Jacobian-Free Newton-Krylov Methods for Nonlinear Implicit Analysis

Fredrik Bengzon, Thomas Borrvall, Anders Jonsson, DYNAmore Nordic AB
Gert Fredriksen, LEGO

Introduction

- For many years, the Newton iterative method in combination with optional BFGS has been the nonlinear implicit solver of choice
  - Full Newton is recommended for strongly nonlinear problems, each iteration is expensive, and performance relies to some extent on “good” tangent implementations
  - BFGS is recommended for weakly to moderately nonlinear problems, iterations are relatively cheap and works reasonably well for many problems, and poor tangents may be slightly corrected by the update, but robustness is affected when encountering unexpected nonlinearities
- There seems to be a gap in the solution portfolio, for many problems full Newton tends to be slow while BFGS tends to lack robustness
  - Is there an alternative?

GMRES – Generalized Minimal RESidual

- Assume we want to solve $\boldsymbol{Ku} = \boldsymbol{F}$ without factorizing $\boldsymbol{K}$
- The characteristic polynomial of $\boldsymbol{K}$ is
  - $p(\lambda) = \det(\lambda \boldsymbol{I} - \boldsymbol{K}) = c_0 + c_1\lambda + c_2\lambda^2 + \cdots + c_n\lambda^n$
- By Cayley-Hamilton theorem, $\boldsymbol{K}$ satisfies $p(\boldsymbol{K}) = \boldsymbol{0}$, so with a bit of rearrangement
  - $\boldsymbol{K}^{-1}\,\boldsymbol{F} = \tilde{c}_1\boldsymbol{F} + \tilde{c}_2\boldsymbol{KF} + \cdots + \tilde{c}_n\boldsymbol{K}^{n-1}\boldsymbol{F}$
- That is, the solution $\boldsymbol{u}$ that we seek is contained in the Krylov space
  - $\mathcal{V}_n(\boldsymbol{K}, \boldsymbol{F}) = \operatorname{span}\{\boldsymbol{F}, \boldsymbol{KF}, \ldots, \boldsymbol{K}^{n-1}\boldsymbol{F}\}$
- Note that this space is not necessarily $\mathcal{R}^n$
  - If $\boldsymbol{F}$ happens to be an eigenvector to $\boldsymbol{K}$ then the $\mathcal{V}_n(\boldsymbol{K}, \boldsymbol{F})$ has dimension 1, and any linear dependence among the vectors will reduce the size of this space accordingly
- The unspoken hope, and the idea behind GMRES, is that a sufficiently accurate solution can be obtained within $\mathcal{V}_m(\boldsymbol{K}, \boldsymbol{F})$ for $m \ll n$

GMRES – Generalized Minimal RESidual

- Matrix multiplications are relatively cheap, so start forming $\boldsymbol{v}_1 = \boldsymbol{F}, \boldsymbol{v}_2 = \boldsymbol{K}\boldsymbol{F}, \boldsymbol{v}_3 = \boldsymbol{K}^2\boldsymbol{F}, \ldots$
- Each new vector must be orthogonalized to the rest, so we will end up with a set of orthonormal vectors that spans the space of interest
  - $\mathcal{V}_m(\boldsymbol{K}, \boldsymbol{F}) = \mathrm{span}\{\boldsymbol{q}_1, \boldsymbol{q}_2, \ldots, \boldsymbol{q}_m\}$
- The solution we look for is the vector $\boldsymbol{v}$ in $\mathcal{V}_m(\boldsymbol{K}, \boldsymbol{F})$ that minimizes $||\boldsymbol{K}\boldsymbol{v} - \boldsymbol{F}||$, which turns out to be a solution to normal equations of dimension m
  - $\boldsymbol{Q}_{m+1}\,\boldsymbol{H}_m = \boldsymbol{K}\,\boldsymbol{Q}_m$
  - $\boldsymbol{H}_m^T \boldsymbol{H}_m \boldsymbol{y} = \boldsymbol{Q}_m^T \boldsymbol{K}^T \boldsymbol{F}$
  - $\boldsymbol{v} = \boldsymbol{Q}_m \boldsymbol{y}$
- Here $\boldsymbol{Q}_j$ is the matrix of collected $\boldsymbol{q}_i$, $i = 1, \ldots j$, and $\boldsymbol{H}_m$ is an $\{m+1\} \times m$ matrix on upper Hessenberg form
- This system is relatively cheap to solve, utilizing a QR-factorization of $\boldsymbol{H}_m^T \boldsymbol{H}_m$

