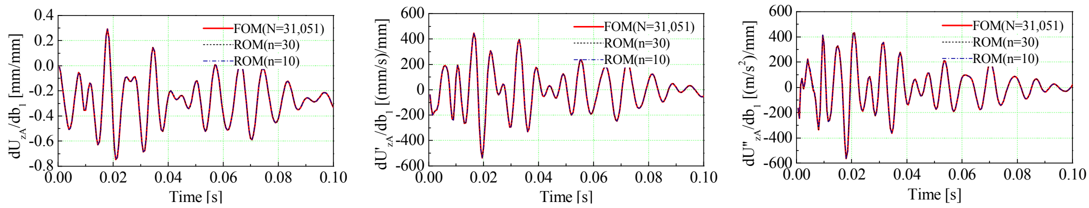
Three parts of the car body are considered as design variables: (1) the panel separating the engine room from the cabin; (2) both front fenders of the car; and (3) the central pillar assembly with side members around the doors (see Fig. 10). In the initial design, the design variables are b_1 = 0.8 mm, b_2 = 1 mm, and b_3 = 1.2 mm, respectively.

The design sensitivities of transient responses calculated using Eqs. (12) and (29) are compared in Figs. 13-18 according to the order of the ROMs. The derivatives of system matrices in the sensitivity equations are approximated by the semi-analytical approach, using the forward difference method with 0.1% design perturbations as the first example.

For simplicity, only the transient responses in the Z-direction are considered. The design variable b_3 has the largest sensitivities of transient responses. In this case, the accuracy of approximate transient sensitivities using the ROM of order 20 is fairly good compared to that of the FOM. For the responses at A, the approximate transient sensitivities perfectly match those obtained from FOM. For the responses at B, while the approximate sensitivities using the ROM (n = 20) is relatively accurate compared to those using the FOM, slight discrepancies occur near the starting time points. The approximate transient sensitivities of responses at B with respect to b_2 are the least accurate and this is because their amplitudes are much smaller than those of other design variables. These discrepancies do not exist if the order of ROM is increased further and the computed transient sensitivities from the ROM of order 60 perfectly match all the sensitivities from FOM.

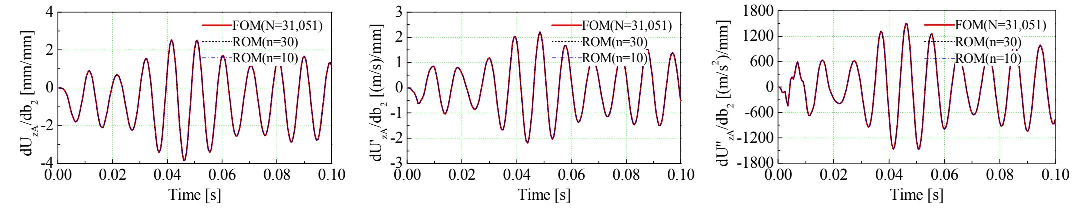
3.3 Comparison of computational cost

We have, heretofore, mainly demonstrated the numerical accuracy of the approximate transient responses and their sensitivities through the numerical examples. In this section, the computational efficiency of ROMs is compared with the



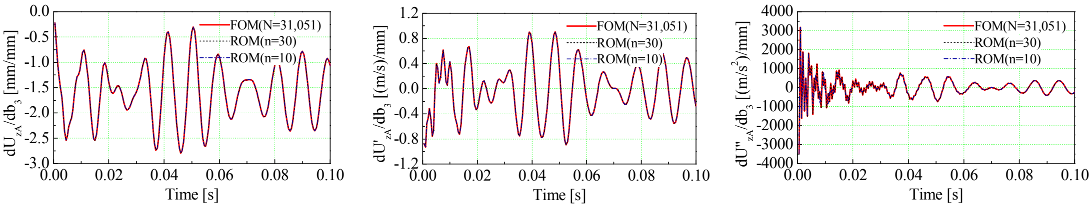
(a) Displacement (b) Velocity (c) Acceleration

Fig. 4. Design sensitivities of transient responses at A w.r.t. b_1 (FOM and ROMs).



