Analytical sensitivity analysis of dynamic problems with direct differentiation of generalized- α time integration

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Abstract

Generalized- α time integration is a generalization of several time integration schemes that can be use in the analysis of dynamic systems. Sensitivity analysis is used in numerical methods of design optimization, uncertainty analysis, parameter fitting and for simply calculating the sensitivities of a design to certain parameters. Analytical sensitivity analysis reduces the computational effort compared with numerical analysis and is therefore essential in efficient gradient-based design optimization. In this study, the sensitivity equations of the generalized- α time integration via direct differentiation are introduced. These are then compared with numerical sensitivities via forward differencing and Newmark- β in terms of accuracy and performance. An example is shown for both linear structural dynamics and flexible multibody dynamics.

Keywords: Sensitivity analysis, Time integration, Structural dynamics, Flexible multibody dynamics

Nomenclature

$(\cdot)$ scalar	$\ddot{q}$ generalized acceleration
$\underline{(\cdot)}$ vector	t time
$\underline{\underline{(\cdot)}}$ two-dimensional matrix	F force
$\underline{\underline{\underline{(\cdot)}}}$ three-dimensional matrix	J Jacobian w.r.t. q
$\underline{\underline{\underline{\underline{(\cdot)}}}}$ fourth-dimensional matrix	R residual
d damping	$\beta, \gamma, \alpha_m, \alpha_f$ time integration constants
k stiffness	λ Lagrangian multiplier
m mass	Φ kinematic constraint
q generalized position	∇ sensitivities w.r.t. x (total derivative)
$\dot{q}$ generalized velocity	∂ partial derivatives w.r.t. x
	$\frac{\partial(\cdot)}{\partial(\cdot)}$ partial derivative

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1. Introduction

Efficient sensitivity analysis is the centerpiece of efficient and effective gradient-based design optimization and can be used in other important analyses such as parameter fitting. In transient problems, sensitivity analysis must be extended to the time integration. A number of studies have been carried out for sensitivity analysis in transient structural dynamics and multibody dynamics, see for example [1, 2, 3, 4, 5] for structural dynamics and [6, 7, 8, 9, 10, 11, 12, 13] for multibody dynamics.

The generalized- α family of time integration methods offers a broad range of time integrators and will therefore be used here. The α -methods add numerical damping to the system to avoid stability problems. This method has found usages in both nonlinear structural dynamics and multibody dynamics. Multibody dynamics addresses the dynamic response with kinematic constraints. Rigid multibody dynamics considers the bodies rigid, while flexible multibody dynamics allows for deformation in the bodies of the system. Applications will be shown to both linear structural dynamics and flexible multibody dynamics.

In the dynamic systems addressed, the transient response (in time domain) is of interest and therefore a temporal discretization is applied. The calculation of the system responses, here position, velocity and acceleration, can be carried out with explicit or implicit time integration methods. Implicit time integration allows for larger time steps than explicit methods, which is bounded by the Courant criterion to remain stable [14]. Newmark introduced an implicit integration scheme, now referred to as Newmark- β in 1959 with two integration parameters γ and β [15]. The Hilber–Hughes–Taylor (HHT) method was introduced in 1977 to improve upon Newmark with the additional integration parameter α_f for numerical damping [16], while the Wood–Bossak–Zienkiewicz (WBZ, also Bossak or Wood) introduced the parameter α_m [17]. Generalized- α was introduced by Chung and Hulbert in 1993 [18] to generalize all these methods with the integration parameters α_m , α_f , β and γ . All parameters can be controlled by a single value, which is the level of numerical damping ρ_∞ ranging from zero, being the highest amount of damping, to unity, being none. The choice of this value can affect the correctness of the response.

This work is concerned with the sensitivity analysis, which is used when one or more parameters effect the system responses. This can be of interest for investigating the sensitivities themselves or for uncertainty analysis and design optimization. Methods for sensitivity analysis include analytical, numerical, complex step and algorithmic approaches [19]. This study will limit itself to analytical sensitivity analysis, which is further divided into direct differentiation (also known as forward sensitivity analysis) and the adjoint variable method (also known as backward sensitivity analysis). The scope here is the investigation of direct differentiation of the generalized- α method. This work is an extension of [20] in which Newmark- β sensitivities are developed and is based on [1, 3]. Newmark- β serves as a comparison.

This work first generally introduces generalized- α time integration. Afterwards the sensitivity equations are introduced for structural dynamics and flexible multibody dynamics, respectively. A numerical example is shown for each and results are provided of both primal and sensitivity analysis in comparison with Newmark- β time integration. We close with a conclusion, including discussion of this work. Further, the derivation of the effective system matrices is provided in the appendix.

2. Sensitivity analysis with generalized- α time integration

In this section we introduce the equations for an acceleration-form (a-form) generalized- α time integration using a predictor–corrector scheme. The acceleration-form refers to the formulation, in which the acceleration is the variable for which is being solved, and is contrasted by the displacement-form (d-form), where the displacement is the primary variable. The predictor–corrector scheme allows for nonlinear terms in the governing equation in which the predictor values are used to determine these values in the nonlinear solver,

Figure 1: Time integration with — acceleration, — $\gamma = 0.5$, — $\gamma = 0.75$

e.g. Newton–Raphson. In this work, we extend this well-established method by directly differentiating both the equations of the time integration as well as the governing equations. We consider both linear structural dynamics as well as flexible multibody dynamics, which is intrinsically nonlinear.

2.1. Generalized- α time integration

In this section, the method for primary and sensitivity analysis with generalized- α time integration is introduced. The basis of which are the Newmark’s equations for the updated position $\underline{q}$ and velocity vectors $\underline{\dot{q}}$ with the calculated value of the acceleration vector $\underline{\ddot{q}}$,

$$\underline{q}_{n+1} = \underbrace{\underline{q}_n + \Delta t \underline{\dot{q}}_n + \left(\frac{1}{2} - \beta\right) \Delta t^2 \underline{\ddot{q}}_n}_{\text{predictor } \underline{q}_{\text{pred}}} + \underbrace{\beta \Delta t^2 \underline{\ddot{q}}_{n+1}}_{\text{corrector}}, \quad (1)$$

$$\underline{\dot{q}}_{n+1} = \underbrace{\underline{\dot{q}}_n + (1 - \gamma) \Delta t \underline{\ddot{q}}_n}_{\text{predictor } \underline{\dot{q}}_{\text{pred}}} + \underbrace{\gamma \Delta t \underline{\ddot{q}}_{n+1}}_{\text{corrector}}, \quad (2)$$

where γ and β are the Newmark integration parameters. Though the simulation will be evaluated at the times t_n and t_{n+1} , values at intermediate points will be approximated. The position $\underline{q}$ and velocity $\underline{\dot{q}}$ use time $t_{n+1} - \alpha_f$ and the acceleration $\underline{\ddot{q}}$ uses time $t_{n+1} - \alpha_m$, giving the linear acceleration approximations (see fig. 1),

$$\underline{q}_{n+1-\alpha_f} = (1 - \alpha_f) \underline{q}_{n+1} + \alpha_f \underline{q}_n, \quad (3)$$

$$\underline{\dot{q}}_{n+1-\alpha_f} = (1 - \alpha_f) \underline{\dot{q}}_{n+1} + \alpha_f \underline{\dot{q}}_n, \quad (4)$$

$$\underline{\ddot{q}}_{n+1-\alpha_m} = (1 - \alpha_m) \underline{\ddot{q}}_{n+1} + \alpha_m \underline{\ddot{q}}_n, \quad (5)$$

where α_m and α_f are integration parameters. A predictor–corrector scheme is used in order to accommodate nonlinear calculation and state-dependency of the system parameters, i.e. system matrices with respect to

position and velocity. The predicted state variables with Newmark's equations are

$$\underline{q}_{\text{pred}} = \underline{q}_n + \Delta t \underline{\dot{q}}_n + \left(\frac{1}{2} - \beta \right) \Delta t^2 \underline{\ddot{q}}_n, \quad (6)$$

$$\underline{\dot{q}}_{\text{pred}} = \underline{\dot{q}}_n + (1 - \gamma) \Delta t \underline{\ddot{q}}_n, \quad (7)$$

and we calculate $\underline{\ddot{q}}_{n+1}$ using the effective system equations (see below for explanation for structural dynamics and flexible multibody dynamics, respectively). The predicted values are then corrected with the Newmark's equations,

$$\underline{q}_{n+1} = \underline{q}_{\text{pred}} + \beta \Delta t^2 \underline{\ddot{q}}_{n+1}, \quad (8)$$

$$\underline{\dot{q}}_{n+1} = \underline{\dot{q}}_{\text{pred}} + \gamma \Delta t \underline{\ddot{q}}_{n+1}. \quad (9)$$

For the sensitivity analysis within the generalized- α time integration, we use direct differentiation of the approximations,

$$\underline{\underline{\nabla q}}_{n+1-\alpha_f} = (1 - \alpha_f) \underline{\underline{\nabla q}}_{n+1} + \alpha_f \underline{\underline{\nabla q}}_n, \quad (10)$$

$$\underline{\underline{\nabla \dot{q}}}_{n+1-\alpha_f} = (1 - \alpha_f) \underline{\underline{\nabla \dot{q}}}_{n+1} + \alpha_f \underline{\underline{\nabla \dot{q}}}_n, \quad (11)$$

$$\underline{\underline{\nabla \ddot{q}}}_{n+1-\alpha_m} = (1 - \alpha_m) \underline{\underline{\nabla \ddot{q}}}_{n+1} + \alpha_m \underline{\underline{\nabla \ddot{q}}}_n, \quad (12)$$

The same direct differentiation is applied to the predictors, which are then defined by

$$\underline{\underline{\nabla q}}_{\text{pred}} = \underline{\underline{\nabla q}}_n + \Delta t \underline{\underline{\nabla \dot{q}}}_n + \left(\frac{1}{2} - \beta \right) \Delta t^2 \underline{\underline{\nabla \ddot{q}}}_n, \quad (13)$$

$$\underline{\underline{\nabla \dot{q}}}_{\text{pred}} = \underline{\underline{\nabla \dot{q}}}_n + (1 - \gamma) \Delta t \underline{\underline{\nabla \ddot{q}}}_n. \quad (14)$$

After calculating $\underline{\underline{\nabla \ddot{q}}}_{n+1}$ by use of the effective sensitivity system (see below for explanation for structural dynamics and flexible multibody dynamics, respectively), the following correctors are used:

$$\underline{\underline{\nabla q}}_{n+1} = \underline{\underline{\nabla q}}_{\text{pred}} + \beta \Delta t^2 \underline{\underline{\nabla \ddot{q}}}_{n+1}, \quad (15)$$

$$\underline{\underline{\nabla \dot{q}}}_{n+1} = \underline{\underline{\nabla \dot{q}}}_{\text{pred}} + \gamma \Delta t \underline{\underline{\nabla \ddot{q}}}_{n+1}. \quad (16)$$

For nonlinear analysis, a Newton solver can be integrated into the solving routine. This will be explained with flexible multibody systems below in § 2.3.

The time integration constants of generalized- α are α_m , α_f , β and γ and through their choice can lead to a number of established time integration methods, including the Newmark family of integrators, Hilber–Hughes–Taylor and Wood–Bossak–Zienkiewicz. Therefore, this can then be referred to as the α -family of time integrators. The equations introduced above in this section can therefore be used generally within this family. Specifically for the generalized- α time integration used here, the choice of integration constants can be tied to a single user-defined parameter, denoted as ρ_∞ [18],

$$\alpha_m = \frac{2\rho_\infty - 1}{\rho_\infty + 1}, \quad (17)$$

$$\alpha_f = \frac{\rho_\infty}{\rho_\infty + 1}, \quad (18)$$

$$\gamma = \frac{1}{2} - \alpha_m + \alpha_f, \quad (19)$$

$$\beta = \frac{1}{4} (1 - \alpha_m + \alpha_f)^2. \quad (20)$$

The value ρ_∞ is sometimes referred to as the (numerical) damping ratio and this is limited to a range of $[0, 1]$. The value $\rho_\infty = 1$ returns Newmark- β retaining frequencies are preserved, while $\rho_\infty = 0$ annihilates all frequencies above $\frac{\Delta t}{T}$ after one time step in which T is the period of the highest frequency of interest. The choice of the numerical damping parameter term for generalized- α time integration is critical for proper results. As this study develops a general framework for this methodology, this will not be addressed here and the reader is referred to [18, 21, 22, 23]. In this study, we use a moderate value of $\rho_\infty = 0.55$, though the sensitivity analysis methodology developed is general and independent of this parameter value.

2.2. Structural dynamics

The governing equation for linear structural dynamics is defined by the following second-order equation of motion:

$$\underline{\underline{m}}\ddot{\underline{q}}(t) + \underline{\underline{d}}\dot{\underline{q}}(t) + \underline{\underline{k}}\underline{q}(t) - \underline{F}(t) = \underline{0}, \quad (21)$$

where $\underline{\underline{m}}$ is the mass matrix, $\underline{\underline{d}}$ is the damping matrix, $\underline{\underline{k}}$ is the stiffness matrix and $\underline{F}$ is the external force vector. For linear structural dynamics the system matrices are constant and independent of position and time. For the solving scheme, we add the residual force vector $\underline{R}(t)$, which is to be zero (to an allowable value) at all times, to the right-hand side. The α -family of integration methods use intermediate point approximations between t_n and t_{n+1} , namely $t_{n+1-\alpha_f}$ and $t_{n+1-\alpha_m}$, revealing

$$\underline{R}_{n+1-\alpha_f} = \underline{\underline{m}}\ddot{\underline{q}}_{n+1-\alpha_m} + \underline{\underline{d}}\dot{\underline{q}}_{n+1-\alpha_f} + \underline{\underline{k}}\underline{q}_{n+1-\alpha_f} - \underline{F}_{n+1-\alpha_f}, \quad (22)$$

where the linear approximation of the intermediate external force is

$$\underline{F}_{n+1-\alpha_f} = (1 - \alpha_f)\underline{F}_{n+1} + \alpha_f\underline{F}_n. \quad (23)$$

The effective equation of motion is defined by

$$\underline{\underline{m}}_{\text{eff}}\ddot{\underline{q}}_{n+1} = \underline{F}_{\text{eff}}, \quad (24)$$

where

$$\underline{\underline{m}}_{\text{eff}} = (1 - \alpha_m)\underline{\underline{m}} + (1 - \alpha_f)\gamma\Delta t\underline{\underline{d}} + (1 - \alpha_f)\beta\Delta t^2\underline{\underline{k}}, \quad (25)$$

$$\begin{aligned} \underline{F}_{\text{eff}} = & \underline{F}_{n+1-\alpha_f} - \alpha_m\underline{\underline{m}}\ddot{\underline{q}}_n + \\ & - \underline{\underline{d}}\left((1 - \alpha_f)\dot{\underline{q}}_{\text{pred}} + \alpha_f\dot{\underline{q}}_n\right) + \\ & - \underline{\underline{k}}\left((1 - \alpha_f)\underline{q}_{\text{pred}} + \alpha_f\underline{q}_n\right). \end{aligned} \quad (26)$$

For the derivation of the effective mass matrix $\underline{\underline{m}}_{\text{eff}}$ and effective force vector $\underline{F}_{\text{eff}}$ for generalized- α method, see § Appendix A.1.