Jacobian-Free GMRES

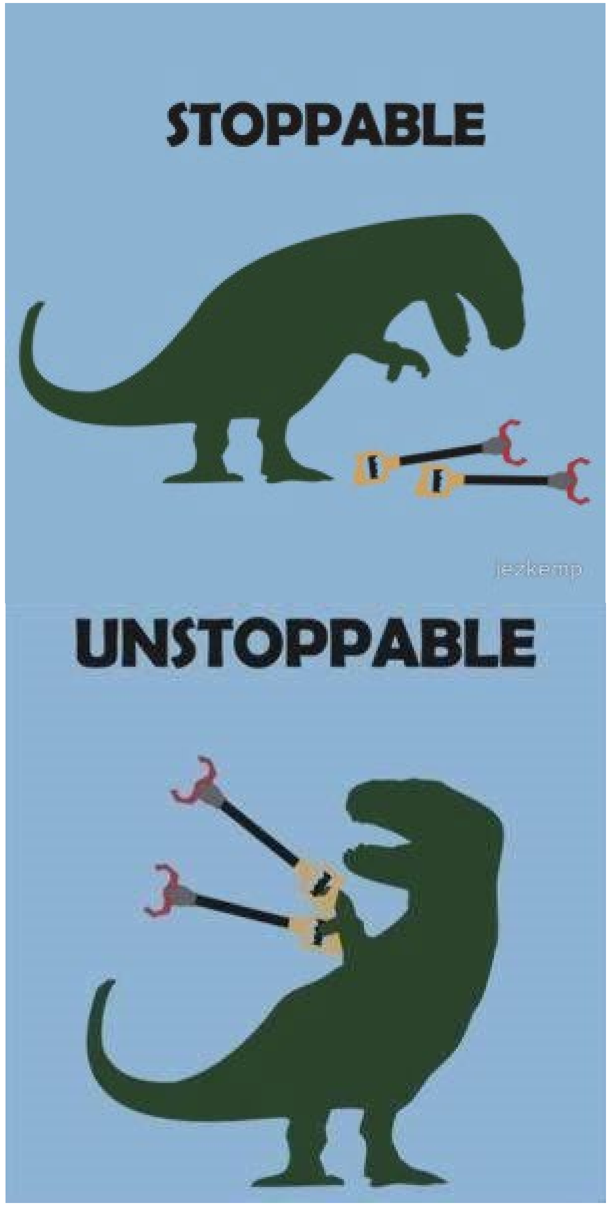
- Instead of forming the Krylov space by recursive multiplications by $\boldsymbol{K}$, we note that for any $\boldsymbol{v}$ and sufficiently small ϵ
  - $\boldsymbol{K}\boldsymbol{v} \approx \frac{\boldsymbol{F}(\boldsymbol{x}+\epsilon\boldsymbol{v})-\boldsymbol{F}(\boldsymbol{x})}{\epsilon}$
- This means that our Krylov space can be formed by recursively applying
  - $\boldsymbol{v}_{j+1} = \frac{\boldsymbol{F}(\boldsymbol{x}+\epsilon\boldsymbol{v}_j)-\boldsymbol{F}(\boldsymbol{x})}{\epsilon}$
- Everything else in the GMRES approach is unchanged, no explicit stiffness required
- To make the method reasonably efficient, we need preconditioning of the system
- Assume $\boldsymbol{P}$ is a good approximation of $\boldsymbol{K}^{-1}$, then we form the Krylov space as
  - $\boldsymbol{v}_{j+1} = \frac{\boldsymbol{F}(\boldsymbol{x}+\epsilon\boldsymbol{P}\boldsymbol{v}_j)-\boldsymbol{F}(\boldsymbol{x})}{\epsilon}$
  - $\mathcal{V}_m(\boldsymbol{K},\boldsymbol{F}) = \text{span}\{\boldsymbol{P}\boldsymbol{v}_1, \boldsymbol{P}\boldsymbol{v}_2, \dots, \boldsymbol{P}\boldsymbol{v}_m\}$
  - $\boldsymbol{v}_1 = \boldsymbol{F}$

Algorithm and Usage

- The complete JFNK algorithm becomes
  - In iteration i, solve for a full Newton step resulting in a factorization of $\boldsymbol{K}_i$
  - In iteration $j, j = i + 1, i + 2, i + 3, \dots, i + \mathrm{ILIMIT}$, obtain the step direction from a JFNK update of dimension KSSIZE using $\boldsymbol{P} = \boldsymbol{K}_i^{-1}$ as the preconditioner
  - Start over with a full stiffness reformation
- The method is activated by NSOLVR=13 on *CONTROL_IMPLICIT_SOLUTION
  - ILIMIT and MAXREF have the same meanings as for BFGS
  - KSSPACE on the same card refers to the size of the Krylov subspace

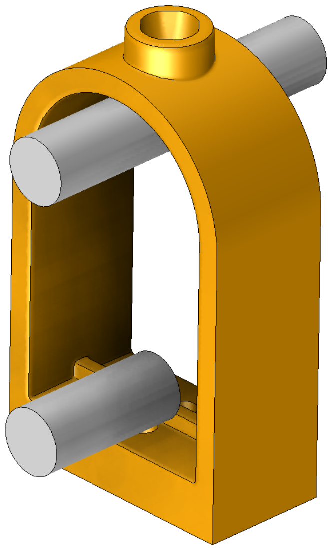
Discussion

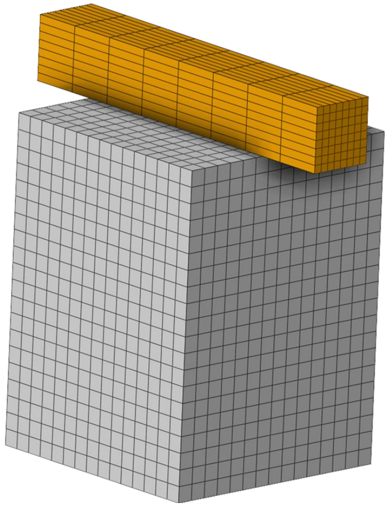
- The stiffness matrix $\boldsymbol{K}$ is the linearization of the force $\boldsymbol{F}$
  - The terrain infinitesimally close to a geometry is examined, and a search direction is based on this information
  - An exact calculation of the stiffness matrix $\boldsymbol{K}$ may be impractical because of complexity and cost
  - Severe nonlinearities may not be captured properly
- The perturbations in JFNK are of size ϵ, so the radius of influence is finite rather than miniscule
  - Contact situations, plasticity, damage and other "far-field" nonlinearities can be "sensed" and accounted for
  - Correction is "richer" compared to BFGS