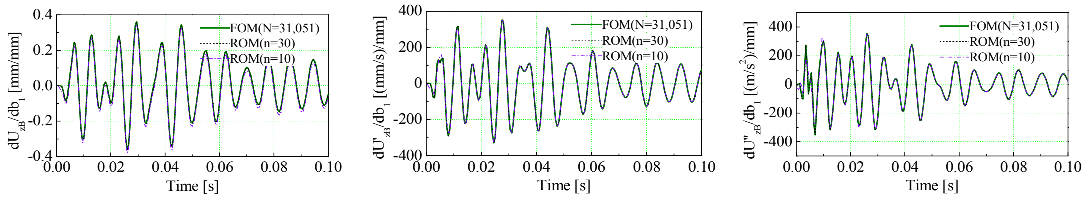
(a) Displacement (b) Velocity (c) Acceleration

Fig. 5. Design sensitivities of transient responses at A w.r.t. b_2 (FOM and ROMs).



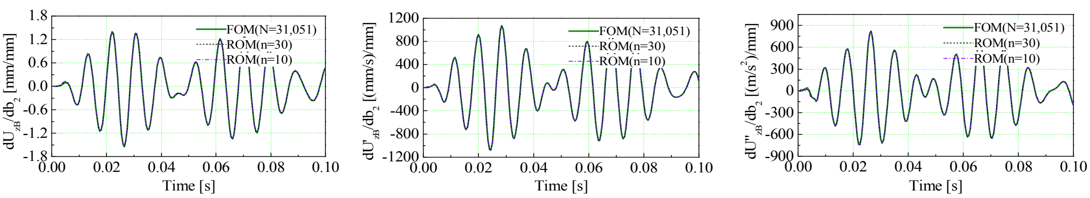
(a) Displacement (b) Velocity (c) Acceleration

Fig. 6. Design sensitivities of transient responses at A w.r.t. b_3 (FOM and ROMs).



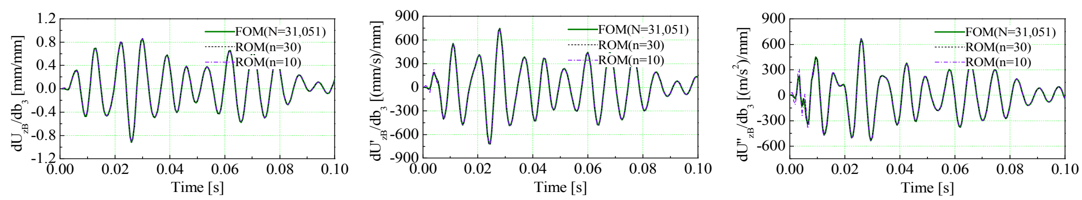
(a) Displacement (b) Velocity (c) Acceleration

Fig. 7. Design sensitivities of transient responses at B w.r.t. b_1 (FOM and ROMs).



(a) Displacement (b) Velocity (c) Acceleration

Fig. 8. Design sensitivities of transient responses at B w.r.t. b_2 (FOM and ROMs).



(a) Displacement (b) Velocity (c) Acceleration

Fig. 9. Design sensitivities of transient responses at B w.r.t. b_3 (FOM and ROMs).

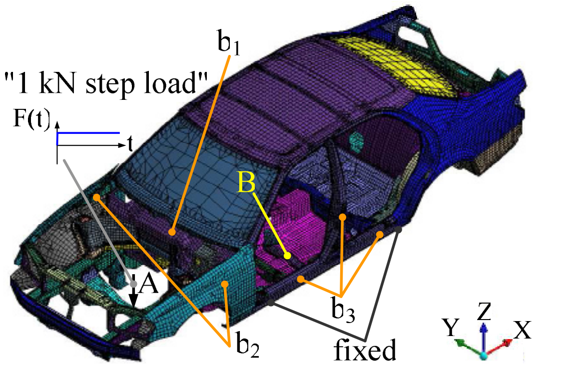
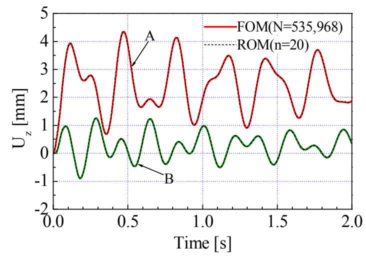
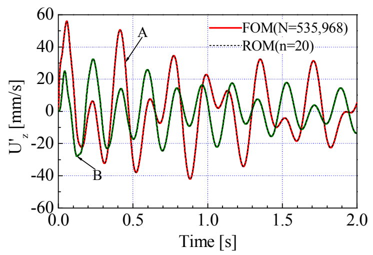


