OPTIMAL PRECONDITIONERS FOR THE SOLUTION OF CONSTRAINED MECHANICAL SYSTEMS IN INDEX-3 FORM

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ABSTRACT

Index-3 differential algebraic equations, such as those governing multibody system dynamics, often pose severe numerical difficulties for small time step sizes. These difficulties can be traced back to the effects of finite precision arithmetics. In this work a solution to this problem is found as a simple preconditioning for the governing equations that eliminates the amplification of errors and the ill conditioning altogether. We develop a theoretical analysis, in particular for the case of the Newmark family of schemes, and show numerical experiments that confirm the predicted behavior.

1 INTRODUCTION

Finite precision arithmetics and non-null convergence tolerances are at the root of well known numerical difficulties in the solution of high index differential algebraic equations (DAEs). Errors and perturbations pollute the numerical solution, resulting in 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.

Typically, proposed remedies in the multibody dynamics literature rely on the reduction of the index from 3 to 2 or even 1. When this is done without appending additional constraints and multipliers, the well known drift of constraint violations is experienced. On the other hand, other approaches such as the GGL method (Gear et al. (1985)) or the more recent Embedded Projection Method (Borri et al. (2006)), avoid the drift effect by introducing additional constraints and multipliers, yielding higher computational costs.

Here we propose a different approach consisting in a preconditioning of the standard index-3 governing equations. A proper scaling of equations and unknowns is found that completely eliminates the pollution problem, achieving perfect independence on the time step size, as observed in the case of ordinary differential equations.

The recipe for the preconditioning is determined on the basis of a theoretical analysis of the perturbation problem in which we model the effects of finite precision arithmetics.

We consider the case of the Newmark family of integration schemes, as representative of a larger class of commonly used time integrators (e.g. modified-α (HHT), generalized-α, etc.). Bottasso et al. (2006) reports in greater detail the proposed formulation, while Bottasso, Bauchau (2005a, 2006) consider the case of BDF methods. Finally, we show some numerical results obtained for a representative multibody problem that confirm the predicted analysis.

2 ASYMPTOTIC ANALYSIS FOR A LINEARIZED DYNAMIC PROBLEM

Any implicit method for the numerical integration of the equations governing the dynamics of a nonlinear 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. Clearly, $\boldsymbol{b}$, $\boldsymbol{J}$ and $\boldsymbol{q}$ all depend on the time step size h.

In the following, we propose a simple approach to account for the effects of *finite* precision arithmetics. To this end, 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

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

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

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

Assuming *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

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

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

Neglecting higher order terms, we get

$$\lim_{h\to 0} \boldsymbol{q}(h,\varepsilon) = -\lim_{h\to 0} \boldsymbol{J}^{-1}(h,0) \lim_{h\to 0} \boldsymbol{b}(h,\varepsilon). \tag{5}$$

Taking norms, we find

$$\left|\lim_{h\to 0} q_i(h,\varepsilon)\right| \le \sum_j \left|\lim_{h\to 0} J^{-1}_{ij}(h,0)\right| \left|\lim_{h\to 0} b_j(h,\varepsilon)\right|, \tag{6a}$$

$$\le \left\|\lim_{h\to 0} \boldsymbol{J}^{-1}(h,0)\right\|_\infty \left\|\lim_{h\to 0} \boldsymbol{b}(h,\varepsilon)\right\|_\infty. \tag{6b}$$

Equation (6b) 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.).

From the analysis carried out above, it appears that a perturbation in the evaluation of the residual $\boldsymbol{b}(h,\varepsilon)$, 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 $\boldsymbol{q}(h,\varepsilon)$, which, therefore, will also not be zero at convergence. Such perturbation can be further amplified by the exact inverse of the Jacobian $\boldsymbol{J}^{-1}(h,0)$. 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.

