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ON THE OPTIMAL SCALING OF INDEX THREE DAES IN MULTIBODY DYNAMICS

Carlo L. Bottasso[1], **Daniel Dopico**[2], **and Lorenzo Trainelli**[1]

[1]Politecnico di Milano
Via La Masa 34, 20156 Milano, Italy
e-mail: carlo.bottasso@polimi.it, lorenzo.trainelli@polimi.it

[2] Escuela Politécnica Superior, University of La Coruña
Mendizábal s/n, 15403 Ferrol, Spain
e-mail: ddopico@udc.es

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Abstract. *We propose a preconditioning strategy for the governing equations of multibody systems in index-3 differential-algebraic form. The method eliminates the amplification of errors and the ill conditioning which affect numerical solutions of high index differential algebraic equations for small time steps. We develop a new theoretical analysis of the perturbation problem and we apply it to the derivation of preconditioners for the Newmark family of integration schemes. The theoretical results are confirmed by numerical experiments.*

1 INTRODUCTION

Errors and perturbations due to finite precision arithmetics pollute the numerical solution of high index differential algebraic equations (DAEs). This pollution causes disastrous effects for small values of the time step size. In fact, state variables and Lagrange multipliers are affected by increasing errors as the time step size decreases. Similarly, the system Jacobian matrix becomes severely ill conditioned.

Various remedies have been offered in the multibody dynamics literature to this problem. Basically, all remedies point to the reduction of the index from 3 to 2 or 1. Examples, among many others, are the well known GGL method [4] or the more recent Embedded Projection Method [1]. However, these approaches require the rewriting of the governing equations. This either increases the cost, since additional constraints and multipliers are introduced, or causes additional problems, like the drift of constraint violations.

A radically different approach consists in the preconditioning of the index-3 governing equations. Reference [7] proposed a simple scaling transformation which led to a partial improvement for both the sensitivity of the solution fields with respect to perturbations and the conditioning of the Jacobian matrix. In References [2, 3] it was shown that the pollution problem can be completely eliminated for BDF schemes by a proper scaling, achieving perfect independence on the time step size. This is the same behavior observed in the case of ordinary differential equations.

In this paper we offer a new theoretical analysis of the perturbation problem. Based on the results of the analysis, we propose a preconditioning strategy for the case of the Newmark family of integration schemes, which is representative of a larger class of commonly used time integrators (e.g. modified-α (HHT), generalized-α, etc.) The procedure amounts to a simple scaling of the unknowns which cures the pollution problem, and another similar scaling of the equations which eliminates the ill conditioning of the Jacobian matrix.

The paper is organized as follows. In Section 2 we present the asymptotic analysis in a general setting, in a way that clearly separates the effects of time discretization and the perturbations which are due to finite precision arithmetics. In Section 3 we start by reviewing the index-3 governing equations together with their time discretization according to the Newmark family of schemes. Next, we analyze two of the various possible implementations of the scheme, and in particular we consider the three-field (displacements, velocities and multipliers) and the two-field (displacements and multipliers) approaches. The former, although probably never employed in practice, is presented since it helps in the understanding of the general features of the proposed methodology, while the latter is obtained by static condensation of the velocities at each time step, and is substantially more efficient in terms of computational costs. For both settings, the asymptotic analysis resulting from Section 2 is carried out. Section 4 discusses the preconditioning strategy for the three and two-field approaches. Numerical results confirming the predicted behaviors are shown in Section 5. Some concluding remarks are finally exposed in Section 6.

2 ASYMPTOTIC ANALYSIS FOR A LINEARIZED DYNAMIC PROBLEM

Any implicit method for the numerical integration of the equations governing the dynamics of a non-linear system leads to the iterative solution of a linearized problem

$$\boldsymbol{J}\,\boldsymbol{q} = -\boldsymbol{b}, \tag{1}$$

in the time step (t_n, t_{n+1}), with time step size $h := t_{n+1} - t_n$. In the preceding equation, $\boldsymbol{q}$ represents the vector of increments for the unknowns in the time step, $\boldsymbol{b}$ represents the residual vector, and $\boldsymbol{J}$ is the Jacobian matrix of the problem, i.e. the tangent matrix of the residual vector with respect to the unknowns.

It goes without saying that $\boldsymbol{b}$, $\boldsymbol{J}$ and $\boldsymbol{q}$ all depend on the time step size h. Furthermore, to model the effects of finite precision arithmetics, we introduce the dependence of all terms appearing in eq. 1 on a small parameter ε. Expanding in Taylor series about $\varepsilon = 0$, we have

$$\boldsymbol{b}(h,\varepsilon) = \boldsymbol{b}(h,0) + \varepsilon \left.\frac{\partial \boldsymbol{b}}{\partial \varepsilon}\right|_{(h,0)} + O(\varepsilon^2), \tag{2a}$$

$$\boldsymbol{J}(h,\varepsilon) = \boldsymbol{J}(h,0) + \varepsilon \left.\frac{\partial \boldsymbol{J}}{\partial \varepsilon}\right|_{(h,0)} + O(\varepsilon^2), \tag{2b}$$

$$\boldsymbol{q}(h,\varepsilon) = \boldsymbol{q}(h,0) + \varepsilon \left.\frac{\partial \boldsymbol{q}}{\partial \varepsilon}\right|_{(h,0)} + O(\varepsilon^2). \tag{2c}$$

For *infinite* precision arithmetics, i.e. for $\varepsilon = 0$, one has at convergence of the Newton process

$$\lim_{h\to 0} \boldsymbol{b}(h,0) = 0, \qquad \lim_{h\to 0} \boldsymbol{q}(h,0) = 0, \tag{3}$$

so that

$$\lim_{h\to 0} \boldsymbol{b}(h,\varepsilon) = \varepsilon \lim_{h\to 0} \left(\frac{\partial \boldsymbol{b}}{\partial \varepsilon}\right)\Bigg|_{(h,0)} + O(\varepsilon^2), \tag{4a}$$

$$\lim_{h\to 0} \boldsymbol{q}(h,\varepsilon) = \varepsilon \lim_{h\to 0} \left(\frac{\partial \boldsymbol{q}}{\partial \varepsilon}\right)\Bigg|_{(h,0)} + O(\varepsilon^2). \tag{4b}$$

Inserting the previous expansions into eq. 1, yields

$$\varepsilon \lim_{h\to 0} \boldsymbol{J}(h,0) \lim_{h\to 0} \left(\frac{\partial \boldsymbol{q}}{\partial \varepsilon}\right)\Bigg|_{(h,0)} = -\varepsilon \lim_{h\to 0} \left(\frac{\partial \boldsymbol{b}}{\partial \varepsilon}\right)\Bigg|_{(h,0)} + O(\varepsilon^2). \tag{5}$$