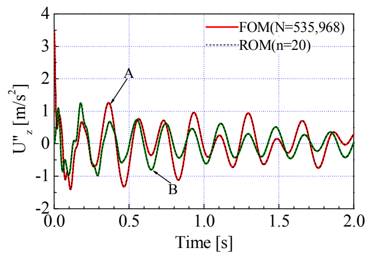
Fig. 10. Finite element model of a car body and the definition of design variables.



(a) Displacement in the Z-direction



(b) Velocity in the Z-direction



(c) Acceleration in the Z-direction

Fig. 11. Transient responses at points A and B (FOM and ROM (n = 20)).

FOM. The calculations were performed using MATLAB on an HP workstation with dual Xeon W5590 processors and 96 GB RAM.

For the stiffened plate problem, the transient simulation using FOM takes about 112 s. On the other hand, ROMs with n = 10, 30, and 50 need highly reduced computational costs, that is, 4.13, 5.46, and 7.02 s, respectively. The computation times for ROMs are less than 6.3% of those for FOM. The computation time of FOM for transient sensitivity with respect to each design variable is roughly 222 s, while the ROM of order 30, for example, takes 5.4 s to generate the Krylov vectors and approximately 0.8 s to calculate the transient sensitivity. The computational cost for calculating transient sensitivity is almost twice that of calculating the transient response because the transient sensitivity calculation needs the solution of state vector x in advance, as depicted in Eq. (2). Transient sensitivity calculations from ROMs with n = 10, 30, and 50 take 4.53, 6.18, and 7.7 s, that is, 2%, 2.8%, and 3.5% of that of the FOM, respectively.

In the case of the car body problem, the transient simulation using FOM takes about 38,430 s. On the other hand, ROMs with n = 20, 60, and 100 need highly reduced computational costs, that is, 94.8, 186.9, and 282.5 s, respectively. The com-

Table 1. Computation times for the transient responses and their sensitivities.

(a) Stiffened plate

Computation time(s)	FOM	ROM		
	N = 31,051	n = 10	n = 30	n = 50
Preparation of the system matrices	-	3	3	3
Generation of ROMs	-	1.1	2.4	3.8
Calculation of transient responses	112	0.03	0.06	0.22
Calculation of transient DSA	222	0.43	0.78	1.1

(b) Car body

Computation time(s)	FOM	ROM		
	N = 535,968	n = 20	n = 60	n = 100
Preparation of the system matrices	-	40	40	40
Generation of ROMs	-	54	145	240
Calculation of transient responses	38,432	0.8	1.9	2.5
Calculation of transient DSA	79,200	4.2	6.8	23.2

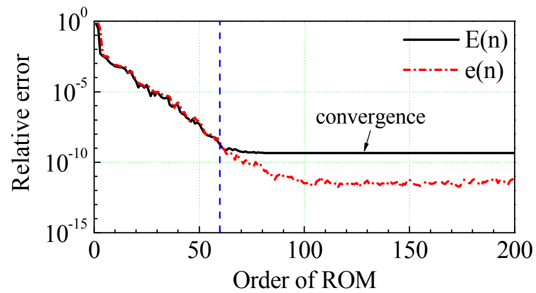
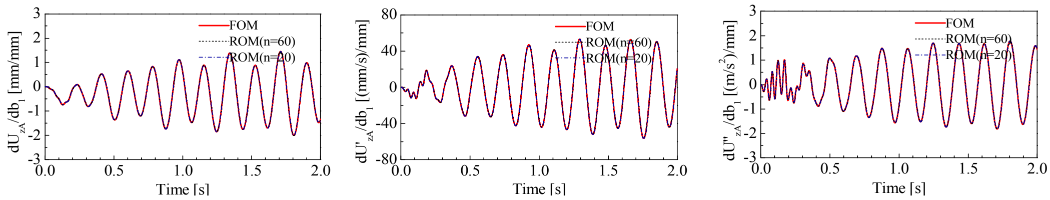
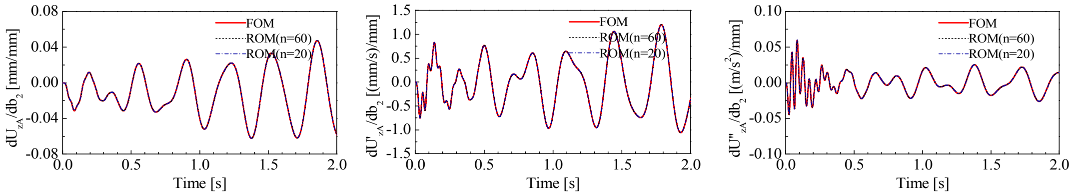