From Eq. (6a) we infer that a solution to this problem can be worked out by appropriate preconditioning of the residual vector and Jacobian matrix, i.e. by considering a scaled problem

$$\bar{\boldsymbol{J}}\,\bar{\boldsymbol{q}} = -\bar{\boldsymbol{b}}, \tag{7}$$

where

$$\bar{\boldsymbol{J}} := \boldsymbol{D}_L \boldsymbol{J}\, \boldsymbol{D}_R, \qquad \bar{\boldsymbol{q}} := \boldsymbol{D}_R^{-1}\,\boldsymbol{q}, \qquad \bar{\boldsymbol{b}} := \boldsymbol{D}_L \boldsymbol{b}, \tag{8}$$

represent the preconditioned Jacobian matrix, preconditioned solution vector and preconditioned residual vector, respectively. Matrices $\boldsymbol{D}_L$ and $\boldsymbol{D}_R$ are the left and right preconditioner, which scale the equations and the unknowns, respectively. This way, by suitably modifying the dependence of these terms on h, asymptotic independence on the time step size of the Newton corrections can be achieved.

3 NEWMARK'S METHOD FOR MULTIBODY SYSTEMS

The equations governing the dynamics of a n degree of freedom multibody system with m holonomic constraints are given by

$$\boldsymbol{M}\,\boldsymbol{v}' = \boldsymbol{f}(\boldsymbol{u},\boldsymbol{v},t) + \boldsymbol{G}(\boldsymbol{u},t)\,\boldsymbol{\lambda}, \tag{9a}$$

$$\boldsymbol{u}' = \boldsymbol{v}, \tag{9b}$$

$$0 = \boldsymbol{\Phi}(\boldsymbol{u},t), \tag{9c}$$

where $\boldsymbol{u}$ represents the n dimensional vector of generalized displacements, $\boldsymbol{v}$ the n dimensional vector of generalized velocities, $\boldsymbol{\lambda}$ the m dimensional vector of Lagrange multipliers that enforce the constraint conditions, $\boldsymbol{f}$ the n dimensional vector of internal and external forces, $\boldsymbol{\Phi}$ the m dimensional vector of constraints, $\boldsymbol{G} := \boldsymbol{\Phi}_{,\boldsymbol{u}}^{T}$ the transpose of the constraint Jacobian, $\boldsymbol{M}$ the $n \times n$ generalized inertia matrix, which can be assumed constant without loss of generality. A prime is used to indicate a derivative with respect to time t.

Equations (9) represent an index-3 differential algebraic system in the state (differential) variables $(\boldsymbol{u},\boldsymbol{v})$ and the multiplier (algebraic) variables $\boldsymbol{\lambda}$.

The following discrete equations result from the application of the Newmark's family of schemes to problem (9) on a time step defined between time t_n and time $t_{n+1} = t_n + h$:

$$\boldsymbol{M}\,\boldsymbol{a}_{n+1} = \boldsymbol{f}_{n+1} + \boldsymbol{G}_{n+1}\boldsymbol{\lambda}_{n+1}, \tag{10a}$$

$$\boldsymbol{v}_{n+1} = \boldsymbol{v}_n + h\left((1-\gamma)\,\boldsymbol{a}_n + \gamma\,\boldsymbol{a}_{n+1}\right), \tag{10b}$$

$$\boldsymbol{u}_{n+1} = \boldsymbol{u}_n + h\,\boldsymbol{v}_n \tag{10c}$$

$$+ \frac{h^2}{2}\left((1-2\,\beta)\,\boldsymbol{a}_n + 2\,\beta\,\boldsymbol{a}_{n+1}\right), \tag{10d}$$

$$0 = \boldsymbol{\Phi}_{n+1}. \tag{10e}$$

In the preceding equations,

$$\boldsymbol{f}_{n+1} := \boldsymbol{f}(\boldsymbol{u}_{n+1},\boldsymbol{v}_{n+1},t_{n+1}), \tag{11a}$$

$$\boldsymbol{G}_{n+1} := \boldsymbol{G}(\boldsymbol{u}_{n+1},t_{n+1}), \tag{11b}$$

$$\boldsymbol{\Phi}_{n+1} := \boldsymbol{\Phi}(\boldsymbol{u}_{n+1},t_{n+1}), \tag{11c}$$

while β and γ represent scalar parameters which define the accuracy and (linear) stability properties of the scheme (see Newmark (1959); Geradin, Cardona (2001) for a detailed discussion).