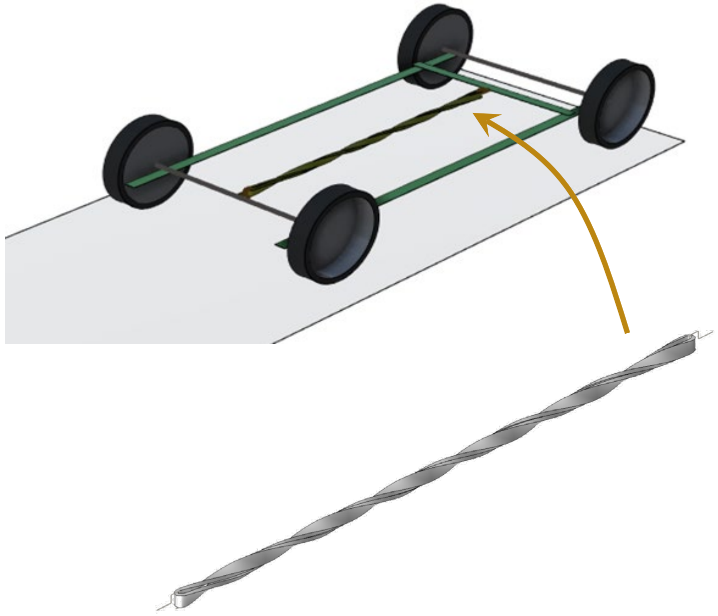


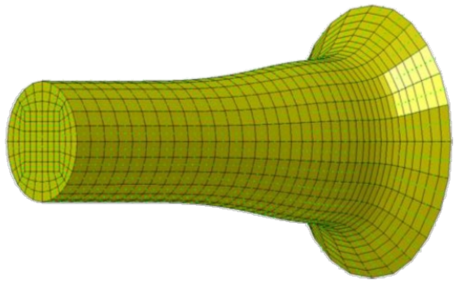
Examples

- Rigid Walls
  - Taylor bar impact
  - LEGO element
  - Prism to rubber
- Mixed element
  - Toy vehicle