The sensitivity analysis is derived using the direct differentiation which is applied to the governing equation (22). This reveals the sensitivity of the force balance for the α -family of integration methods as

$$\begin{aligned} \underline{\underline{\nabla R}}_{n+1-\alpha_f} = & \underline{\underline{\nabla m}}\ddot{\underline{q}}_{n+1-\alpha_m} + \underline{\underline{m}}\underline{\underline{\nabla \ddot{q}}}_{n+1-\alpha_m} + \\ & + \underline{\underline{\nabla d}}\dot{\underline{q}}_{n+1-\alpha_f} + \underline{\underline{d}}\underline{\underline{\nabla \dot{q}}}_{n+1-\alpha_f} + \\ & + \underline{\underline{\nabla k}}\underline{q}_{n+1-\alpha_f} + \underline{\underline{k}}\underline{\underline{\nabla q}}_{n+1-\alpha_f} + \\ & - \underline{\underline{\nabla F}}_{n+1-\alpha_f}, \end{aligned} \quad (27)$$

with the intermediate external force sensitivity is found with the approximation

$$\underline{\underline{F}}_{n+1-\alpha_f} = (1 - \alpha_f) \underline{\underline{F}}_{n+1} + \alpha_f \underline{\underline{F}}_n. \quad (28)$$

The effective equation of motion for sensitivities is defined by the derivative of (24),

$$\underline{\underline{m}}_{\text{eff}} \underline{\underline{\ddot{q}}}_{n+1} = \underline{\underline{F}}_{\text{eff,pseudo}},$$

where

$$\begin{aligned} \underline{\underline{F}}_{\text{eff,pseudo}} = & (1 - \alpha_f) \underline{\underline{F}}_{n+1} + \alpha_f \underline{\underline{F}}_n + \\ & - \left(\underline{\underline{\nabla m}} \left((1 - \alpha_m) \underline{\underline{\dot{q}}}_{n+1} + \alpha_m \underline{\underline{\dot{q}}}_n \right) + \alpha_m \underline{\underline{m}} \underline{\underline{\ddot{q}}}_n \right) + \\ & - \left(\underline{\underline{\nabla d}} \left((1 - \alpha_f) \underline{\underline{\dot{q}}}_{n+1} + \alpha_f \underline{\underline{\dot{q}}}_n \right) + \underline{\underline{d}} \left((1 - \alpha_f) \underline{\underline{\dot{q}}}_{\text{pred}} + \alpha_f \underline{\underline{\dot{q}}}_n \right) \right) + \\ & - \left(\underline{\underline{\nabla k}} \left((1 - \alpha_f) \underline{\underline{q}}_{n+1} + \alpha_f \underline{\underline{q}}_n \right) + \underline{\underline{k}} \left((1 - \alpha_f) \underline{\underline{q}}_{\text{pred}} + \alpha_f \underline{\underline{q}}_n \right) \right). \end{aligned} \quad (29)$$

For the derivation of the effective mass matrix $\underline{\underline{m}}_{\text{eff}}$ and effective pseudo force $\underline{\underline{F}}_{\text{eff,pseudo}}$ for generalized- α method, see § Appendix A.1 and § Appendix A.2.

2.3. Flexible multibody dynamics

Flexible multibody dynamics is the analysis of mechanical systems consisting of flexible bodies constrained by kinematic joints modeled with differential–algebraic equations. This work build on previous work of analytical sensitivity analysis with multibody dynamics, including [24, 25, 13]. In addition to the kinematic constraints w.r.t. structural dynamics, multibody dynamics also must integrate a nonlinear solver in order to consider the position and dependencies of the system matrices and vectors. This will be carried out with Newton steps.

The flexible multibody system is modeled with the floating frame of reference formulation [26, 27, 28]. The generic index-3 differential–algebraic equation for a flexible multibody system with holonomic constraints is written as follows:

$$\underline{\underline{m}}(\underline{q}, t) \underline{\underline{\ddot{q}}}(t) + \underline{\underline{d}}(\underline{q}, t) \underline{\underline{\dot{q}}}(t) + \underline{\underline{k}}(\underline{q}, t) \underline{q}(t) + \underline{\underline{J}}_{\Phi}^T(\underline{q}, t) \underline{\underline{\lambda}}(t) = \underline{\underline{F}}_{\text{ext}}(\underline{q}, \underline{\dot{q}}, t) + \underline{\underline{F}}_v(\underline{q}, \underline{\dot{q}}, t), \quad (30)$$

$$\underline{\underline{\Phi}}(\underline{q}, t) = \underline{0}, \quad (31)$$

where $\underline{q}$, $\underline{\dot{q}}$ and $\underline{\ddot{q}}$ are the generalized position, velocity and acceleration vectors, $\underline{\underline{\lambda}}$ is the vector of Lagrange multipliers of kinematic constraints, the matrices $\underline{\underline{m}}$, $\underline{\underline{d}}$, and $\underline{\underline{k}}$ are the mass, damping and stiffness matrices, $\underline{\underline{J}}_{\Phi}$ is the Jacobian matrix of kinematic constraints, $\underline{\underline{F}}_{\text{ext}}$ is the vector of external forces, $\underline{\underline{F}}_v$ is the quadratic velocity vector and $\underline{\underline{\Phi}}$ is the vector of kinematic constraints at position level. In this work, we will be addressing an index-1 differential–algebraic equation in which the kinematic constraint function is differentiated twice with respect to time,

$$\underline{\underline{m}} \underline{\underline{\ddot{q}}} + \underline{\underline{d}} \underline{\underline{\dot{q}}} + \underline{\underline{k}} \underline{q} + \underline{\underline{J}}_{\Phi}^T \underline{\underline{\lambda}} = \underline{\underline{F}}_{\text{ext}} + \underline{\underline{F}}_v, \quad (32)$$

$$\underline{\underline{J}}_{\Phi} \underline{\underline{\ddot{q}}} = \underline{\underline{F}}_c, \quad (33)$$

where $\underline{\underline{F}}_c$ is the right-hand side of acceleration constraints. The generalized- α method is based on

$$(\underline{\underline{m}} \underline{\underline{\ddot{q}}})_{n+1-\alpha_m} + (\underline{\underline{d}} \underline{\underline{\dot{q}}})_{n+1-\alpha_f} + (\underline{\underline{k}} \underline{q})_{n+1-\alpha_f} + (\underline{\underline{J}}_{\Phi}^T \underline{\underline{\lambda}})_{n+1-\alpha_m} = \underline{\underline{F}}_{\text{ext}, n+1-\alpha_f} + \underline{\underline{F}}_{v, n+1-\alpha_f}, \quad (34)$$

$$(\underline{\underline{J}}_{\Phi} \underline{\underline{\ddot{q}}})_{n+1-\alpha_m} = \underline{\underline{F}}_{c, n+1-\alpha_f}, \quad (35)$$

with the intermediate approximations of all force terms of the equations of motion. These intermediate approximations are shown in § Appendix B.1. Inserting the intermediate approximations of the force terms acting on the flexible multibody system leads to the equations of motion in residual form given by

$$\begin{aligned} \underline{R}_{1,n+1-\alpha_f} = & (1-\alpha_m)\underline{m}_{n+1}\ddot{\underline{q}}_{n+1} + \alpha_m\underline{m}_n\ddot{\underline{q}}_n + (1-\alpha_f)\underline{d}_{n+1}\dot{\underline{q}}_{n+1} + \alpha_f\underline{d}_n\dot{\underline{q}}_n + \\ & + (1-\alpha_f)\underline{k}_{n+1}\underline{q}_{n+1} + \alpha_f\underline{k}_n\underline{q}_n + (1-\alpha_m)\underline{J}_{\Phi,n+1}^T\underline{\lambda}_{n+1} + \alpha_m\underline{J}_{\Phi,n}^T\underline{\lambda}_n + \\ & - (1-\alpha_f)\underline{F}_{\text{ext},n+1} - \alpha_f\underline{F}_{\text{ext},n} - (1-\alpha_f)\underline{F}_{v,n+1} - \alpha_f\underline{F}_{v,n}, \end{aligned} \quad (36)$$

$$\underline{R}_{2,n+1-\alpha_f} = (1-\alpha_m)\underline{J}_{\Phi,n+1}\ddot{\underline{q}}_{n+1} + \alpha_m\underline{J}_{\Phi,n}\ddot{\underline{q}}_n - (1-\alpha_f)\underline{F}_{c,n+1} - \alpha_f\underline{F}_{c,n}. \quad (37)$$

When the system matrices exhibit low-level nonlinearities and with very small time steps, the system matrices undergo negligible change between two times steps. Therefore in this case, these can be assumed to be constant for each residual calculation [29]. The equations of motion are then reduced to

$$\begin{aligned} \underline{R}_{1,n+1-\alpha_f} = & \underline{m}_{n+1-\alpha_m}\ddot{\underline{q}}_{n+1-\alpha_m} + \underline{d}_{n+1-\alpha_f}\dot{\underline{q}}_{n+1-\alpha_f} + \underline{k}_{n+1-\alpha_f}\underline{q}_{n+1-\alpha_f} + \underline{J}_{\Phi,n+1-\alpha_m}^T\underline{\lambda}_{n+1-\alpha_m} + \\ & - (1-\alpha_f)\underline{F}_{\text{ext},n+1} - \alpha_f\underline{F}_{\text{ext},n} - (1-\alpha_f)\underline{F}_{v,n+1} - \alpha_f\underline{F}_{v,n}, \end{aligned} \quad (38)$$

$$\underline{R}_{2,n+1-\alpha_f} = \underline{J}_{\Phi,n+1-\alpha_m}\ddot{\underline{q}}_{n+1-\alpha_m} - \underline{F}_{c,n+1-\alpha_f}. \quad (39)$$

This simplification avoids the need of the system parameters from the previous time step and has a limited impact on the results in the described cases. Nonetheless, the complete formulation, as shown (36) and (37), allowing for larger amounts of nonlinearity and larger time steps is used here.

The effective equation of motion is defined by

$$\begin{bmatrix} \underline{m}_{\text{eff}} & \underline{J}_{\Phi,\text{eff}}^T \\ \underline{J}_{\Phi,\text{eff}} & \underline{0} \end{bmatrix} \begin{bmatrix} \dot{\underline{q}}_{n+1} \\ \underline{\lambda}_{n+1} \end{bmatrix} = \begin{bmatrix} \underline{F}_{a,\text{eff}} \\ \underline{F}_{c,\text{eff}} \end{bmatrix}, \quad (40)$$

where

$$\underline{m}_{\text{eff}} = (1-\alpha_m)\underline{m}_{n+1} + (1-\alpha_f)\gamma\Delta t\underline{d}_{n+1} + (1-\alpha_f)\beta\Delta t^2\underline{k}_{n+1}, \quad (41)$$

$$\underline{J}_{\Phi,\text{eff}} = (1-\alpha_m)\underline{J}_{\Phi,n+1}, \quad (42)$$

$$\begin{aligned} \underline{F}_{a,\text{eff}} = & (1-\alpha_f)\underline{F}_{\text{ext},n+1} + \alpha_f\underline{F}_{\text{ext},n} + (1-\alpha_f)\underline{F}_{v,n+1} + \alpha_f\underline{F}_{v,n} - \alpha_m\underline{m}_n\ddot{\underline{q}}_n + \\ & - (1-\alpha_f)\underline{d}_{n+1}\dot{\underline{q}}_{\text{pred}} - \alpha_f\underline{d}_n\dot{\underline{q}}_n - (1-\alpha_f)\underline{k}_{n+1}\underline{q}_{\text{pred}} - \alpha_f\underline{k}_n\underline{q}_n - \alpha_m\underline{J}_{\Phi,n}^T\underline{\lambda}_n, \end{aligned} \quad (43)$$

$$\underline{F}_{c,\text{eff}} = (1-\alpha_f)\underline{F}_{c,n+1} + \alpha_f\underline{F}_{c,n} - \alpha_m\underline{J}_{\Phi,n}\dot{\underline{q}}_n. \quad (44)$$

The derivation of the effective equation of motion and the terms $\underline{m}_{\text{eff}}$, $\underline{J}_{\Phi,\text{eff}}$, $\underline{F}_{a,\text{eff}}$ and $\underline{F}_{c,\text{eff}}$ is shown in § Appendix B.1.