Therefore, neglecting higher order terms, we get

$$\varepsilon \lim_{h\to 0} \left(\frac{\partial \boldsymbol{q}}{\partial \varepsilon}\right)\Bigg|_{(h,0)} = -\varepsilon \lim_{h\to 0} \boldsymbol{J}(h,0)^{-1} \lim_{h\to 0} \left(\frac{\partial \boldsymbol{b}}{\partial \varepsilon}\right)\Bigg|_{(h,0)}, \tag{6}$$

or, in other words,

$$\lim_{h\to 0} \boldsymbol{q}(h,\varepsilon) = -\lim_{h\to 0} \boldsymbol{J}^{-1}(h,0) \lim_{h\to 0} \boldsymbol{b}(h,\varepsilon). \tag{7}$$

Taking norms, we find

$$\left|\lim_{h\to 0} q_i(h,\varepsilon)\right| \leq \sum_j \left|\lim_{h\to 0} J^{-1}_{ij}(h,0)\right| \left|\lim_{h\to 0} b_j(h,\varepsilon)\right|, \tag{8a}$$

$$\leq \left\|\lim_{h\to 0} \boldsymbol{J}^{-1}(h,0)\right\|_\infty \left\|\lim_{h\to 0} \boldsymbol{b}(h,\varepsilon)\right\|_\infty. \tag{8b}$$

Equation 8b should be interpreted on a block by block basis for problems characterized by different sets of equations (e.g., dynamic equilibrium, kinematic, etc.) and different sets of unknowns (e.g., displacements, velocities, etc.); this will become clearer in the next section.

The previous result can be interpreted as follows: a perturbation in the evaluation of the residual (the term $\boldsymbol{b}(h,\varepsilon)$, which will differ from zero at convergence because of finite precision operations or because the Newton correction has been arrested to a certain given tolerance) will induce a perturbation in the Newton corrections (the term $\boldsymbol{q}(h,\varepsilon)$, which, therefore, will also not be zero at convergence). Such perturbation can be further amplified by the exact inverse of the Jacobian (the term $\boldsymbol{J}^{-1}(h,0)$). When the inverse Jacobian matrix and/or the residual become large as h goes to zero, i.e. when these functions depend on negative powers of h, large perturbations in the Newton corrections are observed.

Equation 8a suggests that a way of solving the problem is to look for appropriate preconditioners which, by suitably modifying the dependence of the residual vector and of the Jacobian matrix on h, will ensure the asymptotic independence on the time step size of the Newton corrections. In general, the scaled system can be written

$$\bar{\boldsymbol{J}}\,\bar{\boldsymbol{q}} = -\bar{\boldsymbol{b}}, \tag{9}$$

where

$$\bar{\boldsymbol{J}} := \boldsymbol{D}_L \boldsymbol{J}\, \boldsymbol{D}_R, \qquad \bar{\boldsymbol{q}} := \boldsymbol{D}_R^{-1}\,\boldsymbol{q}, \qquad \bar{\boldsymbol{b}} := \boldsymbol{D}_L \boldsymbol{b}, \tag{10}$$

represent the preconditioned Jacobian matrix, preconditioned solution vector and preconditioned residual vector, respectively. $\boldsymbol{D}_L$ is the left preconditioner, which scales the equations, while $\boldsymbol{D}_R$ is the right preconditioner, which scales the unknowns.

These ideas are made more precise in the context of the Newmark family of methods in the following section.

3 NEWMARK'S METHOD FOR MULTIBODY SYSTEMS

3.1 Problem definition

The dynamics of a n degree of freedom multibody system with m holonomic constraints is governed by the equations

$$\boldsymbol{M}\,\boldsymbol{v}' = \boldsymbol{f}(\boldsymbol{u},\boldsymbol{v},t) + \boldsymbol{G}(\boldsymbol{u},t)\,\boldsymbol{\lambda}, \tag{11a}$$

$$\boldsymbol{u}' = \boldsymbol{v}, \tag{11b}$$

$$0 = \boldsymbol{\Phi}(\boldsymbol{u},t), \tag{11c}$$

where the notation $(\cdot)' = \mathrm{d}(\cdot)/\mathrm{d}t$ indicates a derivative with respect to time t, $\boldsymbol{u}$ represents the n dimensional vector of generalized displacements, $\boldsymbol{v}$ the n dimensional vector of generalized velocities, and $\boldsymbol{\lambda}$ the m dimensional vector of Lagrange multipliers that enforce the constraint conditions. Furthermore, $\boldsymbol{f}$ is the n dimensional vector of internal and external forces, $\boldsymbol{\Phi}$ is the m dimensional vector of constraints, and $\boldsymbol{G} := \boldsymbol{\Phi}_{,\boldsymbol{u}}^{T}$ is the transpose of the constraint Jacobian. Finally, $\boldsymbol{M}$ represents the $n \times n$ generalized inertia matrix, which can be assumed constant without loss of generality. Equations 11 amount to an index-3 differential algebraic system in the state (differential) variables $(\boldsymbol{u},\boldsymbol{v})$ and the multiplier (algebraic) variables $\boldsymbol{\lambda}$.

The application of the Newmark's family of schemes to problem 11 on a time step defined between time t_n and time $t_{n+1} = t_n + h$ leads to the following discrete equations:

$$\boldsymbol{M}\,\boldsymbol{a}_{n+1} = \boldsymbol{f}_{n+1} + \boldsymbol{G}_{n+1}\boldsymbol{\lambda}_{n+1}, \tag{12a}$$

$$\boldsymbol{v}_{n+1} = \boldsymbol{v}_n + h\,\big((1-\gamma)\,\boldsymbol{a}_n + \gamma\,\boldsymbol{a}_{n+1}\big), \tag{12b}$$

$$\boldsymbol{u}_{n+1} = \boldsymbol{u}_n + h\,\boldsymbol{v}_n + \frac{h^2}{2}\,\big((1-2\,\beta)\,\boldsymbol{a}_n + 2\,\beta\,\boldsymbol{a}_{n+1}\big), \tag{12c}$$

$$0 = \boldsymbol{\Phi}_{n+1}. \tag{12d}$$

In the preceding equations,

$$\boldsymbol{f}_{n+1} := \boldsymbol{f}(\boldsymbol{u}_{n+1}, \boldsymbol{v}_{n+1}, t_{n+1}), \tag{13a}$$
$$\boldsymbol{G}_{n+1} := \boldsymbol{G}(\boldsymbol{u}_{n+1}, t_{n+1}), \tag{13b}$$
$$\boldsymbol{\Phi}_{n+1} := \boldsymbol{\Phi}(\boldsymbol{u}_{n+1}, t_{n+1}), \tag{13c}$$

while β and γ represent scalar parameters which define the accuracy and (linear) stability properties of the scheme (see [6, 5] for a detailed discussion). Equation 12a represents the discrete dynamic equilibrium equation, eqs. 12b,12c define the updates for the $(\boldsymbol{u}, \boldsymbol{v})$ variables, and finally eq. 12d exactly enforces the constraint at the end of the time step.