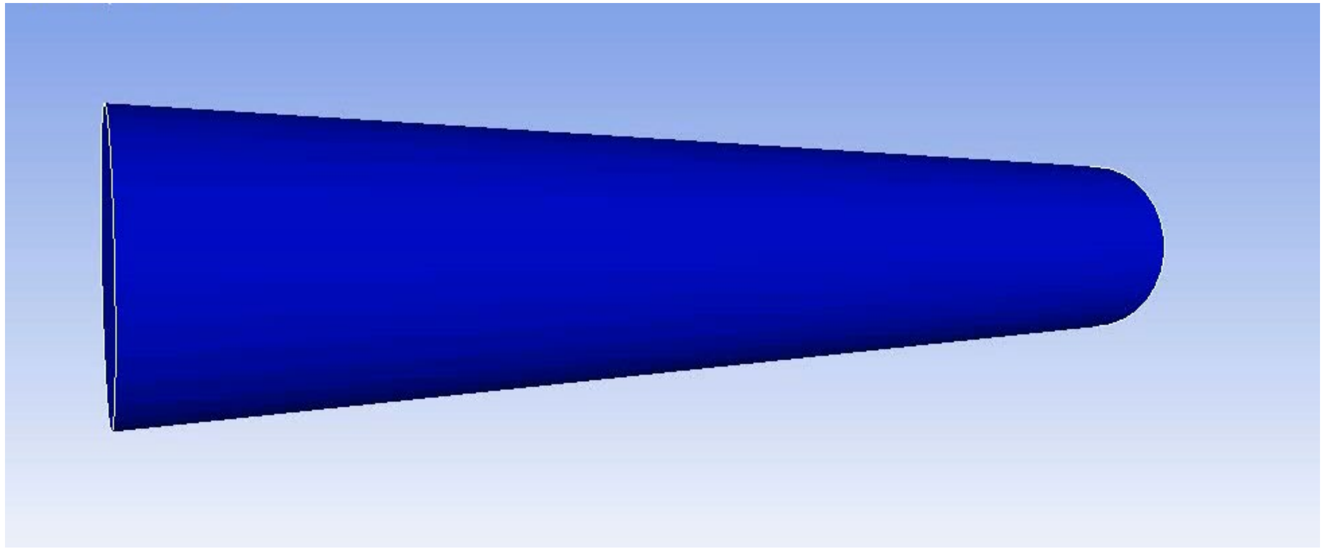


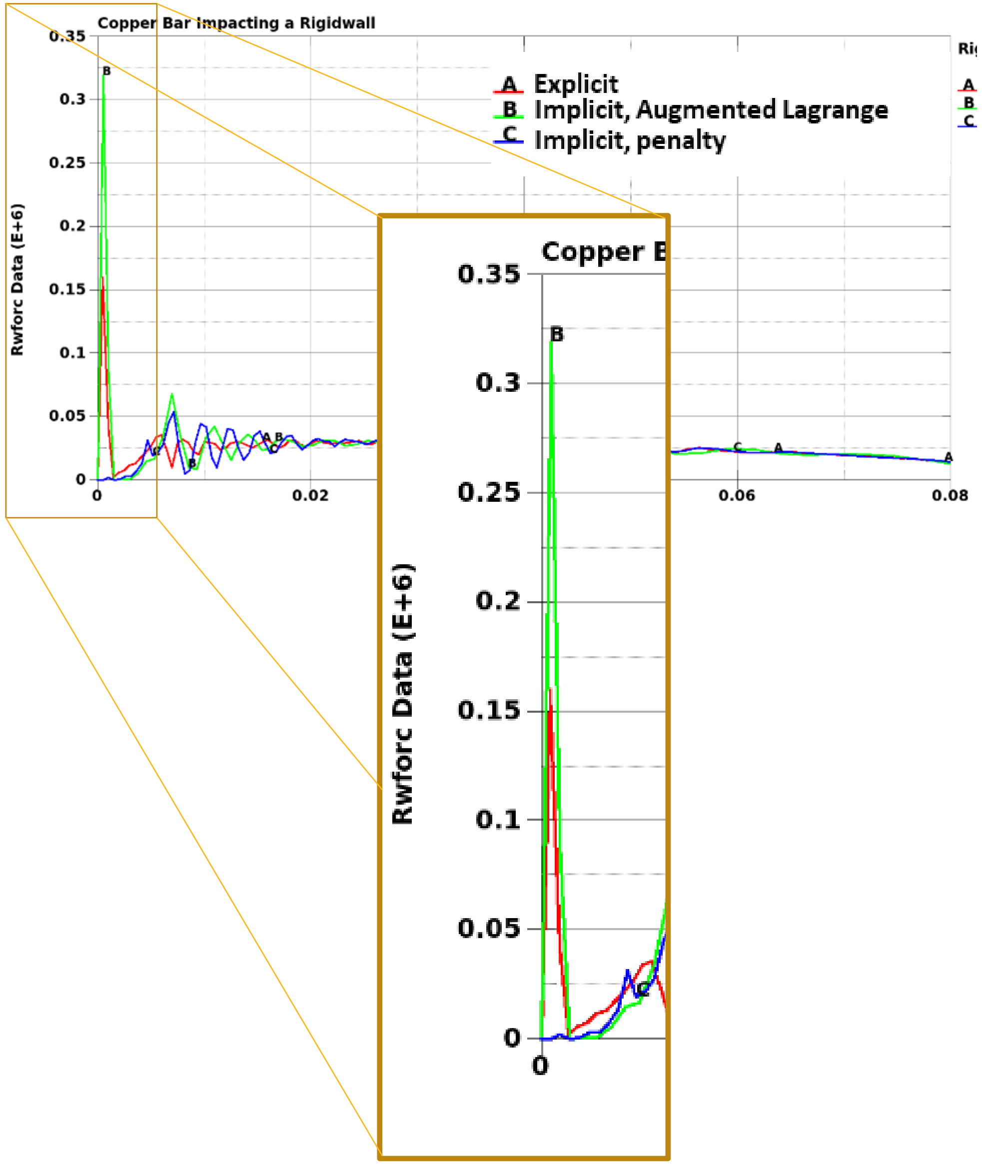




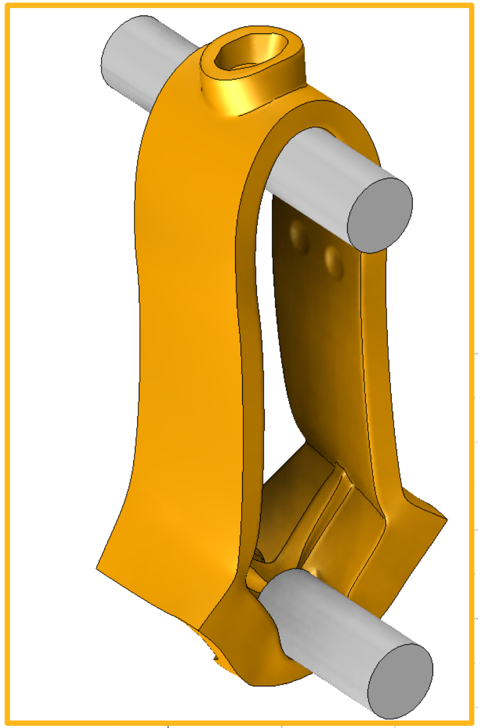
Taylor bar impact

	Symm MF2	NonSym MF2	Symm MUMPS	NonSym MUMPS
JFNK	158	162	454	266
BFGS	n/a	n/a	n/a	1277
FN	379	452	1236	1313