With flexible multibody dynamics, the system parameters including mass, damping, stiffness, constraints and forces are dependent on state variables. Therefore, a nonlinear solver is needed to solve the system and the Newton–Raphson method is used here of the following form:

$$\begin{bmatrix} \frac{\partial \underline{R}_{1,n+1-\alpha_f}}{\partial \dot{\underline{q}}_{n+1}} & \frac{\partial \underline{R}_{1,n+1-\alpha_f}}{\partial \underline{\lambda}_{n+1}} \\ \frac{\partial \underline{R}_{2,n+1-\alpha_f}}{\partial \dot{\underline{q}}_{n+1}} & \frac{\partial \underline{R}_{2,n+1-\alpha_f}}{\partial \underline{\lambda}_{n+1}} \end{bmatrix} \begin{bmatrix} \Delta \dot{\underline{q}}_{n+1} \\ \Delta \underline{\lambda}_{n+1} \end{bmatrix} + \begin{bmatrix} \underline{R}_{1,n+1-\alpha_f} \\ \underline{R}_{2,n+1-\alpha_f} \end{bmatrix} = \underline{0}. \quad (45)$$

With the dependencies shown in (30) and (31), the terms of the Jacobian matrix (tangent operator) of the residuals with respect to $\underline{\ddot{q}}_{n+1}$ and $\underline{\lambda}_{n+1}$ are given by,

$$\begin{aligned}
\frac{\partial \underline{R}_{1,n+1-\alpha_f}}{\partial \underline{\ddot{q}}_{n+1}} = & (1 - \alpha_m) \beta \Delta t^2 \frac{\partial \underline{m}_{n+1}}{\partial \underline{q}_{n+1}} \underline{\ddot{q}}_{n+1} + (1 - \alpha_m) \underline{m}_{n+1} + \\
& + (1 - \alpha_f) \beta \Delta t^2 \frac{\partial \underline{d}_{n+1}}{\partial \underline{q}_{n+1}} \underline{\dot{q}}_{n+1} + (1 - \alpha_f) \gamma \Delta t \underline{d}_{n+1} + \\
& + (1 - \alpha_f) \beta \Delta t^2 \frac{\partial \underline{k}_{n+1}}{\partial \underline{q}_{n+1}} \underline{q}_{n+1} + (1 - \alpha_f) \beta \Delta t^2 \underline{k}_{n+1} + \\
& + (1 - \alpha_m) \beta \Delta t^2 \frac{\partial \underline{J}_{\Phi,n+1}^T}{\partial \underline{q}_{n+1}} \underline{\lambda}_{n+1} + \\
& - (1 - \alpha_f) \left(\beta \Delta t^2 \frac{\partial F_{\text{ext},n+1}}{\partial \underline{q}_{n+1}} + \gamma \Delta t \frac{\partial F_{\text{ext},n+1}}{\partial \underline{\dot{q}}_{n+1}} \right) + \\
& - (1 - \alpha_f) \left(\beta \Delta t^2 \frac{\partial F_{v,n+1}}{\partial \underline{q}_{n+1}} + \gamma \Delta t \frac{\partial F_{v,n+1}}{\partial \underline{\dot{q}}_{n+1}} \right), \tag{46}
\end{aligned}$$

and

$$\begin{aligned}
\frac{\partial \underline{R}_{2,n+1-\alpha_f}}{\partial \underline{\ddot{q}}_{n+1}} = & (1 - \alpha_m) \beta \Delta t^2 \frac{\partial \underline{J}_{\Phi,n+1}}{\partial \underline{q}_{n+1}} \underline{\ddot{q}}_{n+1} + (1 - \alpha_m) \underline{J}_{\Phi,n+1} + \\
& - (1 - \alpha_f) \left(\beta \Delta t^2 \frac{\partial F_{c,n+1}}{\partial \underline{q}_{n+1}} + \gamma \Delta t \frac{\partial F_{c,n+1}}{\partial \underline{\dot{q}}_{n+1}} \right) \tag{47}
\end{aligned}$$

$$\frac{\partial \underline{R}_{1,n+1-\alpha_f}}{\partial \underline{\lambda}_{n+1}} = (1 - \alpha_m) \underline{J}_{\Phi,n+1}^T \tag{48}$$

$$\frac{\partial \underline{R}_{2,n+1-\alpha_f}}{\partial \underline{\lambda}_{n+1}} = \underline{0}. \tag{49}$$

The derivation of these terms is shown in § (Appendix B.2).

The direct differentiation of the equations of motion (36) and (37) leads to the governing equation of the sensitivity analysis,

$$\begin{aligned}
\underline{\nabla R}_{1,n+1-\alpha_f} = & (1 - \alpha_m) \underline{\nabla m}_{n+1} \underline{\ddot{q}}_{n+1} + (1 - \alpha_m) \underline{m}_{n+1} \underline{\nabla \ddot{q}}_{n+1} + \alpha_m \underline{\nabla m}_n \underline{\ddot{q}}_n + \alpha_m \underline{m}_n \underline{\nabla \ddot{q}}_n + \\
& + (1 - \alpha_f) \underline{\nabla d}_{n+1} \underline{\dot{q}}_{n+1} + (1 - \alpha_f) \underline{d}_{n+1} \underline{\nabla \dot{q}}_{n+1} + \alpha_f \underline{\nabla d}_n \underline{\dot{q}}_n + \alpha_f \underline{d}_n \underline{\nabla \dot{q}}_n + \\
& + (1 - \alpha_f) \underline{\nabla k}_{n+1} \underline{q}_{n+1} + (1 - \alpha_f) \underline{k}_{n+1} \underline{\nabla q}_{n+1} + \alpha_f \underline{\nabla k}_n \underline{q}_n + \alpha_f \underline{k}_n \underline{\nabla q}_n + \\
& + (1 - \alpha_m) \underline{\nabla J}_{\Phi,n+1}^T \underline{\lambda}_{n+1} + (1 - \alpha_m) \underline{J}_{\Phi,n+1}^T \underline{\nabla \lambda}_{n+1} + \alpha_m \underline{\nabla J}_{\Phi,n}^T \underline{\lambda}_n + \alpha_m \underline{J}_{\Phi,n}^T \underline{\nabla \lambda}_n + \\
& - (1 - \alpha_f) \underline{\nabla F}_{\text{ext},n+1} - \alpha_f \underline{\nabla F}_{\text{ext},n} - (1 - \alpha_f) \underline{\nabla F}_{v,n+1} - \alpha_f \underline{\nabla F}_{v,n}, \tag{50}
\end{aligned}$$

and

$$\begin{aligned} \underline{\underline{\nabla R}}_{2,n+1-\alpha_f} = & (1-\alpha_m) \underline{\underline{\nabla J}}_{\Phi,n+1} \underline{\underline{\ddot{q}}}_{n+1} + (1-\alpha_m) \underline{\underline{J}}_{\Phi,n+1} \underline{\underline{\nabla \ddot{q}}}_{n+1} + \alpha_m \underline{\underline{\nabla J}}_{\Phi,n} \underline{\underline{\ddot{q}}}_n + \alpha_m \underline{\underline{J}}_{\Phi,n} \underline{\underline{\nabla \ddot{q}}}_n + \\ & - (1-\alpha_f) \underline{\underline{\nabla F}}_{c,n+1} - \alpha_f \underline{\underline{\nabla F}}_{c,n}. \end{aligned} \quad (51)$$

The governing sensitivity equation of the effective system is defined by the derivative of (40),

$$\begin{bmatrix} \underline{\underline{m}}_{\text{eff}} & \underline{\underline{J}}_{\Phi,\text{eff}}^T \\ \underline{\underline{J}}_{\Phi,\text{eff}} & \underline{\underline{0}} \end{bmatrix} \begin{bmatrix} \underline{\underline{\ddot{q}}}_{n+1} \\ \underline{\underline{\lambda}}_{n+1} \end{bmatrix} = \begin{bmatrix} \underline{\underline{F}}_{a,\text{eff,pseudo}} \\ \underline{\underline{F}}_{c,\text{eff,pseudo}} \end{bmatrix}, \quad (52)$$

where

$$\begin{aligned} \underline{\underline{F}}_{a,\text{eff,pseudo}} = & (1-\alpha_f) \underline{\underline{\nabla F}}_{\text{ext},n+1} + \alpha_f \underline{\underline{\nabla F}}_{\text{ext},n} + (1-\alpha_f) \underline{\underline{\nabla F}}_{v,n+1} + \alpha_f \underline{\underline{\nabla F}}_{v,n} + \\ & - (1-\alpha_m) \underline{\underline{\nabla m}}_{n+1} \underline{\underline{\ddot{q}}}_{n+1} - \alpha_m \underline{\underline{\nabla m}}_n \underline{\underline{\ddot{q}}}_n - \alpha_m \underline{\underline{m}}_n \underline{\underline{\nabla \ddot{q}}}_n + \\ & - (1-\alpha_f) \underline{\underline{\nabla d}}_{n+1} \underline{\underline{\dot{q}}}_{n+1} - \alpha_f \underline{\underline{\nabla d}}_n \underline{\underline{\dot{q}}}_n - (1-\alpha_f) \underline{\underline{d}}_{n+1} \underline{\underline{\nabla \dot{q}}}_{\text{pred}} - \alpha_f \underline{\underline{d}}_n \underline{\underline{\nabla \dot{q}}}_n + \\ & - (1-\alpha_f) \underline{\underline{\nabla k}}_{n+1} \underline{\underline{q}}_{n+1} - \alpha_f \underline{\underline{\nabla k}}_n \underline{\underline{q}}_n - (1-\alpha_f) \underline{\underline{k}}_{n+1} \underline{\underline{\nabla q}}_{\text{pred}} - \alpha_f \underline{\underline{k}}_n \underline{\underline{\nabla q}}_n + \\ & - (1-\alpha_m) \underline{\underline{\nabla J}}_{\Phi,n+1}^T \underline{\underline{\lambda}}_{n+1} - \alpha_m \underline{\underline{\nabla J}}_{\Phi,n}^T \underline{\underline{\lambda}}_n - \alpha_m \underline{\underline{J}}_{\Phi,n}^T \underline{\underline{\nabla \lambda}}_n, \end{aligned} \quad (53)$$

$$\begin{aligned} \underline{\underline{F}}_{c,\text{eff,pseudo}} = & (1-\alpha_f) \underline{\underline{\nabla F}}_{c,n+1} + \alpha_f \underline{\underline{\nabla F}}_{c,n} + \\ & - (1-\alpha_m) \underline{\underline{\nabla J}}_{\Phi,n+1} \underline{\underline{\ddot{q}}}_{n+1} - \alpha_m \underline{\underline{\nabla J}}_{\Phi,n} \underline{\underline{\ddot{q}}}_n - \alpha_m \underline{\underline{J}}_{\Phi,n} \underline{\underline{\nabla \ddot{q}}}_n. \end{aligned} \quad (54)$$

The derivation of the effective mass matrix and the effective constraint Jacobian matrix is shown in § (Appendix B.1) and the derivation of the effective pseudo force terms is shown in § (Appendix B.3).

The Newton–Raphson step for the sensitivity analysis is given by

$$\begin{bmatrix} \frac{\partial \underline{\underline{\nabla R}}_{1,n+1-\alpha_f}}{\partial \underline{\underline{\nabla \ddot{q}}}_{n+1}} & \frac{\partial \underline{\underline{\nabla R}}_{1,n+1-\alpha_f}}{\partial \underline{\underline{\nabla \lambda}}_{n+1}} \\ \frac{\partial \underline{\underline{\nabla R}}_{2,n+1-\alpha_f}}{\partial \underline{\underline{\nabla \ddot{q}}}_{n+1}} & \frac{\partial \underline{\underline{\nabla R}}_{2,n+1-\alpha_f}}{\partial \underline{\underline{\nabla \lambda}}_{n+1}} \end{bmatrix} \begin{bmatrix} \underline{\underline{\Delta \nabla \ddot{q}}}_{n+1} \\ \underline{\underline{\Delta \nabla \lambda}}_{n+1} \end{bmatrix} + \begin{bmatrix} \underline{\underline{\nabla R}}_{1,n+1-\alpha_f} \\ \underline{\underline{\nabla R}}_{2,n+1-\alpha_f} \end{bmatrix} = \underline{\underline{0}}. \quad (55)$$

As shown in [20] the Jacobian of the residual sensitivity with respect to $\underline{\underline{\nabla \ddot{q}}}_{n+1}$ and $\underline{\underline{\nabla \lambda}}_{n+1}$ reduces to

$$\begin{bmatrix} \frac{\partial \underline{\underline{\nabla R}}_{1,n+1-\alpha_f}}{\partial \underline{\underline{\nabla \ddot{q}}}_{n+1}} & \frac{\partial \underline{\underline{\nabla R}}_{1,n+1-\alpha_f}}{\partial \underline{\underline{\nabla \lambda}}_{n+1}} \\ \frac{\partial \underline{\underline{\nabla R}}_{2,n+1-\alpha_f}}{\partial \underline{\underline{\nabla \ddot{q}}}_{n+1}} & \frac{\partial \underline{\underline{\nabla R}}_{2,n+1-\alpha_f}}{\partial \underline{\underline{\nabla \lambda}}_{n+1}} \end{bmatrix} = \begin{bmatrix} \frac{\partial \underline{\underline{R}}_{1,n+1-\alpha_f}}{\partial \underline{\underline{\ddot{q}}}_{n+1}} & \frac{\partial \underline{\underline{R}}_{1,n+1-\alpha_f}}{\partial \underline{\underline{\lambda}}_{n+1}} \\ \frac{\partial \underline{\underline{R}}_{2,n+1-\alpha_f}}{\partial \underline{\underline{\ddot{q}}}_{n+1}} & \frac{\partial \underline{\underline{R}}_{2,n+1-\alpha_f}}{\partial \underline{\underline{\lambda}}_{n+1}} \end{bmatrix} \underline{\underline{e}}, \quad (56)$$

wherefore a conventional solver can be used for the solution of the following:

$$\begin{bmatrix} \frac{\partial \underline{\underline{R}}_{1,n+1-\alpha_f}}{\partial \underline{\underline{\ddot{q}}}_{n+1}} & \frac{\partial \underline{\underline{R}}_{1,n+1-\alpha_f}}{\partial \underline{\underline{\lambda}}_{n+1}} \\ \frac{\partial \underline{\underline{R}}_{2,n+1-\alpha_f}}{\partial \underline{\underline{\ddot{q}}}_{n+1}} & \frac{\partial \underline{\underline{R}}_{2,n+1-\alpha_f}}{\partial \underline{\underline{\lambda}}_{n+1}} \end{bmatrix} \begin{bmatrix} \underline{\underline{\Delta \nabla \ddot{q}}}_{n+1} \\ \underline{\underline{\Delta \nabla \lambda}}_{n+1} \end{bmatrix} + \begin{bmatrix} \underline{\underline{\nabla R}}_{1,n+1-\alpha_f} \\ \underline{\underline{\nabla R}}_{2,n+1-\alpha_f} \end{bmatrix} = \underline{\underline{0}}. \quad (57)$$

Figure 2: Structural dynamics example

3. Numerical results

In this section, numerical results will be shown comparing the introduced method of generalized- α time integration with sensitivity analysis (introduced in § 2) with that of Newmark- β . The methods will be compared with applications to both structural dynamics as well as flexible multibody dynamics.

