Politecnico di Milano

OPTIMAL SCALING OF HIGH INDEX DAEs

Carlo L. Bottasso, Lorenzo Trainelli
Politecnico di Milano, Italy

Daniel Dopico
University of La Coruña, Spain

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Outline

- Introduction and background
- Conditioning and sensitivity to perturbations of index-3 DAEs
- Optimal preconditioning by scaling
- Conclusions:

  Index-3 DAEs can be made as easy to integrate as well behaved ODEs!

Motivation

Errors and perturbations due to finite precision arithmetics **pollute** the numerical solution of high index DAEs, such as those arising from multibody dynamics in nonminimal co-ordinates.

This causes disastrous effects on both state variables and Lagrange multipliers for **small values** of the time step size.

We study this phenomenon by means of a novel **asymptotic perturbation analysis** by considering Newmark's method as a representative example within the time integrators adopted in multibody dynamics.

Index-3 Multibody DAEs

Constrained mechanical (multibody) systems in index-3 form:

$$\begin{aligned} \boldsymbol{M}\,\boldsymbol{v}' &= \boldsymbol{f}(\boldsymbol{u},\boldsymbol{v},t) + \boldsymbol{G}(\boldsymbol{u},t)\,\boldsymbol{\lambda}, \\ \boldsymbol{u}' &= \boldsymbol{v}, \\ 0 &= \boldsymbol{\Phi}(\boldsymbol{u},t), \end{aligned}$$

where

- Displacements: $\boldsymbol{u}$
- Velocities: $\boldsymbol{v}$
- Lagrange multipliers: $\boldsymbol{\lambda}$
- Forces: $\boldsymbol{f}$
- Inertia: $\boldsymbol{M}$
- Constraint function: $\boldsymbol{\Phi}$
- Constraint gradient: $\boldsymbol{G} := \boldsymbol{\Phi}_{,\boldsymbol{u}}^{T}$

Newmark's Method

Newmark's method (Newmark, 1959) in three-field $(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{\lambda})$ form:

$$\frac{1}{\gamma\, h}\, \boldsymbol{M}\, (\boldsymbol{v}_{n+1} - \boldsymbol{v}_n) = \boldsymbol{f}_{n+1} + \boldsymbol{G}_{n+1} \boldsymbol{\lambda}_{n+1} - \left(1 - \frac{1}{\gamma}\right) \boldsymbol{M}\, \boldsymbol{a}_n,$$

$$\boldsymbol{u}_{n+1} - \boldsymbol{u}_n = h \left(\frac{\beta}{\gamma}\, \boldsymbol{v}_{n+1} + \left(1 - \frac{\beta}{\gamma}\, \boldsymbol{v}_n\right)\right) - \frac{h^2}{2} \left(1 - \frac{2\,\beta}{\gamma}\right) \boldsymbol{a}_n,$$

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

Accuracy and stability properties determined by the choice of the scheme parameters β and γ.

Refinements and extensions of this basic scheme originate widely diffuse methods: **HHT** (Hilber, Hughes and Taylor, 1977), **generalized-α** (Chung and Hulbert, 1995), etc.

Linearization

Solving with **Newton's method** at each time step:

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

where the iteration matrix is

$$\boldsymbol{J} = \begin{array}{c} \left[\begin{array}{ccc} \boldsymbol{X} & \dfrac{1}{\gamma\,h}\boldsymbol{U} & -\boldsymbol{G} \\ \boldsymbol{I} & -\dfrac{\beta\,h}{\gamma}\boldsymbol{I} & \boldsymbol{0} \\ \boldsymbol{G}^T & \boldsymbol{0} & \boldsymbol{0} \end{array}\right] \\ \begin{array}{ccc} \text{Displacements} & \text{Velocities} & \text{Multipliers} \end{array} \end{array} \begin{array}{l} \}\ \text{Equilibrium eqs.} \\ \}\ \text{Kinematic eqs.} \\ \}\ \text{Constraint eqs.} \end{array} \quad \begin{array}{l} \boldsymbol{X} := -\left(\boldsymbol{f}_{,\boldsymbol{u}}\right)_{n+1} - \left(\left(\boldsymbol{G}\,\boldsymbol{\lambda}\right)_{,\boldsymbol{u}}\right)_{n+1}, \\ \boldsymbol{Y} := -\left(\boldsymbol{f}_{,\boldsymbol{v}}\right)_{n+1}, \\ \boldsymbol{U} := \boldsymbol{M} + \gamma\,h\,\boldsymbol{Y}. \end{array}$$

