A perturbation analysis for the dynamical simulation of mechanical multibody systems, Twenty years later

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Abstract
The equations of motion of constrained mechanical systems form a class of differential-algebraic equations (DAEs)

$$\mathbf{M}(\mathbf{q})\ddot{\mathbf{q}} = \mathbf{f}(\mathbf{q},\dot{\mathbf{q}},\boldsymbol{\lambda}) - \mathbf{G}^{\top}(\mathbf{q})\,\boldsymbol{\lambda}\,, \tag{1a}$$

$$\mathbf{0} = \mathbf{g}(\mathbf{q}) \tag{1b}$$

that has found much interest in applied and numerical mathematics. In multibody dynamics, the variables $\mathbf{q}(t) \in \mathbb{R}^k$ describe the position and orientation of all bodies. The dynamical equations (1a) are characterized by the mass matrix $\mathbf{M}(\mathbf{q})$, the force vector $\mathbf{f}(\mathbf{q},\dot{\mathbf{q}},\boldsymbol{\lambda})$ and the constraint forces $-\mathbf{G}^{\top}(\mathbf{q})\,\boldsymbol{\lambda}$ with Lagrange multipliers $\boldsymbol{\lambda}(t) \in \mathbb{R}^m$ that couple $m \le k$ holonomic constraints $\mathbf{g}(\mathbf{q}) = \mathbf{0}$ to the equilibrium conditions for forces and momenta, $\mathbf{G}(\mathbf{q}) := (\partial \mathbf{g}/\partial \mathbf{q})(\mathbf{q})$.
In 1989, Hairer, Lubich and Roche [1] introduced the perturbation index to classify DAEs w.r.t. “the sensitivity of the solutions to perturbations in the equation” and proved that (1) has perturbation index 3 if $\mathbf{M}(\mathbf{q}) \in \mathbb{R}^{k\times k}$ is symmetric, positive definite and $\mathbf{G}(\mathbf{q}) \in \mathbb{R}^{k\times m}$ has full rank. In 1995, we refined this analysis and developed *A perturbation analysis for the dynamical simulation of mechanical multibody systems* [2] that considers functions $\hat{\mathbf{q}}(t)$, $\hat{\boldsymbol{\lambda}}(t)$ satisfying (1) up to some (small) residuals $\boldsymbol{\delta}(t)$, $\boldsymbol{\theta}(t)$:

$$\mathbf{M}(\hat{\mathbf{q}})\ddot{\hat{\mathbf{q}}} = \mathbf{f}(\hat{\mathbf{q}},\dot{\hat{\mathbf{q}}},\hat{\boldsymbol{\lambda}}) - \mathbf{G}^{\top}(\hat{\mathbf{q}})\,\hat{\boldsymbol{\lambda}} + \boldsymbol{\delta}(t)\,, \tag{2a}$$