3.1. Structural dynamics

The linear structural dynamic problem used here as a demonstration example is based on [30] and shown schematically in fig. 2. This problem is defined by

$$\underbrace{\begin{bmatrix} m_1 & 0 & 0 \\ 0 & m_2 & 0 \\ 0 & 0 & m_3 \end{bmatrix}}_{\underline{m}} \underbrace{\begin{bmatrix} \ddot{q}_1 \\ \ddot{q}_2 \\ \ddot{q}_3 \end{bmatrix}}_{\underline{\ddot{q}}} + \underbrace{\begin{bmatrix} k_1 & -k_1 & 0 \\ -k_1 & k_1 + k_2 & -k_2 \\ 0 & -k_2 & k_2 \end{bmatrix}}_{\underline{k}} \underbrace{\begin{bmatrix} q_1 \\ q_2 \\ q_3 \end{bmatrix}}_{\underline{q}} - \underbrace{\begin{bmatrix} F_1 \\ 0 \\ 0 \end{bmatrix}}_{\underline{F}} = \underbrace{\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}}_{\underline{R}}, \quad (58)$$

with the prescribed displacement,

$$q_1 = \sin \omega t, \quad (59)$$

and the unitless values

$$\begin{aligned} m_1 &= 0, \\ m_2 &= 1, \\ m_3 &= 1, \\ k_1 &= 10^7, \\ k_2 &= 1, \\ \omega &= 1.2. \end{aligned}$$

The masses m_2 and m_3 as well as the stiffnesses k_1 and k_2 are considered design variables with respect to which the design sensitivities are calculated. Considering the prescribed displacement, this problem can be reduced to two degrees of freedom,

$$\underbrace{\begin{bmatrix} m_2 & 0 \\ 0 & m_3 \end{bmatrix}}_{\underline{m}} \underbrace{\begin{bmatrix} \ddot{q}_2 \\ \ddot{q}_3 \end{bmatrix}}_{\underline{\ddot{q}}} + \underbrace{\begin{bmatrix} k_1 + k_2 & -k_2 \\ -k_2 & k_2 \end{bmatrix}}_{\underline{k}} \underbrace{\begin{bmatrix} q_2 \\ q_3 \end{bmatrix}}_{\underline{q}} - \underbrace{\begin{bmatrix} k_1 q_1 \\ 0 \end{bmatrix}}_{\underline{F}} = \underbrace{\begin{bmatrix} 0 \\ 0 \end{bmatrix}}_{\underline{R}}, \quad (60)$$

Figure 3: Responses of the structural dynamic example calculated with — Newmark- β and — generalized- α

which we implement in our in-house solver framework SiMULi in the time $t = [0, 10]$, with time steps $\Delta t = 0.2618$ and the initial conditions

$$\begin{aligned} q_2 &= 0, \\ q_3 &= 0, \\ \dot{q}_2 &= 0, \\ \dot{q}_3 &= 0. \end{aligned}$$

The results for both Newmark- β and generalized- α time integration methods are shown in fig. 3. The numerical damping parameter of generalized- α time integration was set as $\rho_\infty = 0.55$. As expected with generalized- α time integration, the unphysical, high-frequent oscillatory behavior of the response can be avoided. As such, the beneficial effects of numerical damping with generalized- α time integration can be clearly seen in the velocity and acceleration of node 2, while maintaining the integrity of the other responses.

The sensitivity analysis developed above is applied and these results can be seen in fig. 4–6. Again here, the numerical damping allows for usable sensitivities after approximately 15 iterations for those sensitivities susceptible to stability issues, namely the position sensitivities, velocity sensitivities and acceleration sensitivities of node 2, but also velocity sensitivities and acceleration sensitivities of node 3. The number of time steps needed for the damping to take effect can be reduced by increasing the numerical damping parameter ρ_∞ towards unity, though also effecting the other responses to a greater degree. As time continues, the instability grows with Newmark- β time integration and therefore a clear advantage can be seen with generalized- α . It can be clearly seen how gradient-based solvers would struggle to use the gradient information provided with Newmark- β time integration.

For our modest case of four design variables, we show a speedup of two, where the speedup S is defined by the ratio of computational time for finite differencing t_{FD} to that of analytical sensitivities t_{ana} ,

$$S = \frac{t_{\text{FD}}}{t_{\text{ana}}}. \quad (61)$$

The computational time required for analytical sensitivity analysis represents approximately the ideal computational effort twice that of the primal analysis, i.e. analysis without sensitivity analysis. Computation

Figure 4: Position sensitivities ∇q of the structural dynamic example w.r.t. k_1 , k_2 , m_2 and m_3 calculated with — Newmark- β and — generalized- α

Figure 5: Velocity sensitivities $\nabla \dot{q}$ of the structural dynamic example w.r.t. k_1 , k_2 , m_2 and m_3 calculated with — Newmark- β and — generalized- α

Figure 6: Acceleration sensitivities $\nabla \ddot{q}$ of the structural dynamic example w.r.t. k_1 , k_2 , m_2 and m_3 calculated with — Newmark- β and — generalized- α

reduction is the same for both Newmark- β and generalized- α time integration methods, see tab. 1.

3.2. Flexible slider-crank mechanism

The slider crank mechanism as shown in fig. 7 is modeled with flexible multibody dynamics using the floating frame of reference formulation. The mechanism consists of four bodies that are connected by three revolute joints and one prismatic joint. The ground and the slider are considered to be rigid, while the crank shaft and the connecting rod are considered to be flexible and are modeled with Euler-Bernoulli beams. Fig. 8 shows the flexible multibody system of the mechanism. The inertial reference frame coinciding with the reference frame of the ground is shown in blue. The body reference frames of the crank shaft, the connecting rod and the slider are shown in red. The undeformed bodies of the crank shaft and the connecting rod are shown in gray and the deformed bodies are shown in black, where the points represent the nodes of the finite elements. The coordinates that will be investigated in detail for the primal analysis and the sensitivity analysis

Table 1: Computational effort for the structural dynamics example, ¹Intel Core i5-7200U CPU 2.50GHz, ²speedup of analytical sensitivity analysis w.r.t. finite differencing

time integration	sensitivity analysis	calculation time [s] ¹	speedup ²
Newmark- β	none	0.0555	—
Newmark- β	finite differencing	0.2088	—
Newmark- β	analytical	0.1023	2.0410
generalized- α	none	0.0458	—
generalized- α	finite differencing	0.2122	—
generalized- α	analytical	0.0993	2.1370

Figure 7: Slider-crank mechanism

Figure 8: Flexible multibody system of the slider crank mechanism with the undeformed bodies in gray, the deformed bodies in black, the inertial reference frame in blue, the body reference frames in red and the coordinates that are investigated in green

are shown in green. The dimensions of the bodies are listed in tab. 2. The bodies are made of steel and tab. 3 shows the material properties. In this example, the MPa unit system is used with length in mm, mass in t, time in s, force in N, angle in rad and stress in MPa.

The generalized coordinates of a flexible multibody system modeled with the floating frame of reference formulation and Euler–Bernoulli beams are given by

$$\underline{q} = \left[\underline{r}^T \quad \theta_C \quad \underline{\bar{q}}_f^T \right]^T, \quad (62)$$

where $\underline{r}$ is the position of the body reference frame, θ is the orientation of the body reference frame and

Table 2: Dimensions of the bodies

	crank shaft	connecting rod	slider
width	20mm	20mm	30mm
height	30mm	30mm	30mm
length	120mm	180mm	40mm

Table 3: Material properties

property	value
density	$\rho = 7.85 \cdot 10^{-9} \text{ t/mm}^3$
elastic modulus	$E = 210000 \text{ MPa}$
Poisson ratio	$\nu = 0.3$

$\underline{\bar{q}}_f$ are the nodal displacements in body coordinates of each node on the flexible body. Since no damping is considered, the equations of motion of a flexible body are given by

$$\underline{\underline{m}}\ddot{\underline{q}} + \underline{\underline{k}}\underline{q} + \underline{\underline{J}}_\Phi^T \underline{\lambda} = \underline{F}_{\text{ext}} + \underline{F}_v, \quad (63)$$

$$\underline{\underline{J}}_\Phi \ddot{\underline{q}} = \underline{F}_c, \quad (64)$$

where the system matrices of the flexible bodies are given by

$$\underline{\underline{m}} = \begin{bmatrix} \underline{\underline{m}}_{tt} & \underline{\underline{m}}_{tr} & \underline{\underline{m}}_{tf} \\ \underline{\underline{m}}_{tr} & \underline{\underline{m}}_{rr} & \underline{\underline{m}}_{rf} \\ \text{sym.} & & \underline{\underline{m}}_{ff} \end{bmatrix}, \quad \underline{\underline{k}} = \begin{bmatrix} 0 & 0 & 0 \\ & 0 & 0 \\ \text{sym.} & & \underline{\underline{k}}_{ff} \end{bmatrix}, \quad (65)$$

and the system vectors are given by

$$\underline{F}_{\text{ext}} = \begin{bmatrix} \underline{F}_{\text{ext},t} \\ \underline{F}_{\text{ext},r} \\ \underline{F}_{\text{ext},f} \end{bmatrix}, \quad \underline{F}_v = \begin{bmatrix} \underline{F}_{v,t} \\ \underline{F}_{v,r} \\ \underline{F}_{v,f} \end{bmatrix}, \quad (66)$$

with the index denoting translational terms t , rotational terms r and flexible terms f .

For the dynamic simulation of the mechanism, the in-house solver framework SiMULi is used. The simulation is performed in the time interval $t = [0 \text{ s}, 0.025 \text{ s}]$ with time steps $\Delta t = 1 \cdot 10^{-4} \text{ s}$. For the initial conditions, the angular position and velocity of the crank shaft are defined with

$$\begin{aligned} \theta_C &= 0 \text{ rad}, \\ \dot{\theta}_C &= 0 \frac{\text{rad}}{\text{s}}, \end{aligned}$$

and the initial conditions of the other bodies are derived through the kinematic analysis of the system. The dimensions of the cross sections of the crank shaft h_C , w_C and the connecting rod h_R , w_R are used as design variables in the sensitivity analysis.

The results of the simulation of the coordinates that are highlighted in fig. 8 are shown in fig. 9. With Newmark- β , vibrations at high frequencies are observed. With generalized- α , vibrations are observed in the beginning of the simulation that are numerically damped with ongoing simulation time. In addition to the generalized coordinates, the maximum stresses on the upper and lower fiber of the beam elements of the flexible bodies including the crank shaft and the connecting rod are computed. The KS function [31] is used to approximate the maximum stress value with a differentiable function and the results are shown in fig. 10. With Newmark- β , the vibrating behavior of the system causes higher flexible deformation and therefore unrealistic high stress in the components. The numerical damping with generalized- α leads to lower maximum stress values and a more realistic stress distribution over time.

Figure 9: Responses of the slider crank mechanism (values in MPa units, i.e. mm, $\frac{\text{mm}}{\text{s}}$, $\frac{\text{mm}}{\text{s}^2}$ for translations and rad, $\frac{\text{rad}}{\text{s}}$, $\frac{\text{rad}}{\text{s}^2}$ for rotations) calculated with — Newmark- β and — generalized- α

Figure 10: Maximum stress in MPa on the upper and lower fiber of the crank shaft and the connecting rod calculated with — Newmark- β and — generalized- α

Table 4: Computational effort for the slider crank mechanism, ¹Intel Core i7-8700 CPU 3.20GHz, ²speedup of analytical sensitivity analysis w.r.t. finite differencing

time integration	sensitivity analysis	calculation time [mm : ss] ¹	speedup ²
Newmark- β	none	03:44	–
Newmark- β	finite differencing	18:12	–
Newmark- β	analytical	04:29	4.0595
generalized- α	none	02:42	–
generalized- α	finite differencing	13:22	–
generalized- α	analytical	03:30	3.8190

The results of the sensitivity analysis of the coordinates that are highlighted in fig. 8 are shown in fig. 11–13. Similar to above, with Newmark- β the results show a vibrating behavior that would lead to significant problems when using the sensitivities in gradient-based design optimization. With generalized- α , the numerical damping leads to usable sensitivity values after a few time steps. The same behavior also continue with the sensitivity values for the maximum stresses in the crank shaft and the connecting rod shown in fig. 14.

Tab. 4 shows a comparison of the computational effort with different methods. The computational effort with generalized- α is about 30 % lower compared to the computational effort with Newmark- β . The main reason for that is the continuing vibrating behavior with Newmark- β , requiring more iteration steps of the nonlinear solver. The comparison of the sensitivity methods with numerical finite differencing and analytical direct differentiation shows the high efficiency of the analytical method. With the four shown design variables, a speedup as shown in (61) of about $S \approx 4$ of the analytical method compared to the numerical method is obtained. The additional computational effort of analytical sensitivity analysis is just a fraction of the computational effort of the primal analysis. This is because of the simplification shown in (57), which allows to use the Jacobian matrix of the residual built in the primal analysis also for the sensitivity analysis. This allows for a further reduced computational effort.

4. Conclusion

Analytical sensitivity analysis is crucial for efficient design optimization, parameter fitting and uncertainty analysis. In this work the direct differentiation of the generalized- α time integration was derived and implemented for linear structural dynamics and flexible multibody dynamics, the latter of which requiring a nonlinear solve routine. The beneficial effects of the numerical damping provided by the generalized- α method can be clearly seen in comparison with Newmark- β .

The objective of this work is to integrate the analytical sensitivity analysis in gradient-based optimization frameworks. If the functions of interest are nonsmooth, discontinuous and bifurcated, non-gradient-based methods have successfully been used, e.g. design cases with crash analysis. Such cases can be solved with gradient-free optimization algorithms (e.g. [32, 33, 34, 35]) and approximation methods (e.g. [36, 37, 38]).