3.2 Three-field $(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{\lambda})$ form

We consider Newmark's method written in three-field form, the three unknown fields being $(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{\lambda})$. Eliminating $\boldsymbol{a}_{n+1}$ in eqs. 12 we obtain

$$\frac{1}{\gamma\, h}\, \boldsymbol{M}\, (\boldsymbol{v}_{n+1} - \boldsymbol{v}_n) = \boldsymbol{f}_{n+1} + \boldsymbol{G}_{n+1}\boldsymbol{\lambda}_{n+1} - \left(1 - \frac{1}{\gamma}\right)\, \boldsymbol{M}\, \boldsymbol{a}_n, \tag{14a}$$
$$\boldsymbol{u}_{n+1} - \boldsymbol{u}_n = h\, \left(\frac{\beta}{\gamma}\, \boldsymbol{v}_{n+1} + \left(1 - \frac{\beta}{\gamma}\, \boldsymbol{v}_n\right)\right) - \frac{h^2}{2}\, \left(1 - \frac{2\,\beta}{\gamma}\right)\, \boldsymbol{a}_n, \tag{14b}$$
$$0 = \boldsymbol{\Phi}_{n+1}. \tag{14c}$$

Linearizing eqs. 14 leads to problem 1, where the vector of unknown increments $\boldsymbol{q}$ and the residual vector $\boldsymbol{b}$ can be partitioned by blocks as

$$\boldsymbol{q} := \begin{bmatrix} \Delta\boldsymbol{u}_{n+1} \\ \Delta\boldsymbol{v}_{n+1} \\ \Delta\boldsymbol{\lambda}_{n+1} \end{bmatrix}, \qquad \boldsymbol{b} := \begin{bmatrix} \boldsymbol{b}_D \\ \boldsymbol{b}_K \\ \boldsymbol{b}_C \end{bmatrix}, \tag{15}$$

the subscript D indicating the row block of the dynamic equilibrium equations 14a, the subscript K the row block of the kinematic equations 14b, and the subscript C the row block of the constraint equations 14c. The expressions for the residual row blocks are found to be

$$\boldsymbol{b}_D := \frac{1}{\gamma\, h}\, \boldsymbol{M}\, (\boldsymbol{v}_{n+1} - \boldsymbol{v}_n) - (\boldsymbol{f}_{n+1} + \boldsymbol{G}_{n+1}\boldsymbol{\lambda}_{n+1}) + \left(1 - \frac{1}{\gamma}\right)\, \boldsymbol{a}_n, \tag{16a}$$
$$\boldsymbol{b}_K := \boldsymbol{u}_{n+1} - \boldsymbol{u}_n - h\, \left(\frac{\beta}{\gamma}\, \boldsymbol{v}_{n+1} + \left(1 - \frac{\beta}{\gamma}\, \boldsymbol{v}_n\right)\right) + \frac{h^2}{2}\, \left(1 - \frac{2\,\beta}{\gamma}\right)\, \boldsymbol{a}_n, \tag{16b}$$
$$\boldsymbol{b}_C := \boldsymbol{\Phi}_{n+1}. \tag{16c}$$

The Jacobian matrix $\boldsymbol{J}$ reads

$$\boldsymbol{J} = \begin{bmatrix} \boldsymbol{X} & \dfrac{1}{\gamma\, h}\boldsymbol{U} & -\boldsymbol{G} \\ \boldsymbol{I} & -\dfrac{\beta\, h}{\gamma}\boldsymbol{I} & \boldsymbol{0} \\ \boldsymbol{G}^T & \boldsymbol{0} & \boldsymbol{0} \end{bmatrix}, \tag{17}$$

where we wrote $\boldsymbol{G}$ for $\boldsymbol{G}_{n+1}$ for the sake of a lighter notation, while $\boldsymbol{I}$ is the $n \times n$ identity matrix, and finally

$$\boldsymbol{X} := -\left(\boldsymbol{f}_{,\boldsymbol{u}}\right)_{n+1} - \left(\left(\boldsymbol{G}\,\boldsymbol{\lambda}\right)_{,\boldsymbol{u}}\right)_{n+1}, \tag{18a}$$
$$\boldsymbol{Y} := -\left(\boldsymbol{f}_{,\boldsymbol{v}}\right)_{n+1}, \tag{18b}$$
$$\boldsymbol{U} := \boldsymbol{M} + \gamma\, h\, \boldsymbol{Y}. \tag{18c}$$

The inverse Jacobian matrix is readily computed as

$$\boldsymbol{J}^{-1} = \begin{bmatrix} \beta\, h^2 \boldsymbol{W} & \boldsymbol{W}\,\boldsymbol{U} & \boldsymbol{T}^{-1}\boldsymbol{G}\,\boldsymbol{R}^{-1} \\ \gamma\, h\, \boldsymbol{W} & \dfrac{\gamma}{\beta\, h}\,(\boldsymbol{I} - \boldsymbol{W}\,\boldsymbol{U}) & -\dfrac{\gamma}{\beta\, h}\,\boldsymbol{T}^{-1}\boldsymbol{G}\,\boldsymbol{R}^{-1} \\ -\boldsymbol{R}^{-1}\,\boldsymbol{G}^T\boldsymbol{T}^{-1} & \dfrac{1}{\beta\, h^2}\,\boldsymbol{R}^{-1}\,\boldsymbol{G}^T\boldsymbol{T}^{-1}\boldsymbol{U} & \dfrac{1}{\beta\, h^2}\,\boldsymbol{R}^{-1} \end{bmatrix}, \tag{19}$$

having defined

$$\boldsymbol{T} := \boldsymbol{M} + \gamma\, h\, \boldsymbol{Y} + \beta\, h^2 \boldsymbol{X}, \tag{20a}$$
$$\boldsymbol{R} := \boldsymbol{G}^T\boldsymbol{T}^{-1}\boldsymbol{G}, \tag{20b}$$
$$\boldsymbol{S} := \boldsymbol{G}\,\boldsymbol{R}^{-1}\boldsymbol{G}^T, \tag{20c}$$
$$\boldsymbol{W} := \boldsymbol{T}^{-1}(\boldsymbol{I} - \boldsymbol{S}\,\boldsymbol{T}^{-1}). \tag{20d}$$