$$\boldsymbol{\theta} = \mathbf{g}(\hat{\mathbf{q}})\,. \tag{2b}$$

Differentiating the algebraic equations (1b) and (2b) twice, we get systems of linear equations in $\ddot{\mathbf{q}}$, $\boldsymbol{\lambda}$, $\ddot{\hat{\mathbf{q}}}$ and $\hat{\boldsymbol{\lambda}}$ that may be solved to get a bound for $\hat{\boldsymbol{\lambda}}(t) - \boldsymbol{\lambda}(t)$ in terms of $\hat{\mathbf{q}}(t) - \mathbf{q}(t)$, $\dot{\hat{\mathbf{q}}}(t) - \dot{\mathbf{q}}(t)$, $\boldsymbol{\delta}(t)$ and $\ddot{\boldsymbol{\theta}}(t)$. The critical case are high frequency perturbations $\boldsymbol{\theta}(t) = \varepsilon \sin \omega t$ with small amplitude $\varepsilon \ll 1$ that may result in very large errors $\hat{\boldsymbol{\lambda}}(t) - \boldsymbol{\lambda}(t)$ of size $\mathscr{O}(1)\|\ddot{\boldsymbol{\theta}}(t)\| = \mathscr{O}(\varepsilon\omega^2)$.
For the direct time discretization of (1) by Runge-Kutta methods, multi-step methods and methods of Newmark type, we observe a similar amplification of small constraint residuals also in the numerical solution. For a method with time step size h and (small) constraint residuals $\boldsymbol{\theta}_n = \mathbf{g}(\mathbf{q}_n)$, we get $\|\hat{\boldsymbol{\lambda}}_n - \boldsymbol{\lambda}_n\| = \ldots + \mathscr{O}(\theta/h^2)$ with $\theta := \max_l \|\boldsymbol{\theta}_l\|$, i.e., an amplification of constraint residuals by a factor of $1/h^2$. The corresponding error bounds for the solution components $\mathbf{q}_n$ and $\dot{\mathbf{q}}_n$ are much smaller and depend on the structure of the force vector $\mathbf{f}$ in (1a). For systems with $\mathbf{f} = \mathbf{f}(\mathbf{q},\dot{\mathbf{q}})$, we get, e.g., error bounds of size $\mathscr{O}(\theta) + \mathscr{O}\big((\theta/h)^2\big)$ for the position coordinates $\mathbf{q}_n$ and of size $\mathscr{O}(\theta/h)$ for the velocity coordinates $\dot{\mathbf{q}}_n$, see [2, Theorem 7].
An interesting detail of this consistent perturbation analysis for analytical and numerical solution is its invariance w.r.t. algorithmic details like, e.g., scaling strategies for the corrector iteration in implicit time integration methods [3]. More precisely, we will show that the error bounds are optimal w.r.t. the physically relevant variables $\mathbf{q}(t)$, $\dot{\mathbf{q}}(t)$ and $\boldsymbol{\lambda}(t)$ in (1). Furthermore, the perturbation analysis will be extended to equations of motion with a more complex structure including systems with non-holonomic constraints, systems with rank-deficient but positive semi-definite mass matrix $\mathbf{M}(\mathbf{q})$ being positive definite on ker $\mathbf{G}(\mathbf{q})$ and systems having a nonlinear configuration space with Lie group structure.
From the practical viewpoint, the error terms of size $\mathscr{O}(\theta/h^2)$ in $\boldsymbol{\lambda}_n$ may be ignored if the main interest is in the solution trajectory $\mathbf{q}(t)$ at the level of position coordinates and the time step size $h > 0$ is not too small. On the other hand, Lagrange multipliers $\boldsymbol{\lambda}$ and constraint forces $-\mathbf{G}^{\top}(\mathbf{q})\,\boldsymbol{\lambda}$ may be important output quantities to be used, e.g., as inputs for a durability analysis. In that case, more robust numerical schemes have to be used that are based on analytical transformations of the equations of motion (1) before time discretization (*index reduction* [1]).

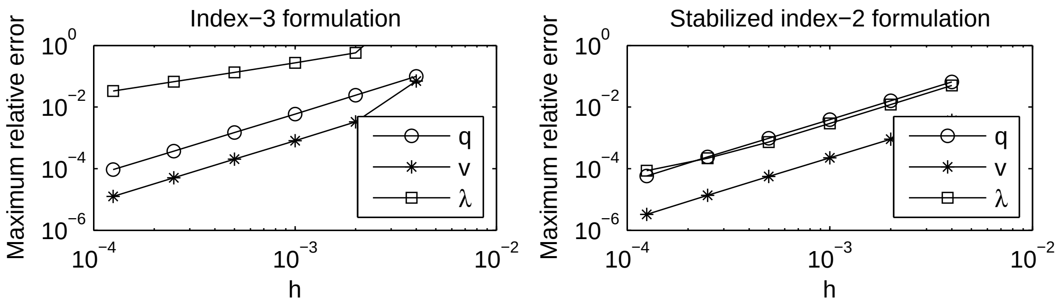

Figure 1: Global error of a generalized-α DAE Lie group integrator, Heavy top benchmark. Left plot: index-3 formulation, right plot: stabilized index-2 formulation.