Equation (10a) represents the discrete dynamic equilibrium equation, Eqs. (10b,10d) define the updates for the $(\boldsymbol{u},\boldsymbol{v})$ variables, and finally Eq. (10e) exactly enforces the constraint at the end of the time step.

4 DISPLACEMENT/MULTIPLIER IMPLEMENTATION

A common implementation of the preceding scheme is the two-field form in terms of $(\boldsymbol{u},\boldsymbol{\lambda})$. All other possible forms of the scheme are discussed in Bottasso et al. (2006). In order to obtain the solving equations for this specific implementation, we eliminate $\boldsymbol{a}_{n+1}$ and $\boldsymbol{v}_{n+1}$ using the updates (10b,10d), to obtain

$$\frac{1}{\beta\,h^2}\,\boldsymbol{M}\,\boldsymbol{u}_{n+1} - \boldsymbol{f}_{n+1} - \boldsymbol{G}_{n+1}\boldsymbol{\lambda}_{n+1} - \boldsymbol{j}_n = 0, \tag{12a}$$

$$\boldsymbol{\Phi}_{n+1} = 0, \tag{12b}$$

where

$$\boldsymbol{j}_n := \boldsymbol{M}\left(\frac{1}{\beta\,h^2}\,\boldsymbol{u}_n + \frac{1}{\beta\,h}\,\boldsymbol{v}_n + \left(1 - \frac{1}{2\,\beta}\right)\,\boldsymbol{a}_n\right). \tag{13}$$

The linearization of Eqs. (12) leads to problem (1), with

$$\boldsymbol{q} := \begin{bmatrix} \Delta\boldsymbol{u}_{n+1} \\ \Delta\boldsymbol{\lambda}_{n+1} \end{bmatrix}, \tag{14a}$$

$$\boldsymbol{b} := \begin{bmatrix} \boldsymbol{b}_D \\ \boldsymbol{b}_C \end{bmatrix}, \tag{14b}$$

$$\boldsymbol{J} = \begin{bmatrix} \frac{1}{\beta\,h^2}\,\boldsymbol{T} & -\boldsymbol{G} \\ \boldsymbol{G}^T & \boldsymbol{0} \end{bmatrix}, \tag{14c}$$

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

$$\boldsymbol{b}_D := \frac{1}{\beta\,h^2}\,\boldsymbol{M}\,\boldsymbol{u}_{n+1} - \boldsymbol{f}_{n+1} - \boldsymbol{G}_{n+1}\boldsymbol{\lambda}_{n+1} - \boldsymbol{j}_n, \tag{15a}$$

$$\boldsymbol{b}_C := \boldsymbol{\Phi}_{n+1}. \tag{15b}$$

The inverse Jacobian matrix can be computed as

$$\boldsymbol{J}^{-1} = \begin{bmatrix} \beta\,h^2\boldsymbol{W} & \boldsymbol{T}^{-1}\boldsymbol{G}\,\boldsymbol{R}^{-1} \\ -\boldsymbol{R}^{-1}\,\boldsymbol{G}^T\boldsymbol{T}^{-1} & \frac{1}{\beta\,h^2}\,\boldsymbol{R}^{-1} \end{bmatrix}. \tag{16}$$