3.3 Asymptotic analysis for the three-field $(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{\lambda})$ form

An estimate of the sensitivity to numerical perturbations of the three-field form of Newmark method can be based on the analysis of Section 2. In particular, we have

$$\lim_{h\to 0} \boldsymbol{J} = \begin{bmatrix} O(h^0) & O(h^{-1}) & O(h^0) \\ O(h^0) & O(h^1) & 0 \\ O(h^0) & 0 & 0 \end{bmatrix}, \tag{21}$$

and

$$\lim_{h\to 0} \boldsymbol{T} = O(h^0), \tag{22a}$$
$$\lim_{h\to 0} \boldsymbol{R} = O(h^0), \tag{22b}$$
$$\lim_{h\to 0} \boldsymbol{S} = O(h^0), \tag{22c}$$
$$\lim_{h\to 0} \boldsymbol{W} = O(h^0), \tag{22d}$$

so that

$$\lim_{h\to 0} \boldsymbol{J}^{-1} = \begin{bmatrix} O(h^2) & O(h^0) & O(h^0) \\ O(h^1) & O(h^{-1}) & O(h^{-1}) \\ O(h^0) & O(h^{-2}) & O(h^{-2}) \end{bmatrix}. \tag{23}$$

This implies that the condition number $C := \|\boldsymbol{J}\|_\infty \|\boldsymbol{J}^{-1}\|_\infty$ of the Jacobian matrix has the following asymptotic behavior

$$\lim_{h\to 0} C = O(h^{-3}). \tag{24}$$

Furthermore, inspecting $\boldsymbol{b}$, we obtain

$$\lim_{h\to 0} \Delta\boldsymbol{b}_D = O(h^0), \tag{25a}$$
$$\lim_{h\to 0} \Delta\boldsymbol{b}_K = O(h^0), \tag{25b}$$
$$\lim_{h\to 0} \Delta\boldsymbol{b}_C = O(h^0). \tag{25c}$$

Therefore, using eq. 8b and considering the block structure of the arrays, we conclude

$$\left|\lim_{h\to 0} \Delta \boldsymbol{u}_{n+1}\right| \leq O(h^0), \tag{26a}$$

$$\left|\lim_{h\to 0} \Delta \boldsymbol{v}_{n+1}\right| \leq O(h^{-1}), \tag{26b}$$

$$\left|\lim_{h\to 0} \Delta \boldsymbol{\lambda}_{n+1}\right| \leq O(h^{-2}). \tag{26c}$$

This result explains the commonly observed ill-conditioned behavior of the velocity components and of the Lagrange multipliers for small values of the step h.

3.4 Two-field $(\boldsymbol{u}, \boldsymbol{\lambda})$ form

Consider now a two-field implementation of Newmark method, and in particular the $(\boldsymbol{u}, \boldsymbol{\lambda})$ case. Given the updates 12b,12c, we eliminate $\boldsymbol{a}_{n+1}$ and $\boldsymbol{v}_{n+1}$ to obtain

$$\frac{1}{\beta\, h^2}\, \boldsymbol{M}\, \boldsymbol{u}_{n+1} - \boldsymbol{f}_{n+1} - \boldsymbol{G}_{n+1}\boldsymbol{\lambda}_{n+1} - \boldsymbol{j}_n = 0, \tag{27a}$$

$$\boldsymbol{\Phi}_{n+1} = 0, \tag{27b}$$

where

$$\boldsymbol{j}_n := \boldsymbol{M}\, \left(\frac{1}{\beta\, h^2}\, \boldsymbol{u}_n + \frac{1}{\beta\, h}\, \boldsymbol{v}_n + \left(1 - \frac{1}{2\,\beta}\right)\, \boldsymbol{a}_n \right). \tag{28}$$

The linearization of eqs. 27 leads to problem 1, with a vector of unknown increments $\boldsymbol{q}$ and a residual vector $\boldsymbol{b}$ given by

$$\boldsymbol{q} := \begin{bmatrix} \Delta \boldsymbol{u}_{n+1} \\ \Delta \boldsymbol{\lambda}_{n+1} \end{bmatrix}, \qquad \boldsymbol{b} := \begin{bmatrix} \boldsymbol{b}_D \\ \boldsymbol{b}_C \end{bmatrix}. \tag{29}$$

The residual row blocks corresponding to the dynamic equilibrium (subscript D) and constraint equations (subscript C) are, respectively,

$$\boldsymbol{b}_D := \frac{1}{\beta\, h^2}\, \boldsymbol{M}\, \boldsymbol{u}_{n+1} - \boldsymbol{f}_{n+1} - \boldsymbol{G}_{n+1}\boldsymbol{\lambda}_{n+1} - \boldsymbol{j}_n, \tag{30a}$$

$$\boldsymbol{b}_C := \boldsymbol{\Phi}_{n+1}. \tag{30b}$$

The Jacobian matrix $\boldsymbol{J}$ reads

$$\boldsymbol{J} = \begin{bmatrix} \frac{1}{\beta\, h^2}\, \boldsymbol{T} & -\boldsymbol{G} \\ \boldsymbol{G}^T & \boldsymbol{0} \end{bmatrix}, \tag{31}$$

and the inverse Jacobian matrix can be computed as

$$\boldsymbol{J}^{-1} = \begin{bmatrix} \beta\, h^2 \boldsymbol{W} & \boldsymbol{T}^{-1}\boldsymbol{G}\, \boldsymbol{R}^{-1} \\ -\boldsymbol{R}^{-1}\, \boldsymbol{G}^T \boldsymbol{T}^{-1} & \frac{1}{\beta\, h^2}\, \boldsymbol{R}^{-1} \end{bmatrix}. \tag{32}$$

3.5 Asymptotic analysis for the two-field $(\boldsymbol{u}, \boldsymbol{\lambda})$ form

Similarly to the three-field case, we get

$$\lim_{h\to 0} \boldsymbol{J} = \begin{bmatrix} O(h^{-2}) & O(h^0) \\ O(h^0) & 0 \end{bmatrix}, \tag{33}$$

and

$$\lim_{h\to 0} \boldsymbol{J}^{-1} = \begin{bmatrix} O(h^2) & O(h^0) \\ O(h^0) & O(h^{-2}) \end{bmatrix}. \tag{34}$$

Therefore, the condition number of the Jacobian matrix has the following asymptotic behavior

$$\lim_{h\to 0} C = O(h^{-4}). \tag{35}$$

Furthermore, inspecting $\boldsymbol{b}$, we obtain

$$\lim_{h\to 0} \Delta \boldsymbol{b}_D = O(h^{-2}), \tag{36a}$$

$$\lim_{h\to 0} \Delta \boldsymbol{b}_C = O(h^0), \tag{36b}$$

and therefore, from eq. 8b, we find

$$\left| \lim_{h\to 0} \Delta \boldsymbol{u}_{n+1} \right| \leq O(h^0), \tag{37a}$$

$$\left| \lim_{h\to 0} \Delta \boldsymbol{\lambda}_{n+1} \right| \leq O(h^{-2}). \tag{37b}$$

3.6 Summary of results of the asymptotic analysis

Table 1 summarizes the results for the various possible forms of the Newmark family of methods. Clearly, the asymptotic behavior of the various fields is always the same, irrespectively of the choice of primary variables. In fact, the $(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{\lambda})$, $(\boldsymbol{u}, \boldsymbol{\lambda})$, $(\boldsymbol{v}, \boldsymbol{\lambda})$ and $(\boldsymbol{a}, \boldsymbol{\lambda})$ forms are obtained from the $(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{a}, \boldsymbol{\lambda})$ form (eqs. 12) by static elimination. This operation, being performed analytically and hence exactly, can not change the dependence on h of the result.