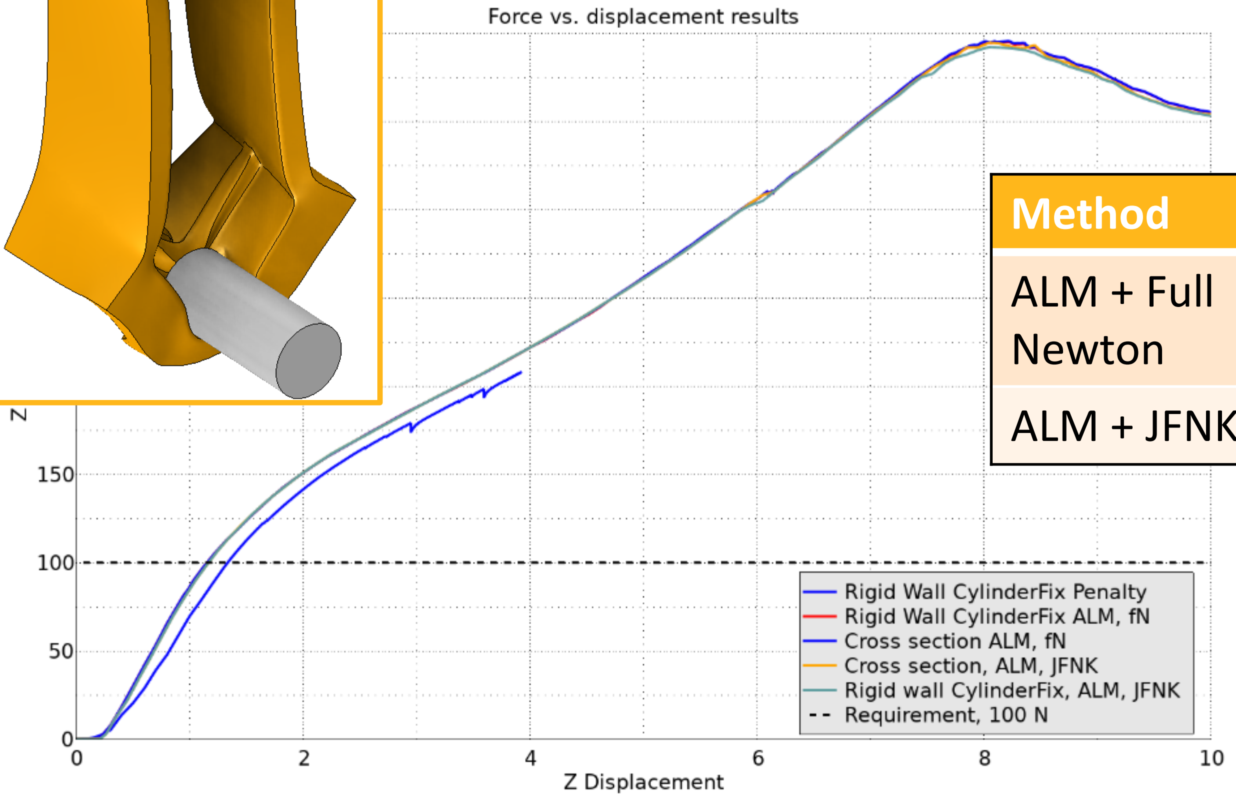




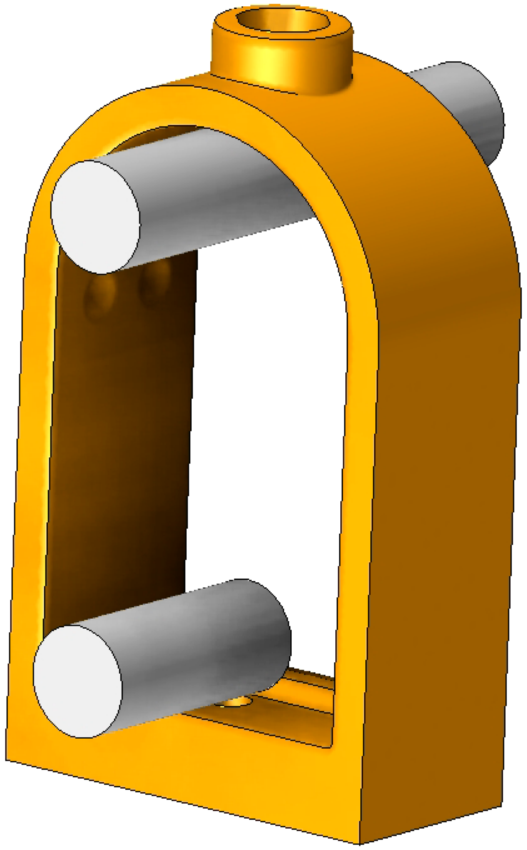
LEGO element test



- Displacement of 10 mm should require 100 N