With the above study and introduction of the direct differentiation of the α -family of time integrators, the authors hope to provide the readers as design engineers a tool in the pursuit of optimal structures and mechanisms under dynamic loading.

Figure 11: Position sensitivities ∇q of the slider crank mechanism w.r.t. h_C , w_C , h_R and w_R (values in MPa system of units) calculated with — Newmark- β and — generalized- α

Figure 12: Velocity sensitivities $\nabla \dot{q}$ of the slider crank mechanism w.r.t. h_C , w_C , h_R and w_R (values in MPa system of units) calculated with — Newmark- β and — generalized- α

Figure 13: Acceleration sensitivities $\nabla \ddot{q}$ of the slider crank mechanism w.r.t. h_C , w_C , h_R and w_R (values in MPa system of units) calculated with — Newmark- β and — generalized- α

Figure 14: Maximum stress sensitivities on the upper and lower fiber of the crank shaft and the connecting rod (values in MPa system of units) calculated with — Newmark- β and — generalized- α

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Appendix A. Derivation of effective equation of motions for structural dynamics

Appendix A.1. Primal analysis

The base for the α -family of integration methods is the equation of motion which for linear structural dynamics is given by

$$\underline{\underline{m}}\ddot{\underline{q}}_{n+1-\alpha_m} + \underline{\underline{d}}\dot{\underline{q}}_{n+1-\alpha_f} + \underline{\underline{k}}\underline{q}_{n+1-\alpha_f} = \underline{F}_{n+1-\alpha_f}, \quad (\text{A.1})$$

and the introduced intermediate values. Inserting the intermediate values into the equation of motion leads to

$$\underline{\underline{m}} \left((1 - \alpha_m) \underline{\dot{q}}_{n+1} + \alpha_m \underline{\dot{q}}_n \right) + \underline{\underline{d}} \left((1 - \alpha_f) \underline{\dot{q}}_{n+1} + \alpha_f \underline{\dot{q}}_n \right) + \underline{\underline{k}} \left((1 - \alpha_f) \underline{q}_{n+1} + \alpha_f \underline{q}_n \right) = (1 - \alpha_f) \underline{F}_{n+1} + \alpha_f \underline{F}_n. \quad (\text{A.2})$$

With Newmark's equations, this becomes

$$\begin{aligned} \underline{\underline{m}} \left((1 - \alpha_m) \underline{\ddot{q}}_{n+1} + \alpha_m \underline{\ddot{q}}_n \right) + \underline{\underline{d}} \left((1 - \alpha_f) \left(\underline{\dot{q}}_{\text{pred}} + \gamma \Delta t \underline{\ddot{q}}_{n+1} \right) + \alpha_f \underline{\dot{q}}_n \right) + \\ + \underline{\underline{k}} \left((1 - \alpha_f) \left(\underline{q}_{\text{pred}} + \beta \Delta t^2 \underline{\ddot{q}}_{n+1} \right) + \alpha_f \underline{q}_n \right) = (1 - \alpha_f) \underline{F}_{n+1} + \alpha_f \underline{F}_n. \end{aligned} \quad (\text{A.3})$$

This can be rearranged to the following format

$$\begin{aligned} ((1 - \alpha_m) \underline{\underline{m}} + (1 - \alpha_f) \gamma \Delta t \underline{\underline{d}} + (1 - \alpha_f) \beta \Delta t^2 \underline{\underline{k}}) \underline{\ddot{q}}_{n+1} = \\ (1 - \alpha_f) \underline{F}_{n+1} + \alpha_f \underline{F}_n - \alpha_m \underline{\underline{m}} \underline{\ddot{q}}_n - \underline{\underline{d}} \left((1 - \alpha_f) \underline{\dot{q}}_{\text{pred}} + \alpha_f \underline{\dot{q}}_n \right) - \underline{\underline{k}} \left((1 - \alpha_f) \underline{q}_{\text{pred}} + \alpha_f \underline{q}_n \right). \end{aligned} \quad (\text{A.4})$$

Therefore, the effective equation of motion is defined by

$$\underline{\underline{m}}_{\text{eff}} \underline{\ddot{q}}_{n+1} = \underline{F}_{\text{eff}}, \quad (\text{A.5})$$

where

$$\underline{\underline{m}}_{\text{eff}} = (1 - \alpha_m) \underline{\underline{m}} + (1 - \alpha_f) \gamma \Delta t \underline{\underline{d}} + (1 - \alpha_f) \beta \Delta t^2 \underline{\underline{k}}, \quad (\text{A.6})$$

$$\underline{F}_{\text{eff}} = (1 - \alpha_f) \underline{F}_{n+1} + \alpha_f \underline{F}_n - \alpha_m \underline{\underline{m}} \underline{\ddot{q}}_n - \underline{\underline{d}} \left((1 - \alpha_f) \underline{\dot{q}}_{\text{pred}} + \alpha_f \underline{\dot{q}}_n \right) - \underline{\underline{k}} \left((1 - \alpha_f) \underline{q}_{\text{pred}} + \alpha_f \underline{q}_n \right). \quad (\text{A.7})$$

Appendix A.2. Sensitivity analysis

The governing equation for sensitivities is the first derivative of the equation of motion,

$$\underline{\underline{\nabla m}} \underline{\ddot{q}}_{n+1} - \alpha_m + \underline{\underline{m}} \underline{\underline{\nabla \ddot{q}}}_{n+1} - \alpha_m + \underline{\underline{\nabla d}} \underline{\dot{q}}_{n+1} - \alpha_f + \underline{\underline{d}} \underline{\underline{\nabla \dot{q}}}_{n+1} - \alpha_f + \underline{\underline{\nabla k}} \underline{q}_{n+1} - \alpha_f + \underline{\underline{k}} \underline{\underline{\nabla q}}_{n+1} - \alpha_f = \underline{\underline{\nabla F}}_{n+1} - \alpha_f, \quad (\text{A.8})$$

where we introduce the intermediate values,

$$\begin{aligned} \underline{\underline{\nabla m}} \left((1 - \alpha_m) \underline{\ddot{q}}_{n+1} + \alpha_m \underline{\ddot{q}}_n \right) + \underline{\underline{m}} \left((1 - \alpha_m) \underline{\underline{\nabla \ddot{q}}}_{n+1} + \alpha_m \underline{\underline{\nabla \ddot{q}}}_n \right) + \\ + \underline{\underline{\nabla d}} \left((1 - \alpha_f) \underline{\dot{q}}_{n+1} + \alpha_f \underline{\dot{q}}_n \right) + \underline{\underline{d}} \left((1 - \alpha_f) \underline{\underline{\nabla \dot{q}}}_{n+1} + \alpha_f \underline{\underline{\nabla \dot{q}}}_n \right) + \\ + \underline{\underline{\nabla k}} \left((1 - \alpha_f) \underline{q}_{n+1} + \alpha_f \underline{q}_n \right) + \underline{\underline{k}} \left((1 - \alpha_f) \underline{\underline{\nabla q}}_{n+1} + \alpha_f \underline{\underline{\nabla q}}_n \right) = \\ (1 - \alpha_f) \underline{\underline{\nabla F}}_{n+1} + \alpha_f \underline{\underline{\nabla F}}_n, \end{aligned} \quad (\text{A.9})$$

and which we update with Newmark's equations

$$\begin{aligned} \underline{\underline{\nabla m}} \left((1 - \alpha_m) \underline{\ddot{q}}_{n+1} + \alpha_m \underline{\ddot{q}}_n \right) + \underline{\underline{m}} \left((1 - \alpha_m) \underline{\underline{\nabla \ddot{q}}}_{n+1} + \alpha_m \underline{\underline{\nabla \ddot{q}}}_n \right) + \\ + \underline{\underline{\nabla d}} \left((1 - \alpha_f) \underline{\dot{q}}_{n+1} + \alpha_f \underline{\dot{q}}_n \right) + \underline{\underline{d}} \left((1 - \alpha_f) \left(\underline{\dot{q}}_{\text{pred}} + \gamma \Delta t \underline{\underline{\nabla \ddot{q}}}_{n+1} \right) + \alpha_f \underline{\underline{\nabla \dot{q}}}_n \right) + \\ + \underline{\underline{\nabla k}} \left((1 - \alpha_f) \underline{q}_{n+1} + \alpha_f \underline{q}_n \right) + \underline{\underline{k}} \left((1 - \alpha_f) \left(\underline{q}_{\text{pred}} + \beta \Delta t^2 \underline{\underline{\nabla \ddot{q}}}_{n+1} \right) + \alpha_f \underline{\underline{\nabla q}}_n \right) = \\ (1 - \alpha_f) \underline{\underline{\nabla F}}_{n+1} + \alpha_f \underline{\underline{\nabla F}}_n. \end{aligned} \quad (\text{A.10})$$

This equation can be rearranged to the following form,

$$\begin{aligned}
& ((1 - \alpha_m) \underline{\underline{m}} + (1 - \alpha_f) \gamma \Delta t \underline{\underline{d}} + (1 - \alpha_f) \beta \Delta t^2 \underline{\underline{k}}) \nabla \ddot{q}_{n+1} = \\
& (1 - \alpha_f) \nabla F_{n+1} + \alpha_f \nabla F_n - \nabla m \left((1 - \alpha_m) \ddot{q}_{n+1} + \alpha_m \ddot{q}_n \right) - \alpha_m \underline{\underline{m}} \nabla \ddot{q}_n + \\
& - \nabla d \left((1 - \alpha_f) \dot{q}_{n+1} + \alpha_f \dot{q}_n \right) - \underline{\underline{d}} \left((1 - \alpha_f) \nabla \dot{q}_{\text{pred}} + \alpha_f \nabla \dot{q}_n \right) + \\
& - \nabla k \left((1 - \alpha_f) q_{n+1} + \alpha_f q_n \right) - \underline{\underline{k}} \left((1 - \alpha_f) \nabla q_{\text{pred}} + \alpha_f \nabla q_n \right). \quad (\text{A.11})
\end{aligned}$$

Therefore, the effective equation of motion for sensitivities is defined by

$$\underline{\underline{m}}_{\text{eff}} \nabla \ddot{q}_{n+1} = \underline{\underline{F}}_{\text{eff,pseudo}}, \quad (\text{A.12})$$

where

$$\underline{\underline{m}}_{\text{eff}} = (1 - \alpha_m) \underline{\underline{m}} + (1 - \alpha_f) \gamma \Delta t \nabla \ddot{q}_{n+1} \underline{\underline{d}} + (1 - \alpha_f) \beta \Delta t^2 \underline{\underline{k}}, \quad (\text{A.13})$$

and

$$\begin{aligned}
\underline{\underline{F}}_{\text{eff,pseudo}} = & (1 - \alpha_f) \nabla F_{n+1} + \alpha_f \nabla F_n - \left(\nabla m \left((1 - \alpha_m) \ddot{q}_{n+1} + \alpha_m \ddot{q}_n \right) + \alpha_m \underline{\underline{m}} \nabla \ddot{q}_n \right) + \\
& - \left(\nabla d \left((1 - \alpha_f) \dot{q}_{n+1} + \alpha_f \dot{q}_n \right) + \underline{\underline{d}} \left((1 - \alpha_f) \nabla \dot{q}_{\text{pred}} + \alpha_f \nabla \dot{q}_n \right) \right) + \\
& - \left(\nabla k \left((1 - \alpha_f) q_{n+1} + \alpha_f q_n \right) + \underline{\underline{k}} \left((1 - \alpha_f) \nabla q_{\text{pred}} + \alpha_f \nabla q_n \right) \right). \quad (\text{A.14})
\end{aligned}$$

Appendix B. Derivation of effective equations of motions for multibody dynamics

Appendix B.1. Primal analysis

The base of the generalized- α method for index-1 differential algebraic equations of a flexible multibody system is given by

$$(\underline{\underline{m}} \ddot{q})_{n+1-\alpha_m} + (\underline{\underline{d}} \dot{q})_{n+1-\alpha_f} + (\underline{\underline{k}} q)_{n+1-\alpha_f} + (\underline{\underline{J}}_{\Phi}^T \lambda)_{n+1-\alpha_m} = \underline{\underline{F}}_{\text{ext},n+1-\alpha_f} + \underline{\underline{F}}_{\text{v},n+1-\alpha_f}, \quad (\text{B.1})$$

$$(\underline{\underline{J}}_{\Phi} \ddot{q})_{n+1-\alpha_m} = \underline{\underline{F}}_{\text{c},n+1-\alpha_f}. \quad (\text{B.2})$$

The intermediate point approximations of the force terms acting on the flexible multibody system are given by

$$(\underline{\underline{m}} \ddot{q})_{n+1-\alpha_m} = (1 - \alpha_m) \underline{\underline{m}}_{n+1} \ddot{q}_{n+1} + \alpha_m \underline{\underline{m}}_n \ddot{q}_n, \quad (\text{B.3})$$

$$(\underline{\underline{d}} \dot{q})_{n+1-\alpha_f} = (1 - \alpha_f) \underline{\underline{d}}_{n+1} \dot{q}_{n+1} + \alpha_f \underline{\underline{d}}_n \dot{q}_n, \quad (\text{B.4})$$

$$(\underline{\underline{k}} q)_{n+1-\alpha_f} = (1 - \alpha_f) \underline{\underline{k}}_{n+1} q_{n+1} + \alpha_f \underline{\underline{k}}_n q_n, \quad (\text{B.5})$$

$$(\underline{\underline{J}}_{\Phi}^T \lambda)_{n+1-\alpha_m} = (1 - \alpha_m) \underline{\underline{J}}_{\Phi,n+1}^T \lambda_{n+1} + \alpha_m \underline{\underline{J}}_{\Phi,n}^T \lambda_n, \quad (\text{B.6})$$

$$(\underline{\underline{J}}_{\Phi} \ddot{q})_{n+1-\alpha_m} = (1 - \alpha_m) \underline{\underline{J}}_{\Phi,n+1} \ddot{q}_{n+1} + \alpha_m \underline{\underline{J}}_{\Phi,n} \ddot{q}_n, \quad (\text{B.7})$$

$$\underline{\underline{F}}_{\text{ext},n+1-\alpha_f} = (1 - \alpha_f) \underline{\underline{F}}_{\text{ext},n+1} + \alpha_f \underline{\underline{F}}_{\text{ext},n}, \quad (\text{B.8})$$

$$\underline{\underline{F}}_{\text{v},n+1-\alpha_f} = (1 - \alpha_f) \underline{\underline{F}}_{\text{v},n+1} + \alpha_f \underline{\underline{F}}_{\text{v},n}, \quad (\text{B.9})$$

$$\underline{\underline{F}}_{\text{c},n+1-\alpha_f} = (1 - \alpha_f) \underline{\underline{F}}_{\text{c},n+1} + \alpha_f \underline{\underline{F}}_{\text{c},n}. \quad (\text{B.10})$$