	$(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{a}, \boldsymbol{\lambda})$	$(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{\lambda})$	$(\boldsymbol{u}, \boldsymbol{\lambda})$	$(\boldsymbol{v}, \boldsymbol{\lambda})$	$(\boldsymbol{a}, \boldsymbol{\lambda})$
$\Delta \boldsymbol{u}$	$O(h^0)$	$O(h^0)$	$O(h^0)$	$O(h^0)*$	$O(h^0)*$
$\Delta \boldsymbol{v}$	$O(h^{-1})$	$O(h^{-1})$	$O(h^{-1})*$	$O(h^{-1})$	$O(h^{-1})*$
$\Delta \boldsymbol{a}$	$O(h^{-2})$	$O(h^{-2})*$	$O(h^{-2})*$	$O(h^{-2})*$	$O(h^{-2})$
$\Delta \boldsymbol{\lambda}$	$O(h^{-2})$	$O(h^{-2})$	$O(h^{-2})$	$O(h^{-2})$	$O(h^{-2})$
C	$O(h^{-4})$	$O(h^{-3})$	$O(h^{-4})$	$O(h^{-3})$	$O(h^{-2})$

Table 1: Summary of results for the four, three and two-field forms (the symbol $*$ denotes a secondary unknown recovered from a primary one.)

On the other hand, the implementation affects the condition number C, as shown in the last row of the same table. Notice however that the effects of perturbations on the solution is *not* measured by the condition number C, but by the asymptotic analysis of Section 2. The only effect of C would be felt when using an iterative solver, whose convergence rate is affected by the conditioning of the matrix. The use of iterative solvers is however quite rare in the context of multibody dynamics problems.

4 OPTIMAL PRECONDITIONING

4.1 Preconditioning for the three-field $(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{\lambda})$ form

Consider the following right preconditioner for the three-field $(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{\lambda})$ form of Newmark's method

$$\boldsymbol{D}_R = \begin{bmatrix} \boldsymbol{I} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \dfrac{\gamma}{\beta\, h}\boldsymbol{I} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \dfrac{1}{\beta\, h^2}\boldsymbol{I} \end{bmatrix}. \tag{38}$$

This scaling of the unknowns, together with $\boldsymbol{D}_L = \boldsymbol{I}$, i.e. no scaling of the equations, completely solves the problem of sensitivity to perturbations. In fact, considering the preconditioned problem 9 and the expressions 16 and 19 for the residuals and the inverse Jacobian, we find:

$$\lim_{h\to 0} \bar{\boldsymbol{J}}^{-1} = \begin{bmatrix} O(h^0) & O(h^0) & O(h^0) \\ O(h^0) & O(h^0) & O(h^0) \\ O(h^0) & O(h^0) & O(h^0) \end{bmatrix}, \tag{39}$$

so that

$$\left| \lim_{h\to 0} \Delta\bar{\boldsymbol{u}}_{n+1} \right| \leq O(h^0), \tag{40a}$$

$$\left| \lim_{h\to 0} \Delta\bar{\boldsymbol{v}}_{n+1} \right| \leq O(h^0), \tag{40b}$$

$$\left| \lim_{h\to 0} \Delta\bar{\boldsymbol{\lambda}}_{n+1} \right| \leq O(h^0). \tag{40c}$$

This way perfect time-step-size independence of perturbations in all the differential and algebraic variables is achieved, as in the case of well behaved ordinary differential equations.

Consider now the right scaling 38 together with the following left scaling

$$\boldsymbol{D}_L = \begin{bmatrix} \beta\, h^2\boldsymbol{I} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{I} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{I} \end{bmatrix}. \tag{41}$$

The combination of the two cures the condition number, and in fact in this case we have

$$\lim_{h\to 0} C = O(h^0). \tag{42}$$

4.2 Preconditioning of the two-field $(\boldsymbol{u}, \boldsymbol{\lambda})$ form

Consider the following right preconditioner:

$$\boldsymbol{D}_R = \begin{bmatrix} \boldsymbol{I} & \boldsymbol{0} \\ \boldsymbol{0} & \dfrac{1}{\beta\, h^2}\boldsymbol{I} \end{bmatrix}. \tag{43}$$

This scaling, together with $\boldsymbol{D}_L = \boldsymbol{I}$, yields to

$$\lim_{h\to 0} \bar{\boldsymbol{J}}^{-1} = \begin{bmatrix} O(h^0) & O(h^0) \\ O(h^0) & O(h^0) \end{bmatrix}, \tag{44}$$

so that we have again perfect time-step-size independence of perturbations in the differential and algebraic variables:

$$\left| \lim_{h \to 0} \Delta \bar{\boldsymbol{u}}_{n+1} \right| \leq O(h^0), \tag{45a}$$

$$\left| \lim_{h \to 0} \Delta \bar{\boldsymbol{\lambda}}_{n+1} \right| \leq O(h^0). \tag{45b}$$

Considering now the right scaling 43 together with the following left scaling

$$\boldsymbol{D}_L = \begin{bmatrix} \beta\, h^2 \boldsymbol{I} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{I} \end{bmatrix}, \tag{46}$$

we have time-step-size independence for the condition number

$$\lim_{h \to 0} C = O(h^0). \tag{47}$$

4.3 Some remarks on preconditioning

It appears that the recipe for curing the numerical difficulties arising from finite precision arithmetics in DAEs can be split into two separate actions:

- a right preconditioning (i.e. a scaling of the unknowns) which cures the sensitivity to perturbations of the solution, and
- a left preconditioning (i.e. a scaling of the equations) which, on top of the former, cures the conditioning of the Jacobian matrix.

As discussed earlier, we stress that the former of these two actions is the one that really matters in the general case, while the latter is relevant only when employing an iterative solver for the solution of problem 1.

As a matter of fact, the right preconditioner works by scaling the unknowns in such a way that, with respect to the time variable, they are all of the same 'order'. Roughly speaking, generalized accelerations and Lagrange multipliers are 'integrated twice' by multiplication for h^2, generalized velocities are 'integrated once' by multiplication for h^1, while generalized coordinates are left unchanged. This appears to be a general rule, and is the same result obtained for a BDF integrator in References [2, 3].

For the left preconditioning, it appears that the recipe is again one of simple multiplication by positive powers of the time step size. In particular, the discretized dynamic equilibrium equation must be 'integrated twice' by multiplication for h^2, in order to reach the same 'order' with respect to the time variable of the kinematic and constraint equations.