At this point, we are in position to estimate the sensitivity to numerical perturbations of the $(\boldsymbol{u},\boldsymbol{\lambda})$ form of Newmark's method based on the analysis of Section 2. In particular, we have

$$\lim_{h\to 0}\boldsymbol{J} = \begin{bmatrix} O(h^{-2}) & O(h^0) \\ O(h^0) & 0 \end{bmatrix}, \tag{17}$$

and

$$\lim_{h\to 0} \boldsymbol{J}^{-1} = \begin{bmatrix} O(h^2) & O(h^0) \\ O(h^0) & O(h^{-2}) \end{bmatrix}. \tag{18}$$

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

$$\lim_{h\to 0} C = O(h^{-4}). \tag{19}$$

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

$$\lim_{h\to 0} \boldsymbol{b}_D = O(h^{-2}), \tag{20a}$$

$$\lim_{h\to 0} \boldsymbol{b}_C = O(h^0), \tag{20b}$$

and therefore, from Eq. (6b), we find

$$\left| \lim_{h\to 0} \Delta \boldsymbol{u}_{n+1} \right| \leq O(h^0), \tag{21a}$$

$$\left| \lim_{h\to 0} \Delta \boldsymbol{\lambda}_{n+1} \right| \leq O(h^{-2}). \tag{21b}$$

As apparent, while the displacement increments are not affected, both the condition number and, more importantly, the multiplier increments show a very unfavorable dependence on time step size, originating the well known numerical difficulties.

5 OPTIMAL PRECONDITIONING

Two simple recipes are now proposed to solve the problem of sensitivity to perturbations in the present framework. Consider first the following right preconditioner:

$$\boldsymbol{D}_R = \begin{bmatrix} \boldsymbol{I} & \boldsymbol{0} \\ \boldsymbol{0} & \dfrac{1}{\beta\, h^2}\, \boldsymbol{I} \end{bmatrix}, \tag{22}$$

together with a trivial left preconditioner, i.e. $\boldsymbol{D}_L = \boldsymbol{I}$. As a result, we get

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

yielding perfect time-step-size independence of perturbations in both the differential and algebraic variables:

$$\left| \lim_{h\to 0} \Delta \bar{\boldsymbol{u}}_{n+1} \right| \leq O(h^0), \tag{24a}$$

$$\left| \lim_{h\to 0} \Delta \bar{\boldsymbol{\lambda}}_{n+1} \right| \leq O(h^0). \tag{24b}$$

Considering now the right scaling (22) together with the following left scaling

$$\boldsymbol{D}_L = \begin{bmatrix} \beta\, h^2 \boldsymbol{I} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{I} \end{bmatrix}, \tag{25}$$

we achieve also time-step-size independence for the condition number

$$\lim_{h\to 0} C = O(h^0). \tag{26}$$

Bottasso et al. (2006) report the optimal scalings for all other possible forms of Newmark's scheme. From the analysis of those results, 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 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 Bottasso, Bauchau (2005a, 2006).

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.

6 NUMERICAL EXAMPLES

In order to illustrate the predictions of the above analysis, we consider Andrews' squeezing mechanism, a planar holonomic multibody system depicted in Figure 1, 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 Schielen (1990). 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 $h = \{1\cdot10^{-3}, 1\cdot10^{-4}, 1\cdot10^{-5}, 1\cdot10^{-6}, 1\cdot10^{-7}\}$, for a duration of the simulation of 0.02 seconds. The problem was 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.

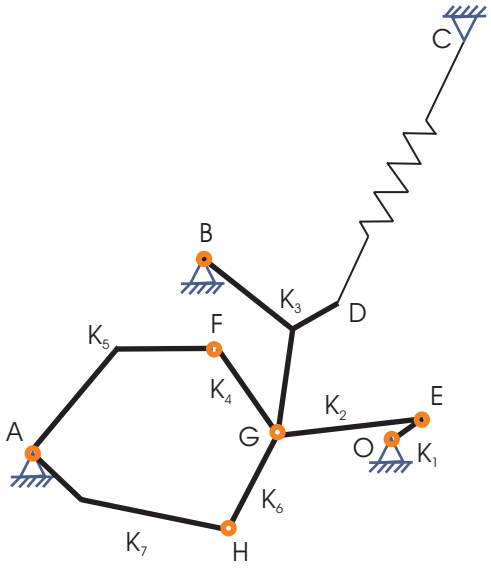

Figure 1: Andrews' squeezing mechanism.