Applying these linear approximations of the generalized- α method to the equations of motion leads to

$$\begin{aligned} (1 - \alpha_m) \underline{\underline{m}}_{n+1} \ddot{\underline{q}}_{n+1} + \alpha_m \underline{\underline{m}}_n \ddot{\underline{q}}_n + (1 - \alpha_f) \underline{\underline{d}}_{n+1} \dot{\underline{q}}_{n+1} + \alpha_f \underline{\underline{d}}_n \dot{\underline{q}}_n + \\ (1 - \alpha_f) \underline{\underline{k}}_{n+1} \underline{q}_{n+1} + \alpha_f \underline{\underline{k}}_n \underline{q}_n + (1 - \alpha_m) \underline{\underline{J}}_{\Phi,n+1}^T \underline{\lambda}_{n+1} + \alpha_m \underline{\underline{J}}_{\Phi,n}^T \underline{\lambda}_n = \\ (1 - \alpha_f) \underline{F}_{\text{ext},n+1} + \alpha_f \underline{F}_{\text{ext},n} + (1 - \alpha_f) \underline{F}_{v,n+1} + \alpha_f \underline{F}_{v,n}, \end{aligned} \quad (\text{B.11})$$

and

$$(1 - \alpha_m) \underline{\underline{J}}_{\Phi,n+1} \ddot{\underline{q}}_{n+1} + \alpha_m \underline{\underline{J}}_{\Phi,n} \ddot{\underline{q}}_n = (1 - \alpha_f) \underline{F}_{c,n+1} + \alpha_f \underline{F}_{c,n}. \quad (\text{B.12})$$

Inserting Newmark's equations gives

$$\begin{aligned} (1 - \alpha_m) \underline{\underline{m}}_{n+1} \ddot{\underline{q}}_{n+1} + \alpha_m \underline{\underline{m}}_n \ddot{\underline{q}}_n (1 - \alpha_f) + \underline{\underline{d}}_{n+1} \left(\dot{\underline{q}}_{\text{pred}} + \gamma \Delta t \ddot{\underline{q}}_{n+1} \right) + \alpha_f \underline{\underline{d}}_n \dot{\underline{q}}_n + \\ + (1 - \alpha_f) \underline{\underline{k}}_{n+1} \left(\underline{q}_{\text{pred}} + \beta \Delta t^2 \ddot{\underline{q}}_{n+1} \right) + \alpha_f \underline{\underline{k}}_n \underline{q}_n + (1 - \alpha_m) \underline{\underline{J}}_{\Phi,n+1}^T \underline{\lambda}_{n+1} + \alpha_m \underline{\underline{J}}_{\Phi,n}^T \underline{\lambda}_n = \\ (1 - \alpha_f) \underline{F}_{\text{ext},n+1} + \alpha_f \underline{F}_{\text{ext},n} + (1 - \alpha_f) \underline{F}_{v,n+1} + \alpha_f \underline{F}_{v,n}, \end{aligned} \quad (\text{B.13})$$

and

$$(1 - \alpha_m) \underline{\underline{J}}_{\Phi,n+1} \ddot{\underline{q}}_{n+1} + \alpha_m \underline{\underline{J}}_{\Phi,n} \ddot{\underline{q}}_n = (1 - \alpha_f) \underline{F}_{c,n+1} + \alpha_f \underline{F}_{c,n}. \quad (\text{B.14})$$

which can be rewritten to

$$\begin{aligned} \left((1 - \alpha_m) \underline{\underline{m}}_{n+1} + (1 - \alpha_f) \gamma \Delta t \underline{\underline{d}}_{n+1} + (1 - \alpha_f) \beta \Delta t^2 \underline{\underline{k}}_{n+1} \right) \ddot{\underline{q}}_{n+1} + (1 - \alpha_m) \underline{\underline{J}}_{\Phi,n+1}^T \underline{\lambda}_{n+1} = \\ (1 - \alpha_f) \underline{F}_{\text{ext},n+1} + \alpha_f \underline{F}_{\text{ext},n} + (1 - \alpha_f) \underline{F}_{v,n+1} + \alpha_f \underline{F}_{v,n} - \alpha_m \underline{\underline{m}}_n \ddot{\underline{q}}_n + \\ - (1 - \alpha_f) \underline{\underline{d}}_{n+1} \dot{\underline{q}}_{\text{pred}} - \alpha_f \underline{\underline{d}}_n \dot{\underline{q}}_n - (1 - \alpha_f) \underline{\underline{k}}_{n+1} \underline{q}_{\text{pred}} - \alpha_f \underline{\underline{k}}_n \underline{q}_n - \alpha_m \underline{\underline{J}}_{\Phi,n}^T \underline{\lambda}_n, \end{aligned} \quad (\text{B.15})$$

and

$$(1 - \alpha_m) \underline{\underline{J}}_{\Phi,n+1} \ddot{\underline{q}}_{n+1} = (1 - \alpha_f) \underline{F}_{c,n+1} + \alpha_f \underline{F}_{c,n} - \alpha_m \underline{\underline{J}}_{\Phi,n} \ddot{\underline{q}}_n. \quad (\text{B.16})$$

The equations of motion of the effective system is given by

$$\begin{bmatrix} \underline{\underline{m}}_{\text{eff}} & \underline{\underline{J}}_{\Phi,\text{eff}}^T \\ \underline{\underline{J}}_{\Phi,\text{eff}} & \underline{\underline{0}} \end{bmatrix} \begin{bmatrix} \ddot{\underline{q}}_{n+1} \\ \underline{\lambda}_{n+1} \end{bmatrix} = \begin{bmatrix} \underline{F}_{a,\text{eff}} \\ \underline{F}_{c,\text{eff}} \end{bmatrix}, \quad (\text{B.17})$$

where

$$\underline{\underline{m}}_{\text{eff}} = (1 - \alpha_m) \underline{\underline{m}}_{n+1} + (1 - \alpha_f) \gamma \Delta t \underline{\underline{d}}_{n+1} + (1 - \alpha_f) \beta \Delta t^2 \underline{\underline{k}}_{n+1}, \quad (\text{B.18})$$

$$\underline{\underline{J}}_{\Phi,\text{eff}} = (1 - \alpha_m) \underline{\underline{J}}_{\Phi,n+1}, \quad (\text{B.19})$$

$$\begin{aligned} \underline{F}_{a,\text{eff}} = (1 - \alpha_f) \underline{F}_{\text{ext},n+1} + \alpha_f \underline{F}_{\text{ext},n} + (1 - \alpha_f) \underline{F}_{v,n+1} + \alpha_f \underline{F}_{v,n} - \alpha_m \underline{\underline{m}}_n \ddot{\underline{q}}_n + \\ - (1 - \alpha_f) \underline{\underline{d}}_{n+1} \dot{\underline{q}}_{\text{pred}} - \alpha_f \underline{\underline{d}}_n \dot{\underline{q}}_n - (1 - \alpha_f) \underline{\underline{k}}_{n+1} \underline{q}_{\text{pred}} - \alpha_f \underline{\underline{k}}_n \underline{q}_n - \alpha_m \underline{\underline{J}}_{\Phi,n}^T \underline{\lambda}_n, \end{aligned} \quad (\text{B.20})$$

$$\underline{F}_{c,\text{eff}} = (1 - \alpha_f) \underline{F}_{c,n+1} + \alpha_f \underline{F}_{c,n} - \alpha_m \underline{\underline{J}}_{\Phi,n} \ddot{\underline{q}}_n. \quad (\text{B.21})$$

Appendix B.2. Nonlinear solver

The base for the nonlinear solver are the residual equations of the flexible multibody system, given by

$$\begin{aligned} \underline{R}_{1,n+1-\alpha_f} = & (1 - \alpha_m) \underline{m}_{n+1} \ddot{\underline{q}}_{n+1} + \alpha_m \underline{m}_n \ddot{\underline{q}}_n + (1 - \alpha_f) \underline{d}_{n+1} \dot{\underline{q}}_{n+1} + \alpha_f \underline{d}_n \dot{\underline{q}}_n + \\ & + (1 - \alpha_f) \underline{k}_{n+1} \underline{q}_{n+1} + \alpha_f \underline{k}_n \underline{q}_n + (1 - \alpha_m) \underline{J}_{\Phi,n+1}^T \underline{\lambda}_{n+1} + \alpha_m \underline{J}_{\Phi,n}^T \underline{\lambda}_n + \\ & - (1 - \alpha_f) \underline{F}_{\text{ext},n+1} - \alpha_f \underline{F}_{\text{ext},n} - (1 - \alpha_f) \underline{F}_{v,n+1} - \alpha_f \underline{F}_{v,n}, \end{aligned} \quad (\text{B.22})$$

$$\underline{R}_{2,n+1-\alpha_f} = (1 - \alpha_m) \underline{J}_{\Phi,n+1} \ddot{\underline{q}}_{n+1} + \alpha_m \underline{J}_{\Phi,n} \ddot{\underline{q}}_n - (1 - \alpha_f) \underline{F}_{c,n+1} - \alpha_f \underline{F}_{c,n}. \quad (\text{B.23})$$

The Newton–Raphson method is used here

$$\begin{bmatrix} \frac{\partial \underline{R}_{1,n+1-\alpha_f}}{\partial \ddot{\underline{q}}_{n+1}} & \frac{\partial \underline{R}_{1,n+1-\alpha_f}}{\partial \underline{\lambda}_{n+1}} \\ \frac{\partial \underline{R}_{2,n+1-\alpha_f}}{\partial \ddot{\underline{q}}_{n+1}} & \frac{\partial \underline{R}_{2,n+1-\alpha_f}}{\partial \underline{\lambda}_{n+1}} \end{bmatrix} \begin{bmatrix} \Delta \ddot{\underline{q}}_{n+1} \\ \Delta \underline{\lambda}_{n+1} \end{bmatrix} + \begin{bmatrix} \underline{R}_{1,n+1-\alpha_f} \\ \underline{R}_{2,n+1-\alpha_f} \end{bmatrix} = \underline{0}, \quad (\text{B.24})$$

where the terms of the Jacobian matrix are given by

$$\begin{aligned} \frac{\partial \underline{R}_{1,n+1-\alpha_f}}{\partial \ddot{\underline{q}}_{n+1}} = & (1 - \alpha_m) \frac{\partial \underline{m}_{n+1}}{\partial \ddot{\underline{q}}_{n+1}} \ddot{\underline{q}}_{n+1} + (1 - \alpha_m) \underline{m}_{n+1} \frac{\partial \ddot{\underline{q}}_{n+1}}{\partial \ddot{\underline{q}}_{n+1}} + \alpha_m \frac{\partial \underline{m}_n}{\partial \ddot{\underline{q}}_{n+1}} \ddot{\underline{q}}_n + \alpha_m \underline{m}_n \frac{\partial \ddot{\underline{q}}_n}{\partial \ddot{\underline{q}}_{n+1}} + \\ & + (1 - \alpha_f) \frac{\partial \underline{d}_{n+1}}{\partial \ddot{\underline{q}}_{n+1}} \dot{\underline{q}}_{n+1} + (1 - \alpha_f) \underline{d}_{n+1} \frac{\partial \dot{\underline{q}}_{n+1}}{\partial \ddot{\underline{q}}_{n+1}} + \alpha_f \frac{\partial \underline{d}_n}{\partial \ddot{\underline{q}}_{n+1}} \dot{\underline{q}}_n + \alpha_f \underline{d}_n \frac{\partial \dot{\underline{q}}_n}{\partial \ddot{\underline{q}}_{n+1}} + \\ & + (1 - \alpha_f) \frac{\partial \underline{k}_{n+1}}{\partial \ddot{\underline{q}}_{n+1}} \underline{q}_{n+1} + (1 - \alpha_f) \underline{k}_{n+1} \frac{\partial \underline{q}_{n+1}}{\partial \ddot{\underline{q}}_{n+1}} + \alpha_f \frac{\partial \underline{k}_n}{\partial \ddot{\underline{q}}_{n+1}} \underline{q}_n + \alpha_f \underline{k}_n \frac{\partial \underline{q}_n}{\partial \ddot{\underline{q}}_{n+1}} + \\ & + (1 - \alpha_m) \frac{\partial \underline{J}_{\Phi,n+1}^T}{\partial \ddot{\underline{q}}_{n+1}} \underline{\lambda}_{n+1} + (1 - \alpha_m) \underline{J}_{\Phi,n+1}^T \frac{\partial \underline{\lambda}_{n+1}}{\partial \ddot{\underline{q}}_{n+1}} + \alpha_m \frac{\partial \underline{J}_{\Phi,n}^T}{\partial \ddot{\underline{q}}_{n+1}} \underline{\lambda}_n + \alpha_m \underline{J}_{\Phi,n}^T \frac{\partial \underline{\lambda}_n}{\partial \ddot{\underline{q}}_{n+1}} + \\ & - (1 - \alpha_f) \frac{\partial \underline{F}_{\text{ext},n+1}}{\partial \ddot{\underline{q}}_{n+1}} - \alpha_f \frac{\partial \underline{F}_{\text{ext},n}}{\partial \ddot{\underline{q}}_{n+1}} - (1 - \alpha_f) \frac{\partial \underline{F}_{v,n+1}}{\partial \ddot{\underline{q}}_{n+1}} - \alpha_f \frac{\partial \underline{F}_{v,n}}{\partial \ddot{\underline{q}}_{n+1}}, \end{aligned} \quad (\text{B.25})$$