Table 2 summarizes the block factors of the optimal left and right preconditioners for the various possible implementations of Newmark's method. The subscripts D, V, K and C for the left preconditioners refers to the dynamic, velocity, kinematic and constraint equations blocks, respectively. The subscripts u, v, a, λ for the right preconditioners refer to the displacement, velocity, acceleration and Lagrange multipliers blocks, respectively.

5 NUMERICAL EXAMPLES

In order to illustrate the predictions of the above analysis, two well known problems were solved: namely, the simple pendulum, and Andrews' squeezing mechanism. Both problems

	$(\boldsymbol{u},\boldsymbol{v},\boldsymbol{a},\boldsymbol{\lambda})$	$(\boldsymbol{u},\boldsymbol{v},\boldsymbol{\lambda})$	$(\boldsymbol{u},\boldsymbol{\lambda})$	$(\boldsymbol{v},\boldsymbol{\lambda})$	$(\boldsymbol{a},\boldsymbol{\lambda})$
$D_{L,D}$ factor	$\beta\,h^2$	$\beta\,h^2$	$\beta\,h^2$	$\gamma\,h^2$	$\beta\,h^2$
$D_{L,V}$ factor	1	–	–	–	–
$D_{L,K}$ factor	1	1	–	–	–
$D_{L,C}$ factor	1	1	1	1	1
$D_{R,u}$ factor	1	1	1	–	1
$D_{R,v}$ factor	$\gamma/\beta\,h$	$\gamma/\beta\,h$	–	$1/\gamma\,h$	–
$D_{R,a}$ factor	$1/\beta\,h^2$	–	–	–	$1/\beta\,h^2$
$D_{R,\lambda}$ factor	$1/\beta\,h^2$	$1/\beta\,h^2$	$1/\beta\,h^2$	$1/\beta\,h^2$	$1/\beta\,h^2$

Table 2: Block factors of the optimal left and right preconditioners for the various possible implementations of Newmark's method.

were solved using the trapezoidal rule (*i.e.* Newmark's method with $\beta = 1/4$, $\gamma = 1/2$) with the two-field $(\boldsymbol{u},\boldsymbol{\lambda})$ approach.

At each time step, the non-linear discretized equations are iteratively solved by using Newton method. At the j-th iteration, one computes the current corrections from the linear system

$$\boldsymbol{J}^j\boldsymbol{q}^j = -\boldsymbol{b}^j. \tag{48}$$

The norm of the corrections $\boldsymbol{q}^j$ decreases at each iteration up to a certain saturation value. In fact, recall that, due to accumulation of roundoff errors, we have

$$\lim_{h\to 0}\boldsymbol{q}(h,\varepsilon) \neq 0. \tag{49}$$

If further iterations are carried out, the norm of the corrections oscillates around its saturation value, and asymptotic convergence is lost. To take into account this effect arising from finite precision arithmetics, we arrested the iterations when the Newton corrections stop decreasing, i.e. when the condition

$$\|\boldsymbol{q}^{j+1}\| \geq \|\boldsymbol{q}^j\| \tag{50}$$

is detected. The last decreasing Newton correction norm indicates the tightest achievable convergence of the Newton iteration process, which can not be further improved no matter how many additional iterations are carried out.

For all problems, we considered the following formulations:

- no preconditioning: the discretized governing equations are left as they are originally cast by applying the trapezoidal rule to eqs. 51;
- left preconditioning: the discretized governing equations are subjected to the scaling of the residuals given by eq. 46;
- right preconditioning: the discretized equations are subjected to the scaling of the unknowns given by eq. 43;
- optimal (i.e. full right/left) preconditioning: the discretized equations are subjected to both the right preconditioning and the left preconditioning.

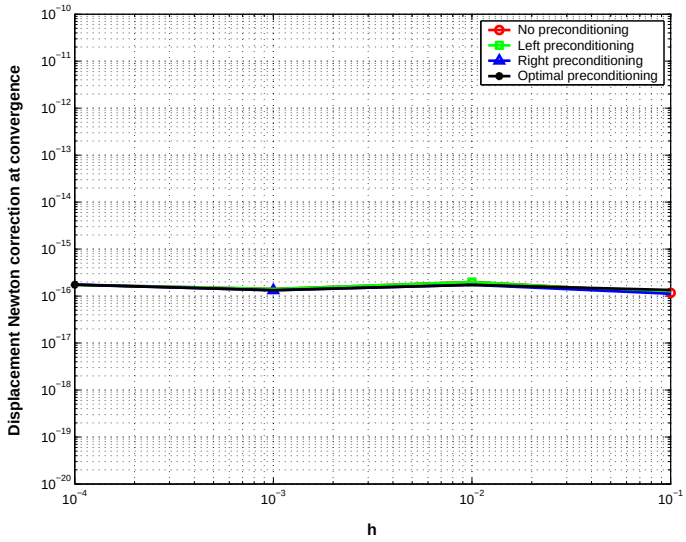

Figure 1: Simple pendulum problem. Last decreasing Newton correction norms of the displacements vs. the time step size with the $(\boldsymbol{u}, \boldsymbol{\lambda})$ approach.

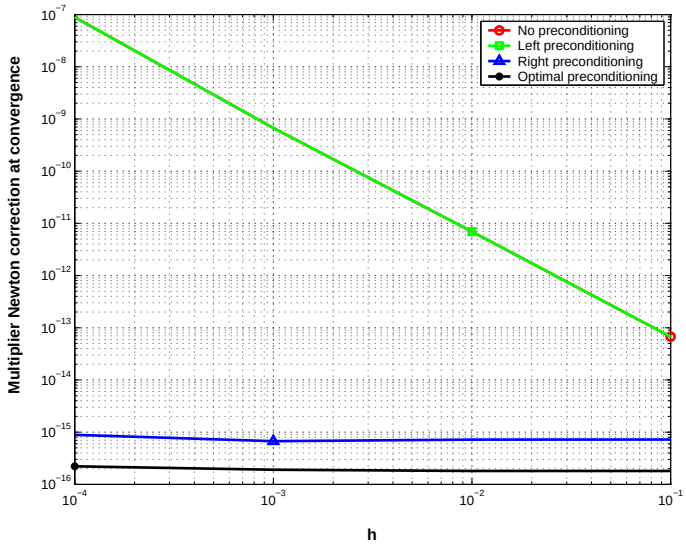

Figure 2: Simple pendulum problem. Last decreasing Newton correction norms of the Lagrange multiplier vs. the time step size with the $(\boldsymbol{u}, \boldsymbol{\lambda})$ approach.