Fig. 12. Relative error and error indicator for transient responses of the car body model.



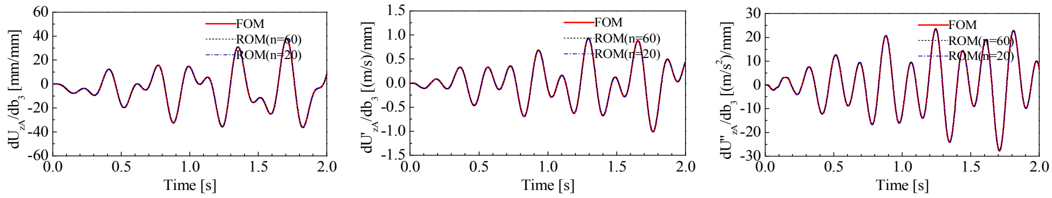
(a) Displacement (b) Velocity (c) Acceleration

Fig. 13. Design sensitivities of transient responses at A w.r.t. b_1 (FOM and ROMs).



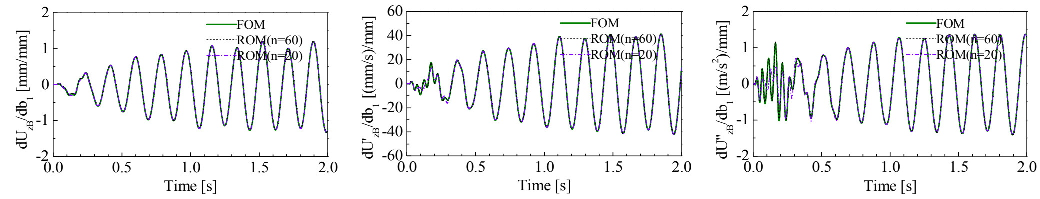
(a) Displacement (b) Velocity (c) Acceleration

Fig. 14. Design sensitivities of transient responses at A w.r.t. b_2 (FOM and ROMs).



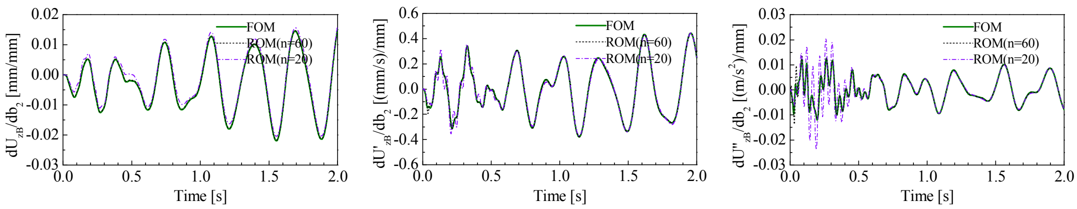
(a) Displacement (b) Velocity (c) Acceleration

Fig. 15. Design sensitivities of transient responses at A w.r.t. b_3 (FOM and ROMs).



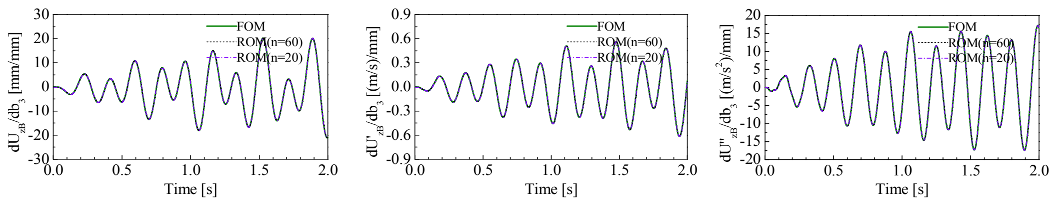
(a) Displacement (b) Velocity (c) Acceleration

Fig. 16. Design sensitivities of transient responses at B w.r.t. b_1 (FOM and ROMs).