Advanced general purpose solvers in industrial multibody system simulation packages make use of the hidden constraints at the level of velocity coordinates $\mathbf{v}(t) := \dot{\mathbf{q}}(t)$. These hidden constraints result from differentiation of $\mathbf{0} = \mathbf{g}\big(\mathbf{q}(t)\big)$ w.r.t. t: $\mathbf{0} = (\mathrm{d}/\mathrm{d}t)\mathbf{g}\big(\mathbf{q}(t)\big) = (\partial \mathbf{g}/\partial \mathbf{q})\big(\mathbf{q}(t)\big)\,\dot{\mathbf{q}}(t) = \mathbf{G}\big(\mathbf{q}(t)\big)\mathbf{v}(t)$. The *stabilized index-2 formulation* (also known as *Gear-Gupta-Leimkuhler formulation*) of the equations of motion [1] considers the hidden constraints as well as the original holonomic constraints (1b) and introduces a new vector $\boldsymbol{\eta}(t) \in \mathbb{R}^m$ of auxiliary variables in the kinematic equations $\dot{\mathbf{q}} = \mathbf{v}$:

$$\mathbf{A}(\mathbf{q})(\dot{\mathbf{q}} - \mathbf{v}) = -\mathbf{G}^\top(\mathbf{q})\,\boldsymbol{\eta}\,, \tag{3a}$$

$$\mathbf{M}(\mathbf{q})\dot{\mathbf{v}} = \mathbf{f}(\mathbf{q},\dot{\mathbf{q}},\boldsymbol{\lambda}) - \mathbf{G}^\top(\mathbf{q})\,\boldsymbol{\lambda}\,, \tag{3b}$$

$$\mathbf{0} = \mathbf{G}(\mathbf{q})\mathbf{v}\,,\ \ \mathbf{0} = \mathbf{g}(\mathbf{q})\,. \tag{3c}$$

The stabilized index-2 formulation (3) is analytically equivalent to the original equations of motion if matrix $\mathbf{A}(\mathbf{q})$ in (3a) is non-singular. Formally, the auxiliary variables $\boldsymbol{\eta}$ vanish identically ($\boldsymbol{\eta}(t) \equiv \mathbf{0}$) but in a practical implementation they remain in the size of discretization errors. Similar results are obtained for the stabilized index-2 formulation of equations of motion with nonholonomic constraints [1].
The main benefit of the index reduced formulation (3) is an improved robustness w.r.t. small perturbations [2]: The error bounds for the Lagrange multipliers are of size $\mathscr{O}(1)\|\dot{\boldsymbol{\theta}}(t)\|$ for the analytical solution $\boldsymbol{\lambda}(t)$ and of size $\mathscr{O}(\theta/h)$ for the numerical solution $\boldsymbol{\lambda}_n$, i.e., they are smaller by a factor of h than the ones for the original index-3 DAE (1). The numerical test results in Fig. 1 illustrate that stabilized index-2 integrators compute often a substantially more accurate numerical solution $\boldsymbol{\lambda}_n$.
The present contribution considers the efficient implementation of time integration methods for the stabilized index-2 formulation (3). Classical index-3 integrators define the numerical solution in time step $t_n \to t_{n+1}$ by corrector equations of dimension $k+m$ in terms of the unknowns $\mathbf{q}_{n+1} \in \mathbb{R}^k$ and $\boldsymbol{\lambda}_{n+1} \in \mathbb{R}^m$, see, e.g., [3, Section 4]. For the stabilized index-2 formulation (3) with $\mathbf{A}(\mathbf{q}) \equiv \mathbf{I}_k$, the dimension of the corrector equations increases to $k+2m$ with unknowns $\mathbf{q}_{n+1}$, $\boldsymbol{\lambda}_{n+1}$ and $\boldsymbol{\eta}_{n+1}$. Alternatively, matrix $\mathbf{A}(\mathbf{q})$ could be set to $\mathbf{A}(\mathbf{q}) := \mathbf{M}(\mathbf{q})$ to get *two* systems of dimension $k+m$ that may be solved efficiently using one and the same approximation of the Jacobian in the Newton-Raphson iteration. We will generalize this approach in a consistent way to equations of motion with rank deficient mass matrix $\mathbf{M}(\mathbf{q})$.
All results are verified by practical implementations of (implicit) Runge-Kutta methods, BDF and Newmark type methods. Easy-to-use plug-ins are developed for the open source Runge-Kutta code RADAU5 and the open source BDF code DASSL to support their straightforward application to the stabilized index-2 formulation (3). The implementation of a stabilized index-2 generalized-α integrator may furthermore be applied to equations of motion in nonlinear configuration spaces with Lie group structure.

References

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