$$\begin{aligned} \frac{\partial \underline{R}_{2,n+1-\alpha_f}}{\partial \ddot{\underline{q}}_{n+1}} = & (1 - \alpha_m) \frac{\partial \underline{J}_{\Phi,n+1}}{\partial \ddot{\underline{q}}_{n+1}} \ddot{\underline{q}}_{n+1} + (1 - \alpha_m) \underline{J}_{\Phi,n+1} \frac{\partial \ddot{\underline{q}}_{n+1}}{\partial \ddot{\underline{q}}_{n+1}} + \alpha_m \frac{\partial \underline{J}_{\Phi,n}}{\partial \ddot{\underline{q}}_{n+1}} \ddot{\underline{q}}_n + \alpha_m \underline{J}_{\Phi,n} \frac{\partial \ddot{\underline{q}}_n}{\partial \ddot{\underline{q}}_{n+1}} + \\ & - (1 - \alpha_f) \frac{\partial \underline{F}_{c,n+1}}{\partial \ddot{\underline{q}}_{n+1}} - \alpha_f \frac{\partial \underline{F}_{c,n}}{\partial \ddot{\underline{q}}_{n+1}}, \end{aligned} \quad (\text{B.26})$$

$$\begin{aligned}
\frac{\partial R_{1,n+1-\alpha_f}}{\partial \underline{\lambda}_{n+1}} = & (1-\alpha_m) \frac{\partial m_{n+1}}{\partial \underline{\lambda}_{n+1}} \ddot{q}_{n+1} + (1-\alpha_m) \underline{m}_{n+1} \frac{\partial \ddot{q}_{n+1}}{\partial \underline{\lambda}_{n+1}} + \alpha_m \frac{\partial m_n}{\partial \underline{\lambda}_{n+1}} \ddot{q}_n + \alpha_m \underline{m}_n \frac{\partial \ddot{q}_n}{\partial \underline{\lambda}_{n+1}} + \\
& + (1-\alpha_f) \frac{\partial d_{n+1}}{\partial \underline{\lambda}_{n+1}} \dot{q}_{n+1} + (1-\alpha_f) \underline{d}_{n+1} \frac{\partial \dot{q}_{n+1}}{\partial \underline{\lambda}_{n+1}} + \alpha_f \frac{\partial d_n}{\partial \underline{\lambda}_{n+1}} \dot{q}_n + \alpha_f \underline{d}_n \frac{\partial \dot{q}_n}{\partial \underline{\lambda}_{n+1}} + \\
& + (1-\alpha_f) \frac{\partial k_{n+1}}{\partial \underline{\lambda}_{n+1}} q_{n+1} + (1-\alpha_f) \underline{k}_{n+1} \frac{\partial q_{n+1}}{\partial \underline{\lambda}_{n+1}} + \alpha_f \frac{\partial k_n}{\partial \underline{\lambda}_{n+1}} q_n + \alpha_f \underline{k}_n \frac{\partial q_n}{\partial \underline{\lambda}_{n+1}} + \\
& + (1-\alpha_m) \frac{\partial \mathbf{J}_{\Phi,n+1}^T}{\partial \underline{\lambda}_{n+1}} \underline{\lambda}_{n+1} + (1-\alpha_m) \underline{\mathbf{J}}_{\Phi,n+1}^T \frac{\partial \underline{\lambda}_{n+1}}{\partial \underline{\lambda}_{n+1}} + \alpha_m \frac{\partial \mathbf{J}_{\Phi,n}^T}{\partial \underline{\lambda}_{n+1}} \underline{\lambda}_n + \alpha_m \underline{\mathbf{J}}_{\Phi,n}^T \frac{\partial \underline{\lambda}_n}{\partial \underline{\lambda}_{n+1}} + \\
& - (1-\alpha_f) \frac{\partial F_{\text{ext},n+1}}{\partial \underline{\lambda}_{n+1}} - \alpha_f \frac{\partial F_{\text{ext},n}}{\partial \underline{\lambda}_{n+1}} - (1-\alpha_f) \frac{\partial F_{v,n+1}}{\partial \underline{\lambda}_{n+1}} - \alpha_f \frac{\partial F_{v,n}}{\partial \underline{\lambda}_{n+1}}, \tag{B.27}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial R_{2,n+1-\alpha_f}}{\partial \underline{\lambda}_{n+1}} = & (1-\alpha_m) \frac{\partial \mathbf{J}_{\Phi,n+1}}{\partial \underline{\lambda}_{n+1}} \ddot{q}_{n+1} + (1-\alpha_m) \underline{\mathbf{J}}_{\Phi,n+1} \frac{\partial \ddot{q}_{n+1}}{\partial \underline{\lambda}_{n+1}} + \alpha_m \frac{\partial \mathbf{J}_{\Phi,n}}{\partial \underline{\lambda}_{n+1}} \ddot{q}_n + \alpha_m \underline{\mathbf{J}}_{\Phi,n} \frac{\partial \ddot{q}_n}{\partial \underline{\lambda}_{n+1}} + \\
& - (1-\alpha_f) \frac{\partial F_{c,n+1}}{\partial \underline{\lambda}_{n+1}} - \alpha_f \frac{\partial F_{c,n}}{\partial \underline{\lambda}_{n+1}}. \tag{B.28}
\end{aligned}$$

The derivatives of the system parameters of the previous time step with respect to state variables of the next time step will disappear. The dependencies of the system parameters are shown in (30) and (31) and applying the chain rule for the differentiation leads to

$$\begin{aligned}
\frac{\partial R_{1,n+1-\alpha_f}}{\partial \ddot{q}_{n+1}} = & (1-\alpha_m) \left(\frac{\partial m_{n+1}}{\partial q_{n+1}} \frac{\partial q_{n+1}}{\partial \ddot{q}_{n+1}} \right) \ddot{q}_{n+1} + (1-\alpha_m) \underline{m}_{n+1} \frac{\partial \ddot{q}_{n+1}}{\partial \ddot{q}_{n+1}} + \\
& + (1-\alpha_f) \left(\frac{\partial d_{n+1}}{\partial q_{n+1}} \frac{\partial q_{n+1}}{\partial \ddot{q}_{n+1}} \right) \dot{q}_{n+1} + (1-\alpha_f) \underline{d}_{n+1} \frac{\partial \dot{q}_{n+1}}{\partial \ddot{q}_{n+1}} + \\
& + (1-\alpha_f) \left(\frac{\partial k_{n+1}}{\partial q_{n+1}} \frac{\partial q_{n+1}}{\partial \ddot{q}_{n+1}} \right) q_{n+1} + (1-\alpha_f) \underline{k}_{n+1} \frac{\partial q_{n+1}}{\partial \ddot{q}_{n+1}} + \\
& + (1-\alpha_m) \left(\frac{\partial \mathbf{J}_{\Phi,n+1}^T}{\partial q_{n+1}} \frac{\partial q_{n+1}}{\partial \ddot{q}_{n+1}} \right) \underline{\lambda}_{n+1} + (1-\alpha_m) \underline{\mathbf{J}}_{\Phi,n+1}^T \frac{\partial \underline{\lambda}_{n+1}}{\partial \ddot{q}_{n+1}} + \\
& - (1-\alpha_f) \left(\frac{\partial F_{\text{ext},n+1}}{\partial q_{n+1}} \frac{\partial q_{n+1}}{\partial \ddot{q}_{n+1}} + \frac{\partial F_{\text{ext},n+1}}{\partial \dot{q}_{n+1}} \frac{\partial \dot{q}_{n+1}}{\partial \ddot{q}_{n+1}} \right) + \\
& - (1-\alpha_f) \left(\frac{\partial F_{v,n+1}}{\partial q_{n+1}} \frac{\partial q_{n+1}}{\partial \ddot{q}_{n+1}} + \frac{\partial F_{v,n+1}}{\partial \dot{q}_{n+1}} \frac{\partial \dot{q}_{n+1}}{\partial \ddot{q}_{n+1}} \right), \tag{B.29}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial R_{2,n+1-\alpha_f}}{\partial \ddot{q}_{n+1}} = & (1-\alpha_m) \left(\frac{\partial \mathbf{J}_{\Phi,n+1}}{\partial q_{n+1}} \frac{\partial q_{n+1}}{\partial \ddot{q}_{n+1}} \right) \ddot{q}_{n+1} + (1-\alpha_m) \underline{\mathbf{J}}_{\Phi,n+1} \frac{\partial \ddot{q}_{n+1}}{\partial \ddot{q}_{n+1}} + \\
& - (1-\alpha_f) \left(\frac{\partial F_{c,n+1}}{\partial q_{n+1}} \frac{\partial q_{n+1}}{\partial \ddot{q}_{n+1}} + \frac{\partial F_{c,n+1}}{\partial \dot{q}_{n+1}} \frac{\partial \dot{q}_{n+1}}{\partial \ddot{q}_{n+1}} \right), \tag{B.30}
\end{aligned}$$

$$\begin{aligned} \frac{\partial R_{1,n+1-\alpha_f}}{\partial \underline{\lambda}_{n+1}} &= (1 - \alpha_m) \underline{m}_{n+1} \frac{\partial \underline{\ddot{q}}_{n+1}}{\partial \underline{\lambda}_{n+1}} + (1 - \alpha_f) \underline{d}_{n+1} \frac{\partial \underline{\dot{q}}_{n+1}}{\partial \underline{\lambda}_{n+1}} + \\ &+ (1 - \alpha_f) \underline{k}_{n+1} \frac{\partial \underline{q}_{n+1}}{\partial \underline{\lambda}_{n+1}} + (1 - \alpha_m) \underline{J}_{\Phi,n+1}^T \frac{\partial \underline{\lambda}_{n+1}}{\partial \underline{\lambda}_{n+1}}, \end{aligned} \quad (\text{B.31})$$

$$\frac{\partial R_{2,n+1-\alpha_f}}{\partial \underline{\lambda}_{n+1}} = (1 - \alpha_m) \underline{J}_{\Phi,n+1} \frac{\partial \underline{\ddot{q}}_{n+1}}{\partial \underline{\lambda}_{n+1}}. \quad (\text{B.32})$$

The derivatives of the state variables respect to $\underline{\ddot{q}}_{n+1}$ and $\underline{\lambda}_{n+1}$ are given by

$$\begin{aligned} \frac{\partial \underline{q}_{n+1}}{\partial \underline{\ddot{q}}_{n+1}} &= \beta \Delta t^2 \underline{e}, & \frac{\partial \underline{q}_{n+1}}{\partial \underline{\lambda}_{n+1}} &= \underline{0}, \\ \frac{\partial \underline{\dot{q}}_{n+1}}{\partial \underline{\ddot{q}}_{n+1}} &= \gamma \Delta t \underline{e}, & \frac{\partial \underline{\dot{q}}_{n+1}}{\partial \underline{\lambda}_{n+1}} &= \underline{0}, \\ \frac{\partial \underline{\ddot{q}}_{n+1}}{\partial \underline{\ddot{q}}_{n+1}} &= \underline{e}, & \frac{\partial \underline{\ddot{q}}_{n+1}}{\partial \underline{\lambda}_{n+1}} &= \underline{0}, \\ \frac{\partial \underline{\lambda}_{n+1}}{\partial \underline{\ddot{q}}_{n+1}} &= \underline{0}, & \frac{\partial \underline{\lambda}_{n+1}}{\partial \underline{\lambda}_{n+1}} &= \underline{e}, \end{aligned} \quad (\text{B.33})$$

leading to the terms of the Jacobian matrix given by

$$\begin{aligned} \frac{\partial R_{1,n+1-\alpha_f}}{\partial \underline{\ddot{q}}_{n+1}} &= (1 - \alpha_m) \beta \Delta t^2 \frac{\partial \underline{m}_{n+1}}{\partial \underline{q}_{n+1}} \underline{\ddot{q}}_{n+1} + (1 - \alpha_m) \underline{m}_{n+1} + \\ &+ (1 - \alpha_f) \beta \Delta t^2 \frac{\partial \underline{d}_{n+1}}{\partial \underline{q}_{n+1}} \underline{\dot{q}}_{n+1} + (1 - \alpha_f) \gamma \Delta t \underline{d}_{n+1} + \\ &+ (1 - \alpha_f) \beta \Delta t^2 \frac{\partial \underline{k}_{n+1}}{\partial \underline{q}_{n+1}} \underline{q}_{n+1} + (1 - \alpha_f) \beta \Delta t^2 \underline{k}_{n+1} + \\ &+ (1 - \alpha_m) \beta \Delta t^2 \frac{\partial \underline{J}_{\Phi,n+1}^T}{\partial \underline{q}_{n+1}} \underline{\lambda}_{n+1} + \\ &- (1 - \alpha_f) \left(\beta \Delta t^2 \frac{\partial F_{\text{ext},n+1}}{\partial \underline{q}_{n+1}} + \gamma \Delta t \frac{\partial F_{\text{ext},n+1}}{\partial \underline{\dot{q}}_{n+1}} \right) + \\ &- (1 - \alpha_f) \left(\beta \Delta t^2 \frac{\partial F_{v,n+1}}{\partial \underline{q}_{n+1}} + \gamma \Delta t \frac{\partial F_{v,n+1}}{\partial \underline{\dot{q}}_{n+1}} \right), \end{aligned} \quad (\text{B.34})$$

$$\begin{aligned} \frac{\partial R_{2,n+1-\alpha_f}}{\partial \underline{\ddot{q}}_{n+1}} &= (1 - \alpha_m) \beta \Delta t^2 \frac{\partial \underline{J}_{\Phi,n+1}}{\partial \underline{q}_{n+1}} \underline{\ddot{q}}_{n+1} + (1 - \alpha_m) \underline{J}_{\Phi,n} + \\ &- (1 - \alpha_f) \left(\beta \Delta t^2 \frac{\partial F_{c,n+1}}{\partial \underline{q}_{n+1}} + \gamma \Delta t \frac{\partial F_{c,n+1}}{\partial \underline{\dot{q}}_{n+1}} \right), \end{aligned} \quad (\text{B.35})$$

$$\frac{\partial R_{1,n+1-\alpha_f}}{\partial \lambda_{n+1}} = (1 - \alpha_m) \underline{J}_{\Phi,n+1}^T, \quad (\text{B.36})$$

$$\frac{\partial R_{2,n+1-\alpha_f}}{\partial \lambda_{n+1}} \underset{=}{=} 0. \quad (\text{B.37})$$