(a) Displacement (b) Velocity (c) Acceleration

Fig. 17. Design sensitivities of transient responses at B w.r.t. b_2 (FOM and ROMs).



(a) Displacement (b) Velocity (c) Acceleration

Fig. 18. Design sensitivities of transient responses at B w.r.t. b_3 (FOM and ROMs).

putation time for the ROM of order 60 (which is accurate enough for both transient response and its sensitivity), is less than 0.49% of that for the FOM. The computation time of FOM for transient sensitivity with respect to each design variable is roughly 79,200 s, while the ROM of order 60, for example, takes 185 s to generate the Krylov vectors and 6.8 s to calculate the transient sensitivity. Transient sensitivity calculations from ROMs with n = 20, 60, and 100 take 98.2, 191.8, and 303.2 s, that is, 0.13%, 0.24%, and 0.38% of that of the FOM, respectively.

A considerable reduction is obtained in the computational costs for transient responses and their sensitivity because of the use of ROMs. The use of ROMs becomes more efficient as the size of FOM increases. The extra computational cost to prepare the system matrices and generate ROMs is minor compared to the time integration of the FOMs. Note that the computation times in Table 1 may vary slightly, depending on the configuration of the computer used for operation, such as the I/O rates of the hard disk drives and the number of processes.

4. Conclusion

Calculation of transient dynamic responses and their sensitivities using the Krylov subspace-based MOR, shows that a considerable reduction in computation time and a good agreement with those provided by the FOM can be achieved. In the methodology, the ROMs generated from the original FOM using implicit moment-matching through the Arnoldi process are used to calculate the transient response and its design sensitivity. Newmark's time integration method is employed to calculate transient responses and their design sensitivities. Concretely, the following conclusions can be drawn from this study.

(1) For a stiffened plate with 31,051 DOF, a ROM of order 10 gives fairly accurate approximations of displacement and velocity compared to those from the FOM. In the case of a car body with 535,992 DOF, all the transient responses from a ROM of order 20 are visually almost indistinguishable from the exact transient responses using the FOM. However, it is noted that one needs to increase the order of ROM further if the accuracy level of approximate displacement is necessary for approximate acceleration.

(2) For the proper order of ROM in terms of accuracy and efficiency, the relation $E(n) \approx e(n)$ can be used to determine an optimal order of ROM because the structural dynamic examples in this paper have shown that the $E(n) \approx e(n)$ relation is valid.

(3) The assumption that the Krylov basis vectors are treated as constant with respect to the perturbation of a design variable seems feasible for transient responses as well as the frequency response case. With this assumption, the transient sensitivities calculated from a ROM with n = 30 for the stiffened plate and n = 60 for the car body perfectly match all the transient sensitivities from the FOMs. However, if the same order of ROM is used, the accuracy of the transient sensitivities slightly decreases compared to that of the transient responses only.

(4) In general, the calculation of Krylov basis vectors for the projection matrix is computationally less expensive than modal eigenvectors. Even numerical computation for Krylov vectors is slightly less expensive than that of LDRVs because of the mass orthonormality of LDRVs; therefore, the proposed method is significantly efficient in approximating transient response and its sensitivity, provided that the same formulation in time integration is used.

Therefore, large-size transient FE models which have the problem of high computational cost in gradient-based optimization iterations because of repeated transient analysis can be efficiently handled using calculation of transient response and its design sensitivity analysis through the suggested model order reduction.

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Jeong Sam Han received his B.S. degree in Mechanical Engineering from Kyungpook National University, Korea, in 1995. He then went on to receive his M.S. and Ph.D. degrees from KAIST, Korea, in 1997 and 2003, respectively. Dr. Han is currently a professor at the Department of Mechanical Design Engineering at Andong National University, Korea. His research interests cover the areas of model order reduction, structural optimization, and rotordynamics, etc.