and the right hand side is

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

Perturbation Analysis

In the linearized problem $\boldsymbol{J}\,\boldsymbol{q} = -\boldsymbol{b}$, all terms depend on the time step size h. Additionally, they are affected by **finite precision**.

We model the effects of finite precision arithmetics by means of the small parameter ε , with $\varepsilon = 0$ corresponding to the ideal exact (infinite precision) arithmetics.

By Taylor series about $\varepsilon = 0$ we get:

$$\lim_{h\to 0} \boldsymbol{b}(h,0) = 0$$

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

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

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

$$\lim_{h\to 0} \boldsymbol{q}(h,0) = 0$$

Perturbation Analysis

Inserting the previous expressions into $\boldsymbol{J}\,\boldsymbol{q} = -\boldsymbol{b}$ and neglecting higher order terms, at convergence we get:

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

so that, taking norms,

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

The previous result clearly states that, if $\boldsymbol{J}^{-1}$ and/or $\boldsymbol{b}$ depend on negative powers of h, **accuracy will be very poor for small time steps.**

As a consequence, the order of convergence of the integration scheme will be degraded.

Application to Newmark

Apply perturbation analysis to three-field form:

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

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

$$\lim_{h\to 0} \boldsymbol{b} = \begin{Bmatrix} O(h^{-1}) \\ O(h^0) \\ O(h^0) \end{Bmatrix}.$$

Accuracy of the solution:

$$\boxed{\left|\lim_{h\to 0} \Delta \boldsymbol{u}_{n+1}\right| \leq O(h^0), \quad \left|\lim_{h\to 0} \Delta \boldsymbol{v}_{n+1}\right| \leq O(h^{-1}), \quad \left|\lim_{h\to 0} \Delta \boldsymbol{\lambda}_{n+1}\right| \leq O(h^{-2}).}$$

Remark: severe <u>loss of accuracy</u> (ill conditioning) for small h!

Application to Newmark

Application of the perturbation analysis to **other** possible forms of Newmark's method (four-field, two-field) yields similar results:

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

(The asterisk marks a recovered field.)

Remark: this analysis is easily extended to <u>other</u> integration methods, for example BDF-type integrators (Bottasso et al., 2006). Again, similar results are observed.

Index-3 Multibody DAEs

Solutions proposed in the literature:

- **Reduction of the index**
  - ✓ Only velocity level constraints

  but drift and need for stabilization
  - ✓ GGL "stabilized index-2" (Gear et al. 1985)
  - ✓ Embedded Projection Method (Borri and Trainelli, 2000)

  but increased cost and complexity

- **Scaling**

  simple and straightforward to implement

  (related work: Petzold and Lötstedt, 1986; Cardona and Geradin, 1994; Negrut, 2005).

Left and Right Preconditioning

Based on the fundamental result derived above,

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

appropriate preconditiong by **scaling equations** and **unknowns** of Newton's problem can modify the dependencies of $\boldsymbol{J}^{-1}$ and $\boldsymbol{b}$:

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

with

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

where

$\boldsymbol{D}_L$ = left preconditioner, scales the equations;

$\boldsymbol{D}_R$ = right preconditioner, scales the unknowns.

Remark: scale back unknowns once at convergence of Newton's iterations for the current time step.