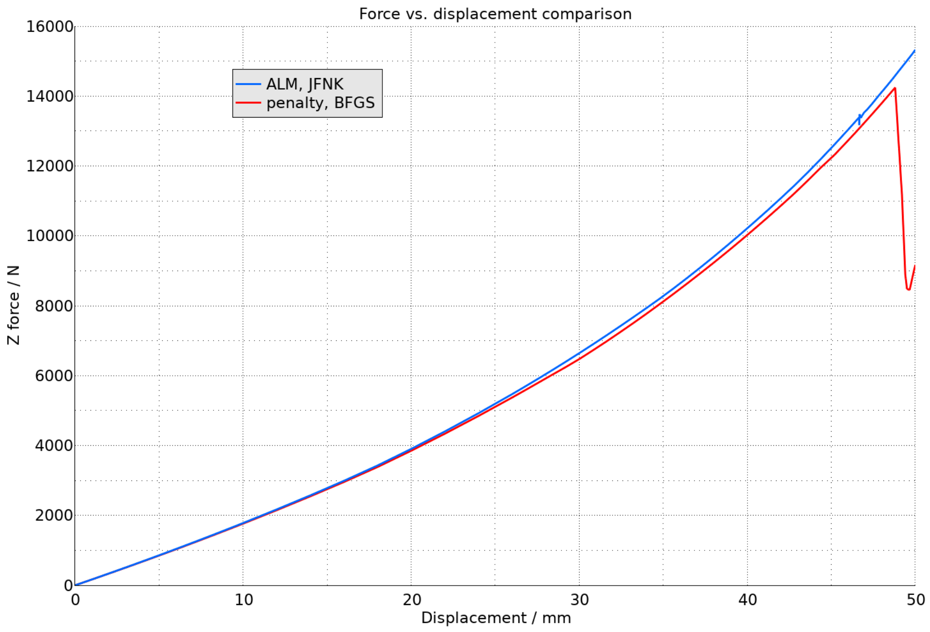


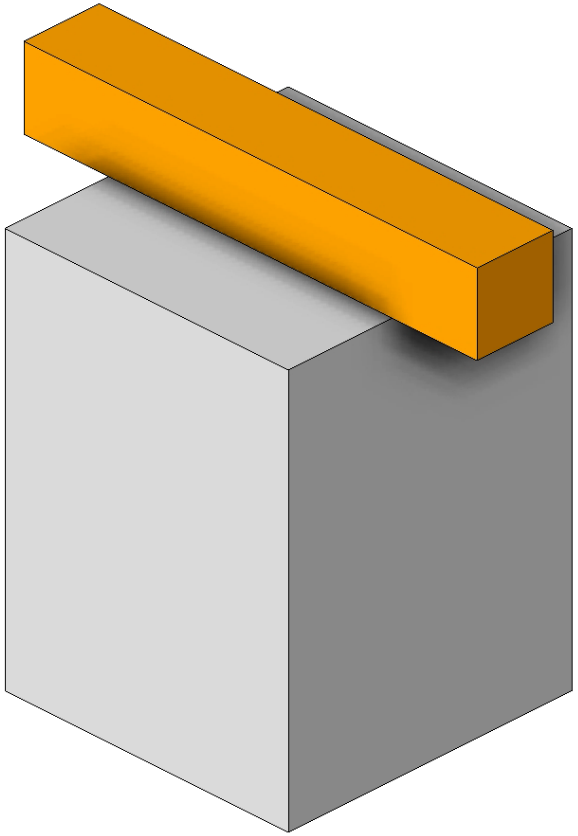
Method	Iterations
ALM + Full Newton	14338
ALM + JFNK	3446