5.1 The simple pendulum

The problem is governed by the following equations:

$$v_x' = \lambda\, u_x, \tag{51a}$$
$$v_y' = \lambda\, u_y - 1, \tag{51b}$$
$$u_x' = v_x, \tag{51c}$$
$$u_y' = v_y, \tag{51d}$$
$$0 = \frac{1}{2}\,(u_x^2 + u_y^2 - 1), \tag{51e}$$

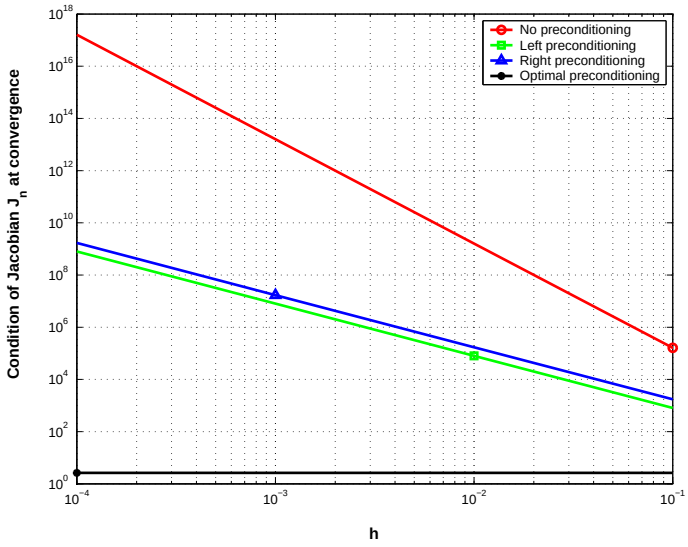

Figure 3: Simple pendulum problem. Condition number for the Jacobian matrix at convergence vs. the time step size with the $(\boldsymbol{u}, \boldsymbol{\lambda})$ approach.

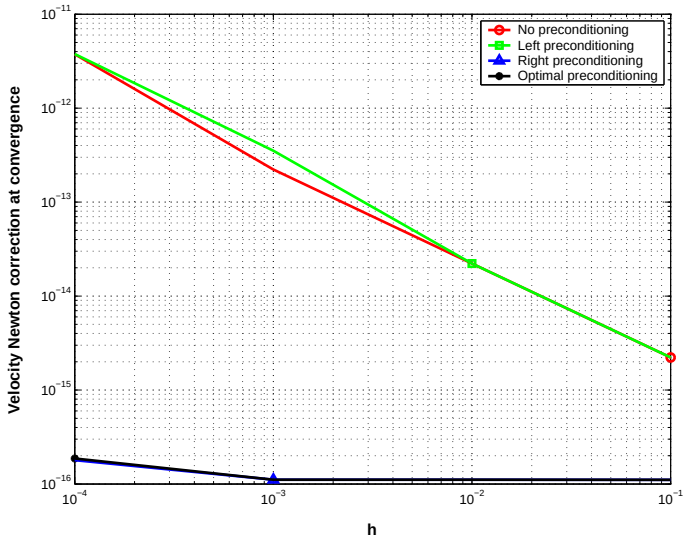

Figure 4: Simple pendulum problem. Last decreasing Newton correction norms of the velocities vs. the time step size with the $(\boldsymbol{v}, \boldsymbol{\lambda})$ approach.

where u_x and u_y are the Cartesian coordinates of the point mass, v_x and v_y the corresponding velocity components, while λ the intensity of the reaction force. Bar length, point mass and acceleration of gravity are all equal to 1. The point mass is initially at rest with $u_x = 1$, $u_y = 0$, and falls under the action of gravity. The problem was solved in the time interval $[0, 1 \cdot 10^{-3}]$, and we used time-step sizes $h = \{1 \cdot 10^{-1}, 1 \cdot 10^{-2}, 1 \cdot 10^{-3}, 1 \cdot 10^{-4}\}$.

Figure 1 shows the behavior of the coordinate correction norm as a function of h. It appears that the non-preconditioned and the preconditioned solutions are all insensitive to the time step size, as predicted. The case of the Lagrange multipliers, however, is very different: figure 2 shows that non-preconditioned multiplier corrections (as well as the left-preconditioned ones) display an $O(h^{-2})$ behavior, while the right-preconditioned and the optimally preconditioned

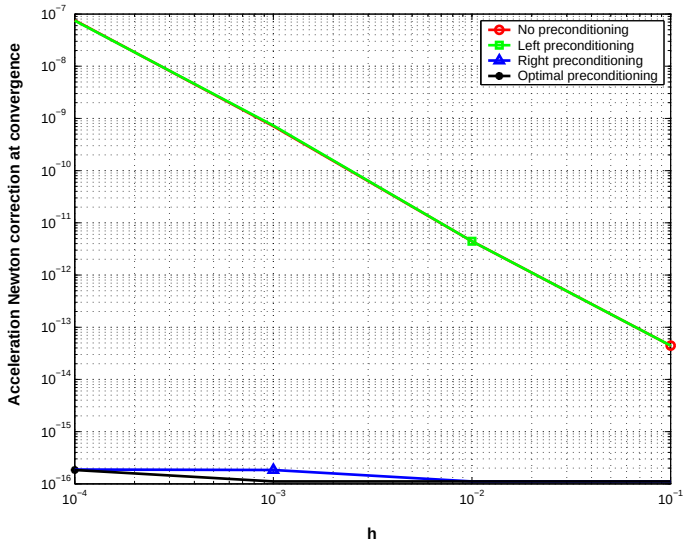

Figure 5: Simple pendulum problem. Last decreasing Newton correction norms of the accelerations vs. the time step size with the $(\boldsymbol{a}, \boldsymbol{\lambda})$ approach.

corrections are insensitive to the time step size. Figure 3 shows the condition number of the Jacobian matrix: in this case, the non-preconditioned values are $O(h^{-4})$, the left- only and right-only preconditioned values are $O(h^{-2})$, while the optimally preconditioned values achieve time step size insensitivity. These results are consistent with table 1.

In order to complete the picture, in figures 4 and 5 we give the results of the same analysis carried out with the two-field $(\boldsymbol{v}, \boldsymbol{\lambda})$ and $(\boldsymbol{a}, \boldsymbol{\lambda})$ approaches. Figure 4 shows the behavior of the velocity correction norm and figure 5 that of the acceleration correction norm as functions of h. In the former figure, we see that non-preconditioned velocity corrections (as well as the left-preconditioned ones) are $O(h^{-1})$, while the right-preconditioned and optimally preconditioned corrections are insensitive to the time step size. In the latter figure, the non-preconditioned velocity corrections (as well as the left-preconditioned ones) are $O(h^{-2})$, while the right-preconditioned and optimally preconditioned corrections are again insensitive to the time step size. Again, all results are consistent with table 1.