Optimal Newmark Preconditioning

Left scaling:

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

Scale equilibrium eqs. by h^2

Right scaling:

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

Scale velocities by h

Scale Lagrange multipliers by h^2

Accuracy of the solution:

$$\left| \lim_{h \to 0} \Delta \bar{\boldsymbol{u}}_{n+1} \right| \leq O(h^0), \quad \left| \lim_{h \to 0} \Delta \bar{\boldsymbol{v}}_{n+1} \right| \leq O(h^0), \quad \left| \lim_{h \to 0} \Delta \bar{\boldsymbol{\lambda}}_{n+1} \right| \leq O(h^0).$$

Remark: <u>accuracy</u> (conditioning) independent of time step size, as for well behaved ODEs. Similar results for <u>all other forms</u> of the scheme.

Optimal Preconditioning

A general rule?

As seen, velocities are scaled by h , while Lagrange multipliers by h^2 and displacements are left unchanged.

Right preconditioning restores **the same 'order'** in the time variable for all fields: roughly speaking, Lagrange multipliers are 'twice integrated' and velocities 'singly integrated' to match the dimensions of displacements.

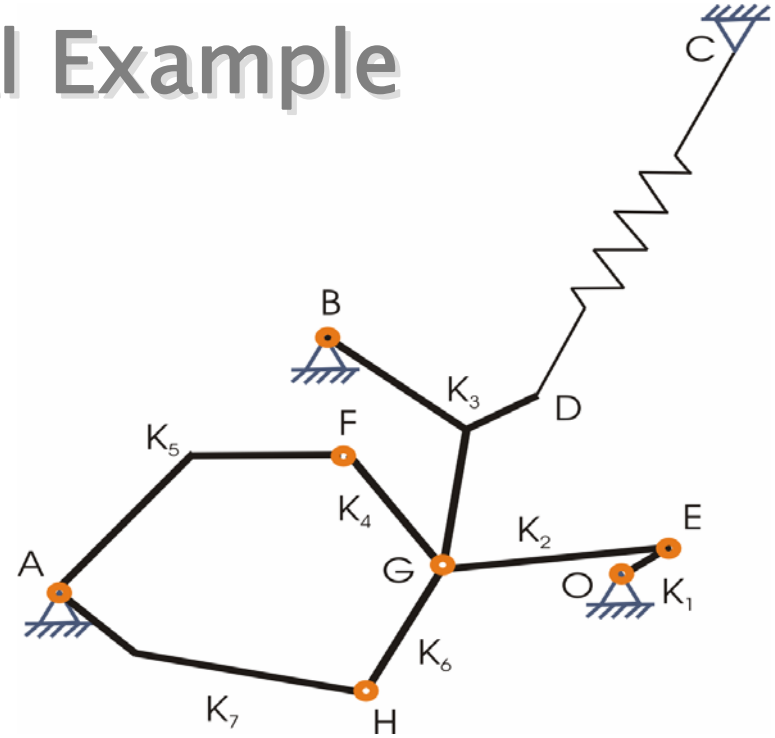
Left preconditioning clearly depends on how discretized equations are written. Again, the recipe calls to **match** the time 'dimension' of the equations.

Same results are found in the case of BDF-type integrators (Bottasso et al., 2006).

Numerical Example

Andrews' squeezing mechanism

(with 2-D Cartesian coordinates)