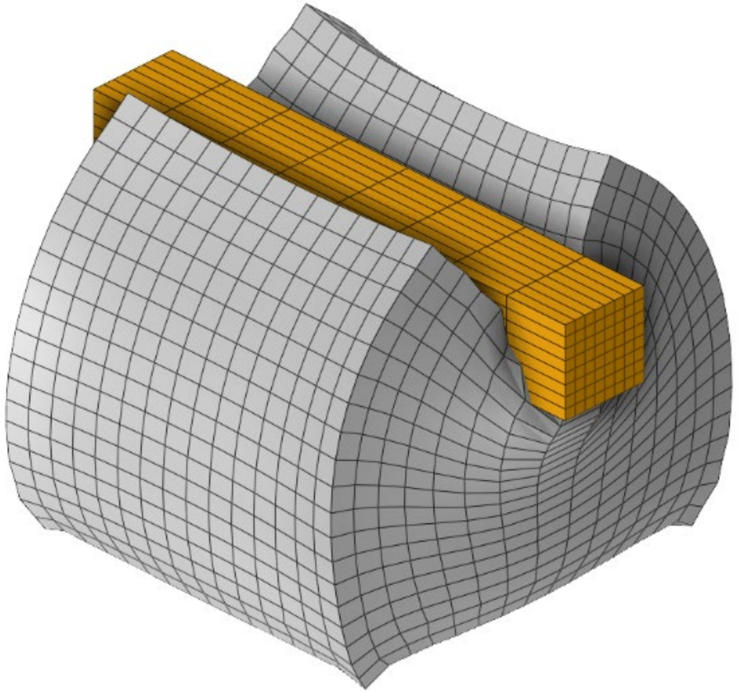
Prismatic indentation

Method	Iterations
ALM + Full Newton	2677
ALM + JFNK	439



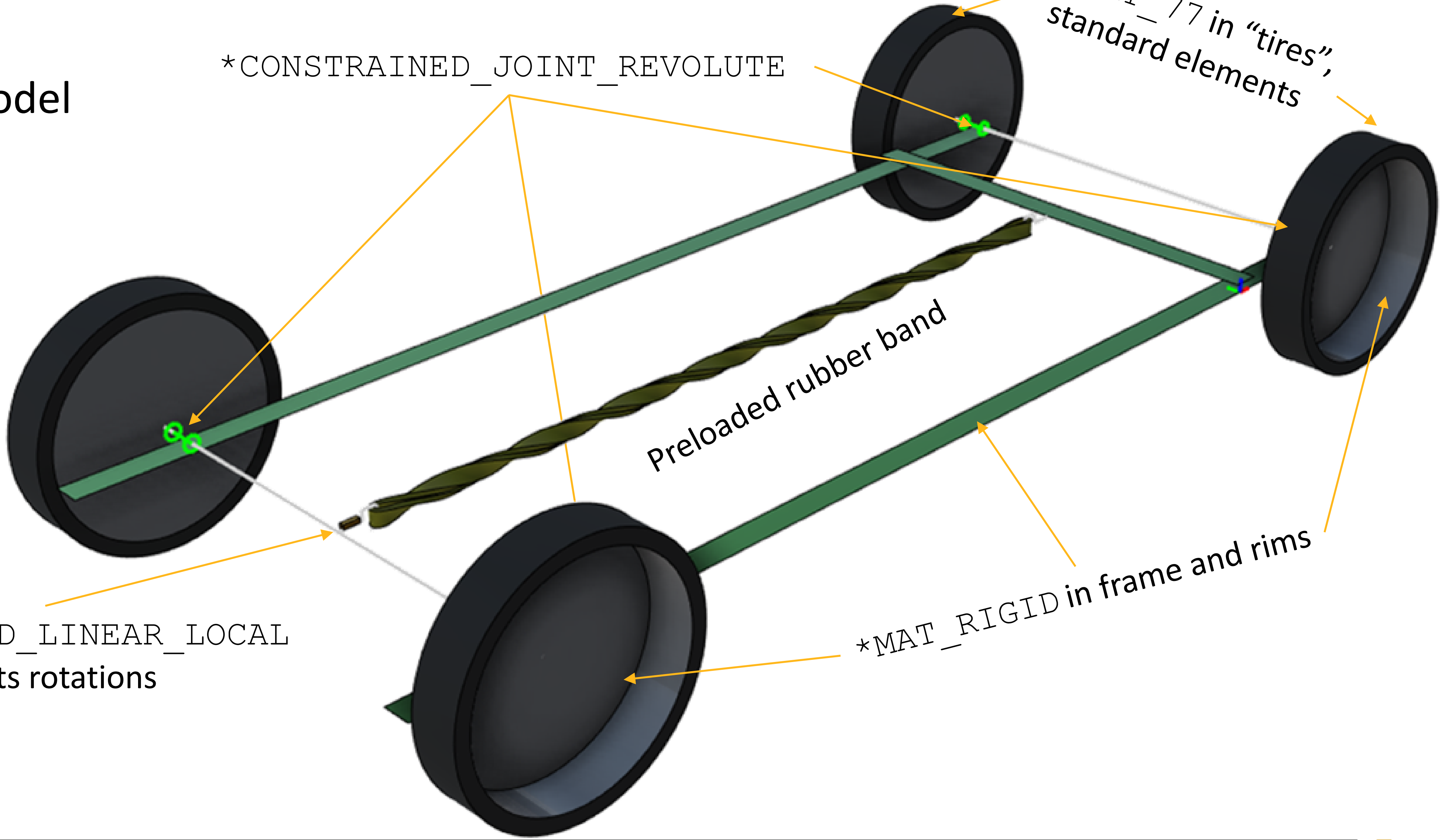


- 50 mm indentation

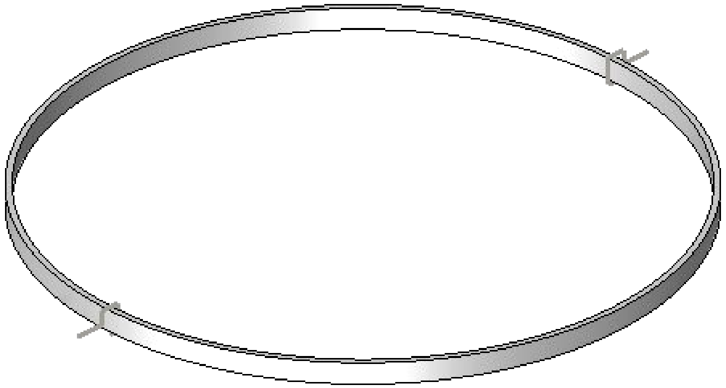


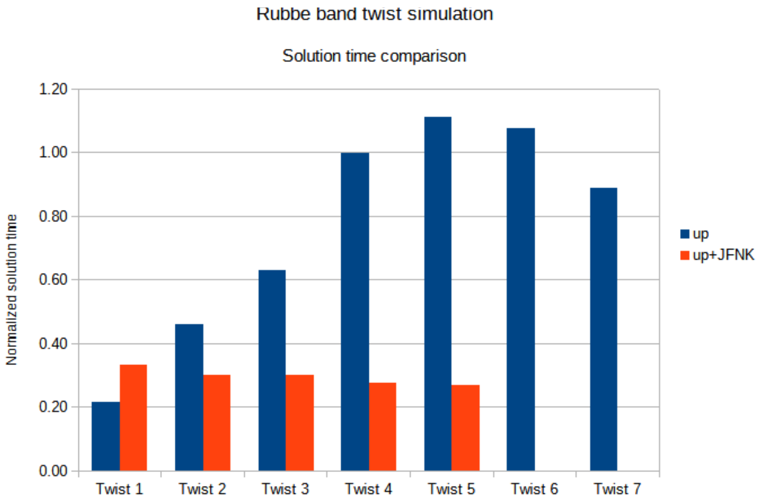
Toy vehicle

- Car model

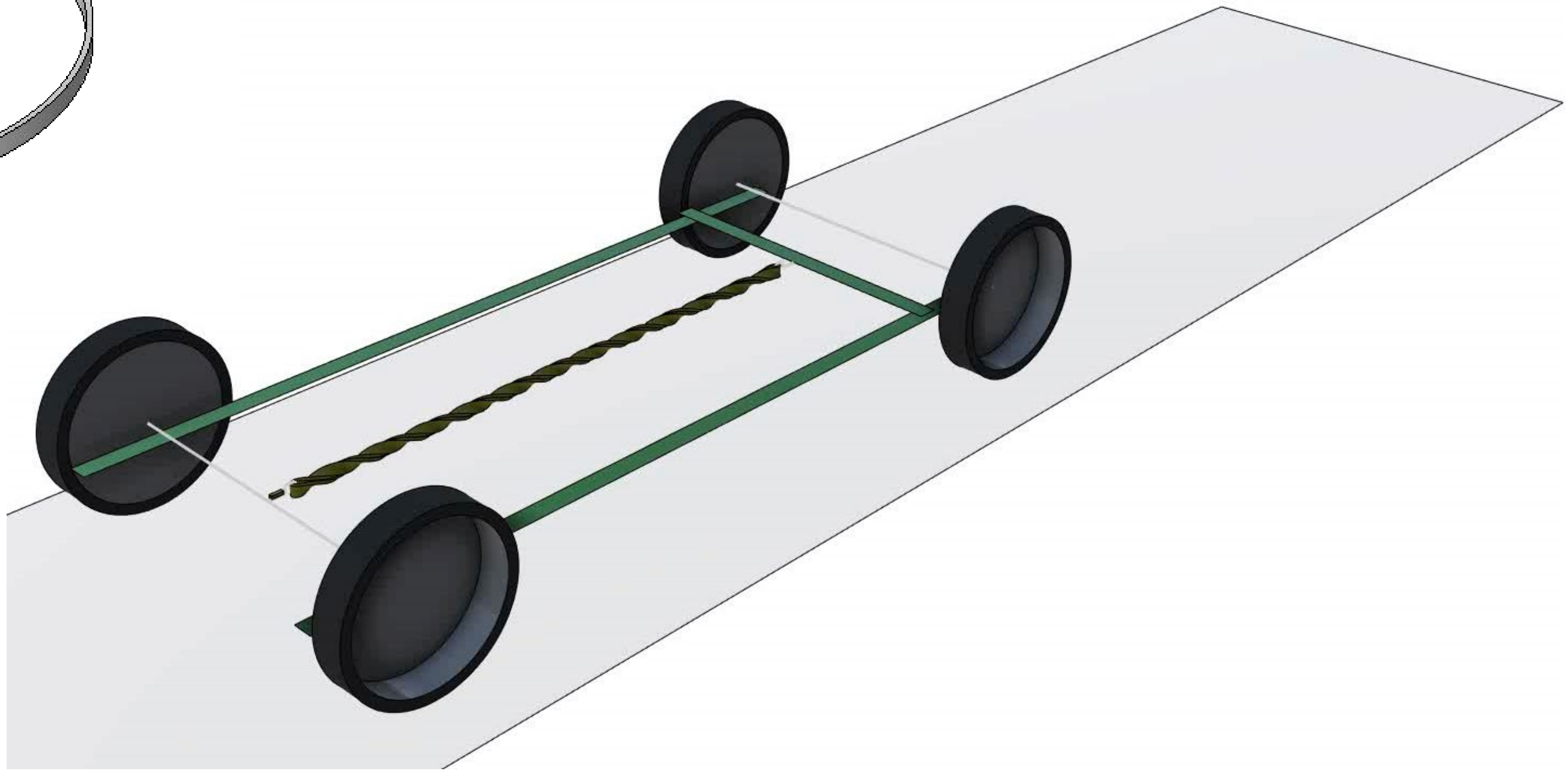


Toy vehicle





- Twisting of the band
  - Multistage analysis
  - One revolution at a time
  - Final state passed on as dynain.lsda



Summary

- New non-linear solver implemented
  - Jacobian-Free Newton-Krylov
  - Suited for saddle-point type problems (ALM) and “large particularly nonlinear” problems
- Tested for some non-trivial situations
  - Promising prospects but more work is needed, perhaps in collaboration with linear algebra team
  - Important to maintain the “explicit” efficiency for the method to be advantageous