Appendix B.3. Sensitivity analysis

The derivative of the equations of motion leads to the governing equation of the sensitivities given by

$$\begin{aligned}
& (1-\alpha_m)\underline{\underline{\nabla m}}_{n+1}\ddot{q}_{n+1} + (1-\alpha_m)\underline{\underline{m}}_{n+1}\underline{\underline{\nabla \ddot{q}}}_{n+1} + \alpha_m\underline{\underline{\nabla m}}_n\ddot{q}_n + \alpha_m\underline{\underline{m}}_n\underline{\underline{\nabla \ddot{q}}}_n + \\
& + (1-\alpha_f)\underline{\underline{\nabla d}}_{n+1}\dot{q}_{n+1} + (1-\alpha_f)\underline{\underline{d}}_{n+1}\underline{\underline{\nabla \dot{q}}}_{n+1} + \alpha_f\underline{\underline{\nabla d}}_n\dot{q}_n + \alpha_f\underline{\underline{d}}_n\underline{\underline{\nabla \dot{q}}}_n + \\
& + (1-\alpha_f)\underline{\underline{\nabla k}}_{n+1}q_{n+1} + (1-\alpha_f)\underline{\underline{k}}_{n+1}\underline{\underline{\nabla q}}_{n+1} + \alpha_f\underline{\underline{\nabla k}}_nq_n + \alpha_f\underline{\underline{k}}_n\underline{\underline{\nabla q}}_n + \\
& + (1-\alpha_m)\underline{\underline{\nabla J}}_{\Phi,n+1}^T\underline{\underline{\lambda}}_{n+1} + (1-\alpha_m)\underline{\underline{J}}_{\Phi,n+1}^T\underline{\underline{\nabla \lambda}}_{n+1} + \alpha_m\underline{\underline{\nabla J}}_{\Phi,n}^T\underline{\underline{\lambda}}_n + \alpha_m\underline{\underline{J}}_{\Phi,n}^T\underline{\underline{\nabla \lambda}}_n = \\
& (1-\alpha_f)\underline{\underline{\nabla F}}_{\text{ext},n+1} + \alpha_f\underline{\underline{\nabla F}}_{\text{ext},n} + (1-\alpha_f)\underline{\underline{\nabla F}}_{v,n+1} + \alpha_f\underline{\underline{\nabla F}}_{v,n}, \quad (\text{B.38})
\end{aligned}$$

and

$$(1 - \alpha_m) \underline{\underline{\nabla \mathbf{J}_{\Phi, n+1} \ddot{\mathbf{q}}_{n+1}}} + (1 - \alpha_m) \underline{\mathbf{J}_{\Phi, n+1} \nabla \ddot{\mathbf{q}}_{n+1}} + \alpha_m \underline{\underline{\nabla \mathbf{J}_{\Phi, n} \ddot{\mathbf{q}}_n}} + \alpha_m \underline{\mathbf{J}_{\Phi, n} \nabla \ddot{\mathbf{q}}_n} = (1 - \alpha_f) \underline{\underline{\nabla F_{c, n+1}}} + \alpha_f \underline{\underline{\nabla F_{c, n}}}. \quad (\text{B.39})$$

Including Newmark's equations leads to

$$\begin{aligned}
& (1 - \alpha_m) \underline{\underline{\underline{\nabla m}}}_{n+1} \underline{\underline{\underline{\ddot{q}}}}_{n+1} + (1 - \alpha_m) \underline{\underline{\underline{m}}}_{n+1} \underline{\underline{\underline{\nabla \ddot{q}}}}_{n+1} + \alpha_m \underline{\underline{\underline{\nabla m}}}_n \underline{\underline{\underline{\ddot{q}}}}_n + \alpha_m \underline{\underline{\underline{m}}}_n \underline{\underline{\underline{\nabla \ddot{q}}}}_n + \\
& + (1 - \alpha_f) \underline{\underline{\underline{\nabla d}}}_{n+1} \underline{\underline{\underline{\dot{q}}}}_{n+1} + (1 - \alpha_f) \underline{\underline{\underline{d}}}_{n+1} \left(\underline{\underline{\underline{\nabla \dot{q}}}}_{\text{pred}} + \gamma \Delta t \underline{\underline{\underline{\nabla \ddot{q}}}}_{n+1} \right) + \alpha_f \underline{\underline{\underline{\nabla d}}}_n \underline{\underline{\underline{\dot{q}}}}_n + \alpha_f \underline{\underline{\underline{d}}}_n \underline{\underline{\underline{\nabla \dot{q}}}}_n + \\
& + (1 - \alpha_f) \underline{\underline{\underline{\nabla k}}}_{n+1} \underline{\underline{\underline{q}}}_{n+1} + (1 - \alpha_f) \underline{\underline{\underline{k}}}_{n+1} \left(\underline{\underline{\underline{\nabla q}}}_{\text{pred}} + \beta \Delta t^2 \underline{\underline{\underline{\nabla \ddot{q}}}}_{n+1} \right) + \alpha_f \underline{\underline{\underline{\nabla k}}}_n \underline{\underline{\underline{q}}}_n + \alpha_f \underline{\underline{\underline{k}}}_n \underline{\underline{\underline{\nabla q}}}_n + \\
& + (1 - \alpha_m) \underline{\underline{\underline{\nabla J}}}_{\Phi, n+1}^T \underline{\underline{\underline{\lambda}}}_{n+1} + (1 - \alpha_m) \underline{\underline{\underline{J}}}_{\Phi, n+1}^T \underline{\underline{\underline{\nabla \lambda}}}_{n+1} + \alpha_m \underline{\underline{\underline{\nabla J}}}_{\Phi, n}^T \underline{\underline{\underline{\lambda}}}_n + \alpha_m \underline{\underline{\underline{J}}}_{\Phi, n}^T \underline{\underline{\underline{\nabla \lambda}}}_n = \\
& (1 - \alpha_f) \underline{\underline{\underline{\nabla F}}}_{\text{ext}, n+1} + \alpha_f \underline{\underline{\underline{\nabla F}}}_{\text{ext}, n} + (1 - \alpha_f) \underline{\underline{\underline{\nabla F}}}_{v, n+1} + \alpha_f \underline{\underline{\underline{\nabla F}}}_{v, n}, \quad (\text{B.40})
\end{aligned}$$

and

$$(1 - \alpha_m) \underline{\underline{\nabla}} \mathbf{J}_{\Phi, n+1} \underline{\underline{\ddot{q}}}_{n+1} + (1 - \alpha_m) \underline{\underline{\mathbf{J}}}_{\Phi, n+1} \underline{\underline{\nabla}} \underline{\underline{\ddot{q}}}_{n+1} + \alpha_m \underline{\underline{\nabla}} \mathbf{J}_{\Phi, n} \underline{\underline{\dot{q}}}_n + \alpha_m \underline{\underline{\mathbf{J}}}_{\Phi, n} \underline{\underline{\nabla}} \underline{\underline{\ddot{q}}}_n = (1 - \alpha_f) \underline{\underline{\nabla}} F_{c, n+1} + \alpha_f \underline{\underline{\nabla}} F_{c, n}, \quad (\text{B.41})$$

which can be rewritten to

$$\begin{aligned}
& \left((1 - \alpha_m) \underline{\underline{m}}_{n+1} + (1 - \alpha_f) \gamma \Delta t \underline{\underline{d}}_{n+1} + (1 - \alpha_f) \beta \Delta t^2 \underline{\underline{k}}_{n+1} \right) \underline{\underline{\nabla \ddot{q}}}_{n+1} + (1 - \alpha_m) \underline{\underline{J}}_{\Phi, n+1}^T \underline{\underline{\nabla \lambda}}_{n+1} = \\
& (1 - \alpha_f) \underline{\underline{\nabla F}}_{\text{ext}, n+1} + \alpha_f \underline{\underline{\nabla F}}_{\text{ext}, n} + (1 - \alpha_f) \underline{\underline{\nabla F}}_{v, n+1} + \alpha_f \underline{\underline{\nabla F}}_{v, n} + \\
& - (1 - \alpha_m) \underline{\underline{\nabla m}}_{n+1} \underline{\underline{\ddot{q}}}_{n+1} - \alpha_m \underline{\underline{\nabla m}}_n \underline{\underline{\ddot{q}}}_n - \alpha_m \underline{\underline{m}}_n \underline{\underline{\nabla \ddot{q}}} + \\
& - (1 - \alpha_f) \underline{\underline{\nabla d}}_{n+1} \underline{\underline{\dot{q}}}_{n+1} - \alpha_f \underline{\underline{\nabla d}}_n \underline{\underline{\dot{q}}}_n - (1 - \alpha_f) \underline{\underline{d}}_{n+1} \underline{\underline{\nabla \dot{q}}}_{\text{pred}} - \alpha_f \underline{\underline{d}}_n \underline{\underline{\nabla \dot{q}}} + \\
& - (1 - \alpha_f) \underline{\underline{\nabla k}}_{n+1} \underline{\underline{q}}_{n+1} - \alpha_f \underline{\underline{\nabla k}}_n \underline{\underline{q}}_n - (1 - \alpha_f) \underline{\underline{k}}_{n+1} \underline{\underline{\nabla q}}_{\text{pred}} - \alpha_f \underline{\underline{k}}_n \underline{\underline{\nabla q}} + \\
& - (1 - \alpha_m) \underline{\underline{\nabla J}}_{\Phi, n+1}^T \underline{\underline{\lambda}}_{n+1} - \alpha_m \underline{\underline{\nabla J}}_{\Phi, n}^T \underline{\underline{\lambda}}_n - \alpha_m \underline{\underline{J}}_{\Phi, n}^T \underline{\underline{\nabla \lambda}}_n, \quad (\text{B.42})
\end{aligned}$$

and

$$\begin{aligned}
& (1 - \alpha_m) \underline{\underline{J}}_{\Phi, n+1} \underline{\underline{\nabla \ddot{q}}}_{n+1} = \\
& (1 - \alpha_f) \underline{\underline{\nabla F}}_{c, n+1} + \alpha_f \underline{\underline{\nabla F}}_{c, n} - (1 - \alpha_m) \underline{\underline{\nabla J}}_{\Phi, n+1} \underline{\underline{\ddot{q}}}_{n+1} - \alpha_m \underline{\underline{\nabla J}}_{\Phi, n} \underline{\underline{\ddot{q}}}_n - \alpha_m \underline{\underline{J}}_{\Phi, n} \underline{\underline{\nabla \ddot{q}}}. \quad (\text{B.43})
\end{aligned}$$

The governing equation of sensitivity analysis of the effective system is given by

$$\begin{bmatrix} \underline{\underline{m}}_{\text{eff}} & \underline{\underline{J}}_{\Phi, \text{eff}}^T \\ \underline{\underline{J}}_{\Phi, \text{eff}} & \underline{\underline{0}} \end{bmatrix} \begin{bmatrix} \underline{\underline{\nabla \dot{q}}}_{n+1} \\ \underline{\underline{\nabla \lambda}}_{n+1} \end{bmatrix} = \begin{bmatrix} \underline{\underline{F}}_{a, \text{eff}, \text{pseudo}} \\ \underline{\underline{F}}_{c, \text{eff}, \text{pseudo}} \end{bmatrix}, \quad (\text{B.44})$$

where

$$\begin{aligned}
\underline{\underline{F}}_{a, \text{eff}, \text{pseudo}} = & (1 - \alpha_f) \underline{\underline{\nabla F}}_{\text{ext}, n+1} + \alpha_f \underline{\underline{\nabla F}}_{\text{ext}, n} + (1 - \alpha_f) \underline{\underline{\nabla F}}_{v, n+1} + \alpha_f \underline{\underline{\nabla F}}_{v, n} + \\
& - (1 - \alpha_m) \underline{\underline{\nabla m}}_{n+1} \underline{\underline{\ddot{q}}}_{n+1} - \alpha_m \underline{\underline{\nabla m}}_n \underline{\underline{\ddot{q}}}_n - \alpha_m \underline{\underline{m}}_n \underline{\underline{\nabla \ddot{q}}} + \\
& - (1 - \alpha_f) \underline{\underline{\nabla d}}_{n+1} \underline{\underline{\dot{q}}}_{n+1} - \alpha_f \underline{\underline{\nabla d}}_n \underline{\underline{\dot{q}}}_n - (1 - \alpha_f) \underline{\underline{d}}_{n+1} \underline{\underline{\nabla \dot{q}}}_{\text{pred}} - \alpha_f \underline{\underline{d}}_n \underline{\underline{\nabla \dot{q}}} + \\
& - (1 - \alpha_f) \underline{\underline{\nabla k}}_{n+1} \underline{\underline{q}}_{n+1} - \alpha_f \underline{\underline{\nabla k}}_n \underline{\underline{q}}_n - (1 - \alpha_f) \underline{\underline{k}}_{n+1} \underline{\underline{\nabla q}}_{\text{pred}} - \alpha_f \underline{\underline{k}}_n \underline{\underline{\nabla q}} + \\
& - (1 - \alpha_m) \underline{\underline{\nabla J}}_{\Phi, n+1}^T \underline{\underline{\lambda}}_{n+1} - \alpha_m \underline{\underline{\nabla J}}_{\Phi, n}^T \underline{\underline{\lambda}}_n - \alpha_m \underline{\underline{J}}_{\Phi, n}^T \underline{\underline{\nabla \lambda}}, \quad (\text{B.45})
\end{aligned}$$

$$\underline{\underline{F}}_{c, \text{eff}, \text{pseudo}} = (1 - \alpha_f) \underline{\underline{\nabla F}}_{c, n+1} + \alpha_f \underline{\underline{\nabla F}}_{c, n} - (1 - \alpha_m) \underline{\underline{\nabla J}}_{\Phi, n+1} \underline{\underline{\ddot{q}}}_{n+1} - \alpha_m \underline{\underline{\nabla J}}_{\Phi, n} \underline{\underline{\ddot{q}}}_n - \alpha_m \underline{\underline{J}}_{\Phi, n} \underline{\underline{\nabla \ddot{q}}}. \quad (\text{B.46})$$