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

$$\boldsymbol{J}^j \boldsymbol{q}^j = -\boldsymbol{b}^j. \tag{27}$$

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

$$\lim_{h\to 0} \boldsymbol{q}(h, \varepsilon) \neq 0. \tag{28}$$

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

$$\|\boldsymbol{q}^{j+1}\| \geq \|\boldsymbol{q}^j\| \tag{29}$$

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.

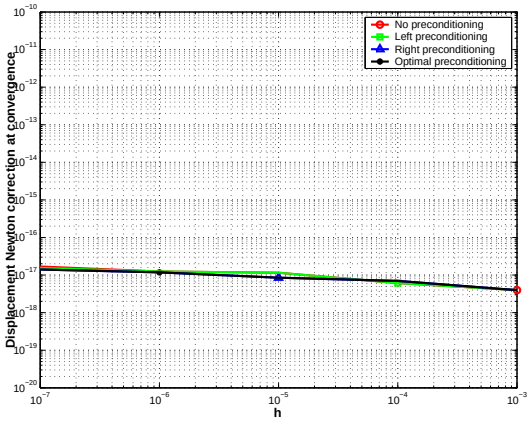

Figure 2: Last decreasing Newton correction norms of the coordinates vs. the time step size with the $(\boldsymbol{u}, \boldsymbol{\lambda})$ approach.

Figures 2, 3 and 4 show, respectively, the coordinate correction norm, the Lagrange multipliers correction norm, and the condition number as functions of the time step. The results exactly agree with the ones predicted by the analysis.

7 CONCLUDING REMARKS

In this work we have presented an 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.

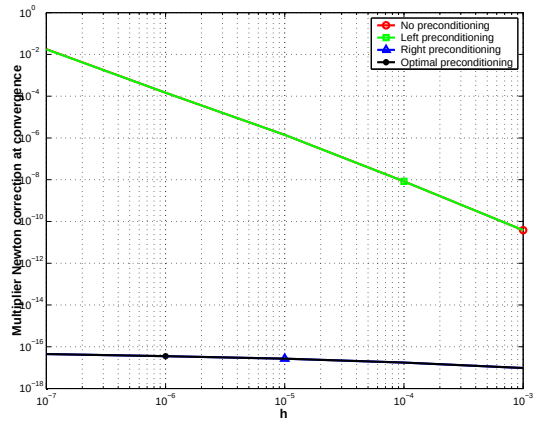

Figure 3: Last decreasing Newton correction norms of the Lagrange multiplier vs. the time step size with the $(\boldsymbol{u}, \boldsymbol{\lambda})$ approach.

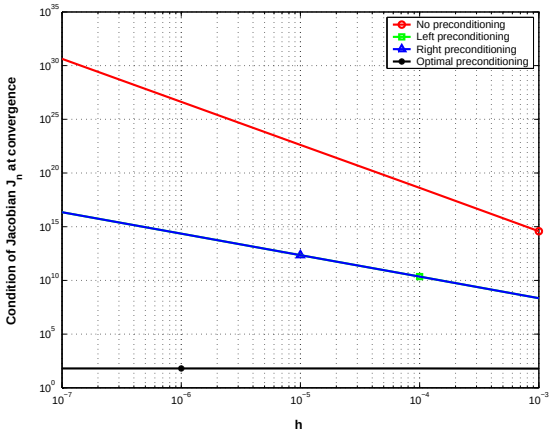

Figure 4: Condition number for the Jacobian matrix at convergence vs. the time step size with the $(\boldsymbol{u}, \boldsymbol{\lambda})$ approach.

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. 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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