At each Newton iteration, solve

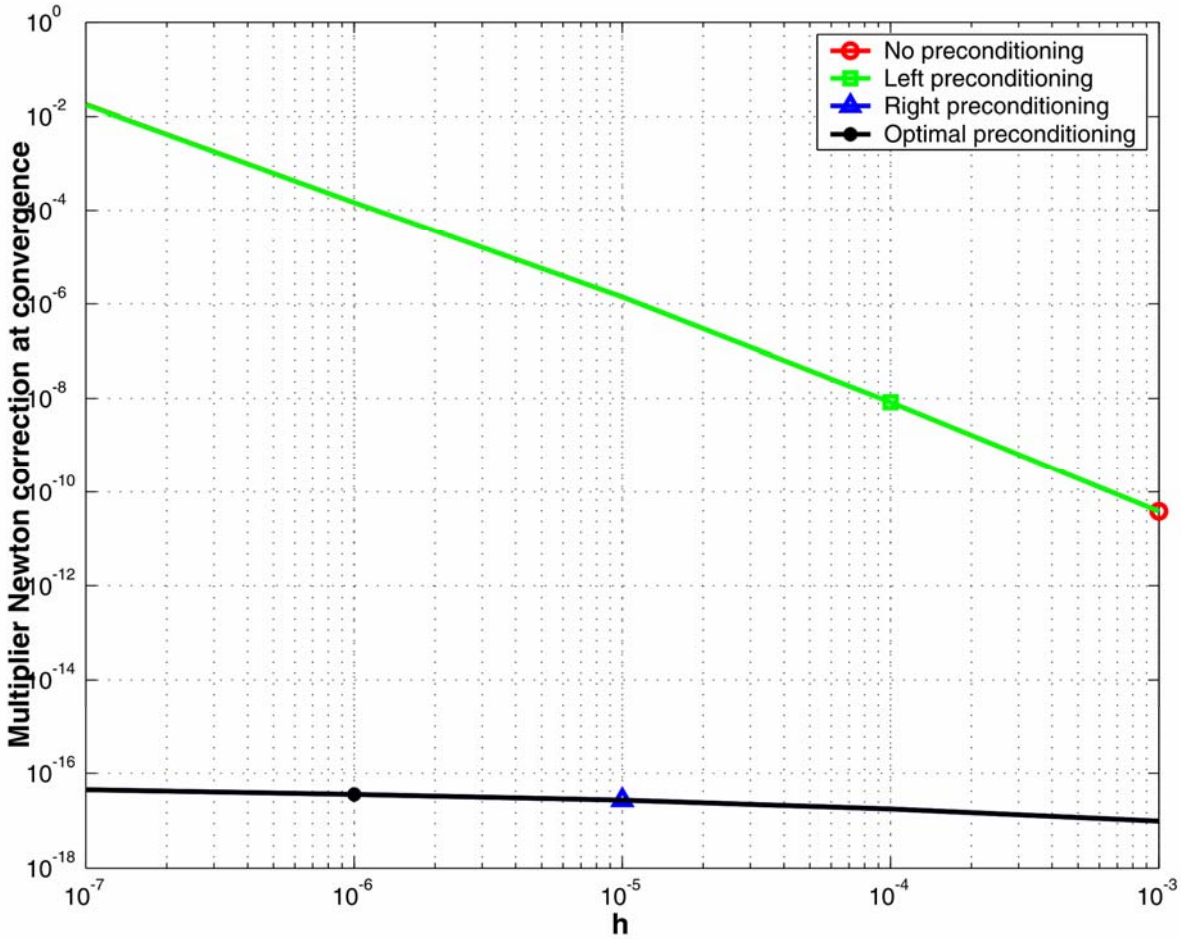
$$\boldsymbol{J}^j \boldsymbol{q}^j = -\boldsymbol{b}^j$$

Stop at **first non-decreasing** Newton correction, i.e.:

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

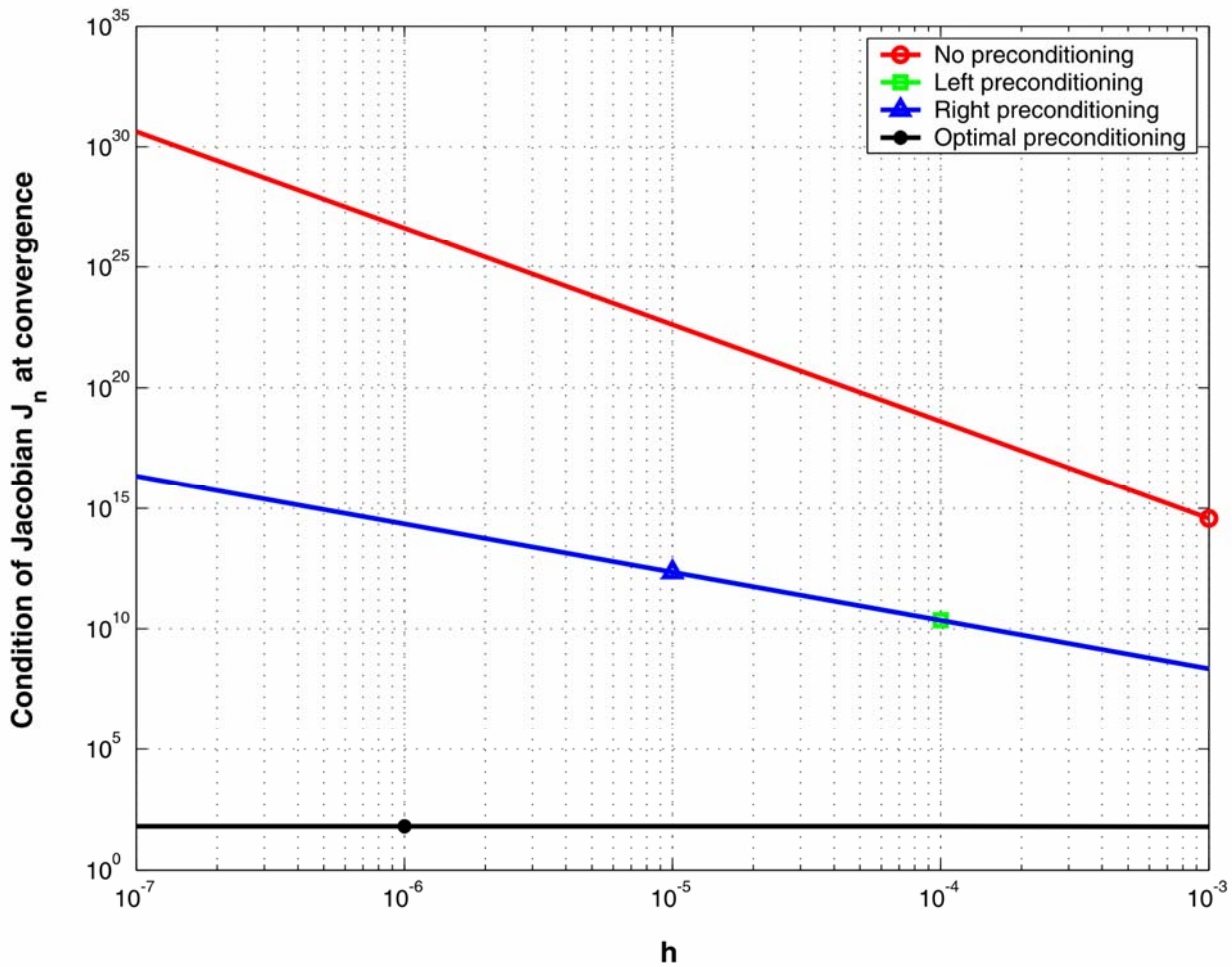
This is a measure of the **tightest achievable convergence** of Netwon's method (in fact, corrections reach <u>saturation</u> due to finite precision.)

Numerical Example



Convergence order for the Lagrange multipliers

Numerical Example



Convergence order for the condition number $C := \|\boldsymbol{J}\|_\infty \|\boldsymbol{J}^{-1}\|_\infty$

Conclusions

Index-3 DAEs can be made **as easy to solve** numerically as well behaved ODEs!

- **Recipe** for Newmark's method:
  - Use any form of the algorithm (two-field forms are more computationally convenient)
  - Use left and right scaling of primary unknowns
  - Recover scaled quantities at convergence
- **Trivial** to implement in existing codes
- The methodology **extends** to other integrators (HHT, BDF, etc.)