5.2 Andrews' squeezing mechanism

Next, we consider the well known Andrew's squeezing mechanism, a planar holonomic multibody system depicted in figure 6, and consisting of seven rigid bodies connected via revolute joints, loaded by a spring at point D and actuated by a constant torque driver at point O. The model is described in detail in Reference [8]. The problem is here formulated in terms of the 2-D cartesian coordinates of the points E through H of the figure, along with the Lagrange multipliers which enforce the constant distance constraints between the points. We used the time-step sizes $h = \{1 \cdot 10^{-3}, 1 \cdot 10^{-4}, 1 \cdot 10^{-5}, 1 \cdot 10^{-6}, 1 \cdot 10^{-7}\}$, for a duration of the simulation of 0.02 seconds.

Figures 7, 8 and 9 show, respectively, the coordinate correction norm, the Lagrange multipliers correction norm, and the condition number as functions of the time step. Here again the results exactly agree with the ones predicted by the analysis and with those of the previous example.

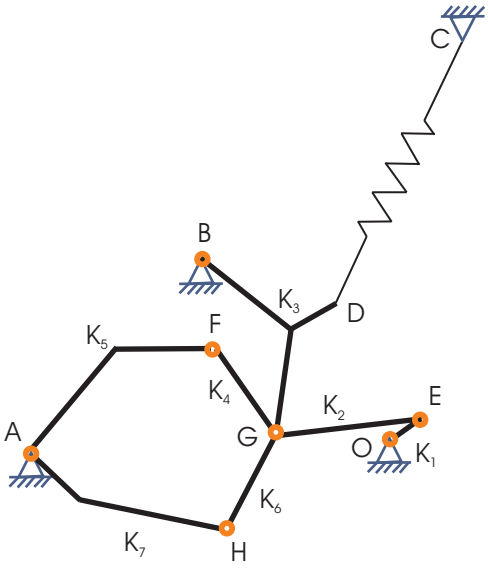

Figure 6: Andrews' squeezing mechanism.

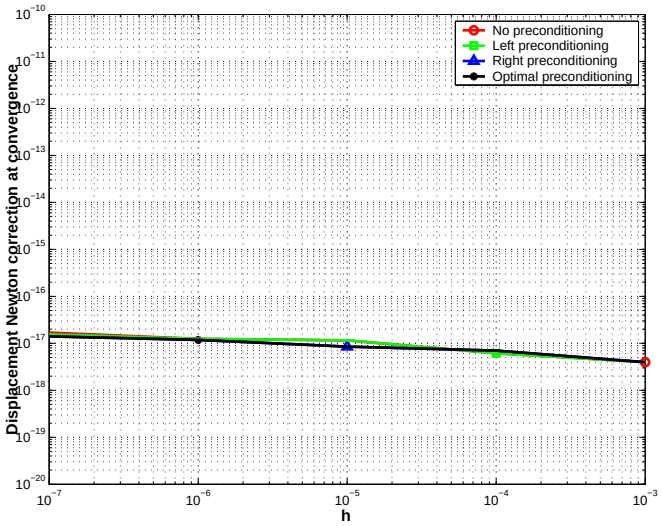

Figure 7: Andrews' mechanism. Last decreasing Newton correction norms of the coordinates vs. the time step size with the $(\boldsymbol{u}, \boldsymbol{\lambda})$ approach.

6 CONCLUDING REMARKS

In this work we have presented a novel analysis of the sensitivity to perturbations arising from finite precision arithmetics in the solution of index-3 differential-algebraic problems. The effects of finite precision arithmetics are modeled by using a small number, and an asymptotic analysis is carried out. Estimates for the perturbations in the unknowns are obtained by determining the dependence on the time step size of the residual vector and of the Jacobian matrix of the linearized problem.

Based on this result, preconditioners are readily identified which cure the pollution problem at its root. We analyzed the Newmark family of integrators, as a representative example of second order integrators for finite-element multibody system analysis. The preconditioners

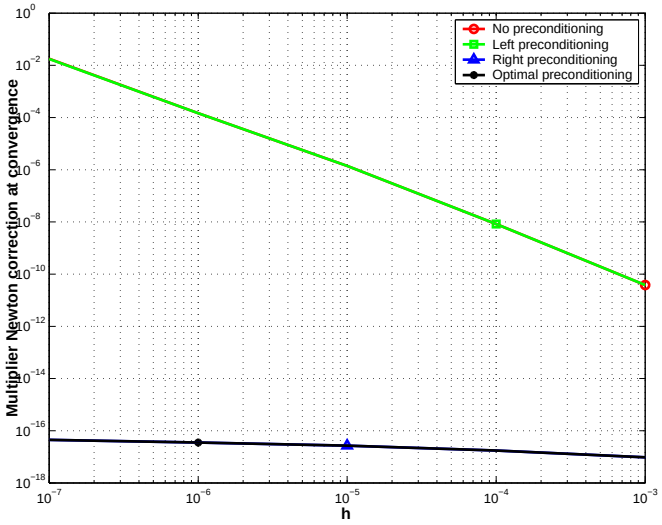

Figure 8: Andrews' mechanism. Last decreasing Newton correction norms of the Lagrange multiplier vs. the time step size with the $(\boldsymbol{u}, \boldsymbol{\lambda})$ approach.

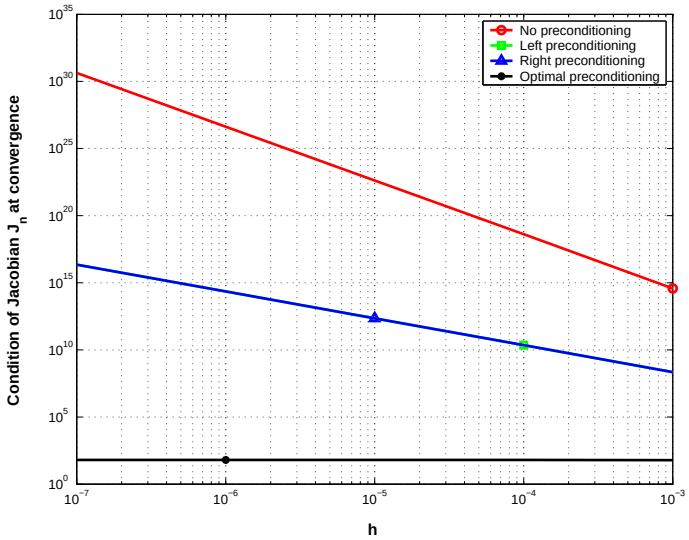

Figure 9: Andrews' mechanism. Condition number for the Jacobian matrix at convergence vs. the time step size with the $(\boldsymbol{u}, \boldsymbol{\lambda})$ approach.

were described in detail in this work for two forms of the equations. All other possible forms lead however to the same identical results, namely that it is always possible to eliminate the problem by simple scaling.

Numerical examples were used to confirm the analysis and illustrate the beneficial effects of the preconditioning strategy. The proposed methodology has the potential merit, with respect to other possible approaches, of being trivial to implement in an existing code. In fact it does not require any re-writing of the governing equations and/or the introduction of additional unknowns as commonly done with index-reduction approaches.

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