FEM advanced course

Lecture 1 - Intro & solution methods for non-linear algebraic equations

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Course material

1. Peter Wriggers, *Nonlinear Finite Element Methods*, Springer-Verlag 2008, https://link.springer.com/book/10.1007/978-3-540-71001-1
2. Reijo Kouhia, *Computational techniques for the non-linear analysis of structures*, https://webpages.tuni.fi/rakmek/personnel/kouhia/papers/lecture_notes/comp_stab.pdf

Other good books

- K.J. Bathe, *Finite Element Procedures*. 2nd ed. 2014. https://web.mit.edu/kjb/www/Books/FEP_2nd_Edition_4th_Printing.pdf
- N.-H. Kim, *Introduction to Nonlinear Finite Element Analysis*, Springer, 2015. https://link.springer.com/book/10.1007/978-1-4419-1746-1
- T. Belytschko, W.K. Liu, B. Moran, K. Elkhodary, *Nonlinear Finite Elements for Continua and Structures*, Wiley, 2013.
- M. Kleiber, *Incremental Finite Element Modelling in Non-linear Solid Mechanics*, Ellis-Horwood, 1989.
- J.T. Oden, *Finite Elements of Nonlinear Continua*, McGraw-Hill 1972, Dover 2006.
- J.N. Reddy, *An Introduction to Nonlinear Finite Element Analysis*, Oxford University Press. 2004.
- S. Krenk, *Non-linear Modeling and Analysis of Solids and Structures*, Cambridge University Press. 2009. https://doi.org/10.1017/CBO9780511812163

Course content

1. Solution methods of non-linear algebraic equations.
2. Kinematical equations.
3. Balance equations and stress measures.
4. Constitutive models.
5. Variational problem.
6. Linearization.
7. Spatial discretization.
8. Solution methods for static/stationary problems.
9. Time integration methods. Vibration analysis.
10. Solution methods for stability analysis.
11. Formulation of structural elements: truss, beam, plate, shell, 3D-continuum.
12. Introduction to contact problems.

Course timetable

- Lecture 1. Solution methods of non-linear algebraic equations.
- Lecture 2. Kinematical and balance equations, stress measures, linearization.
- Lecture 3. Elastic constitutive models.
- Lecture 4. Objective rates, total- and updated Lagrangian formulations.
- Lecture 5. Truss element with TL-formulation.
- Lecture 6. Truss element with UL-formulation. Timoshenko beam model.
- Lecture 7. Reissner goemetrically exact beam model.
- Lecture 8. Path-following methods.
- Lecture 9. Plate, shell and 3D-solid elements.
- Lecture 10. Solution methods for stability and vibration analysis.
- Lecture 11. Solution methods for transient problems.
- Lecture 12. Integation of elasto-plastic problems.
- Lecture 13. Introduction to contact problems.
- Lecture 14. Possible visiting lecture.

Non-linear algebraic equations

First scalar equations in a single variable x:

$$f(x) = 0. \tag{1}$$

Only iterative numerical solution is possible for general equations.

Newton's method, known also as Newton-Raphson method, is based on linearization.

Start from an initial guess x_0, linearize wrt x_0

$$f(x) \approx f(x_0) + f'(x_0)\delta x = 0 \quad \Rightarrow \delta x = -f(x_0)/f'(x_0), \tag{2}$$

and update $x_1 = x_0 + \delta x$. Then proceed as x_1 as a linearization point.

Algorithm Newton for a single variable

1. Select an initial value x_0 and compute $r_0 = |f(x_0)|$
2. Set $i = 0$
3. Iterate until convergence
   (i) Compute $f'(x_i)$
   (ii) Solve $f'(x_i)\delta x = -f(x_i)$
   (iii) Update $x_{i+1} = x_i + \delta x$
   (iv) Set $i = i + 1$
   (v) Compute $f(x_i)$
   (vi) If $|f(x_i)| < \epsilon_\mathrm{r} r_0 + \epsilon_\mathrm{a}$ and $|\delta x| < \epsilon_\mathrm{r}|x_i| + \epsilon_\mathrm{a}$ convergence

ϵ_r is the relative and ϵ_a the absolute convergence tolerance for the residual $|f|$.

A good book for the mathematical and algorithmic aspects is:
C.T. Kelley, *Iterative Methods for Linear and Nonlinear Equations*, Siam, 1995, https://archive.siam.org/books/textbooks/fr16_book.pdf, where Chapter 5 is devoted to Newton's method.

Example 1

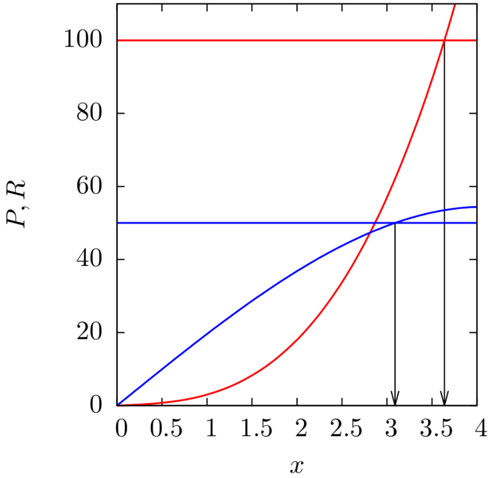
A non-linear spring with a force displacement relation $R(x) = k_1 x + k_3 x^3$ and a load P, define a non-linear equilibrium equation

$$f(x) = R(x) - P = 0 \quad \Rightarrow k_1 x + k_3 x^3 - P = 0.$$

Two cases:

1. Softening spring: $k_1 = 20, k_3 = -0.4$, load $P = 50$
2. Stiffening spring: $k_1 = 1, k_3 = 2$, load $P = 100$

Use both full Newton and chord (modified) Newton.



Example 1 - Softening spring, results

$\epsilon_{\rm r} = 10^{-5}, \epsilon_{\rm a} = 10^{-10}$.

Full Newton

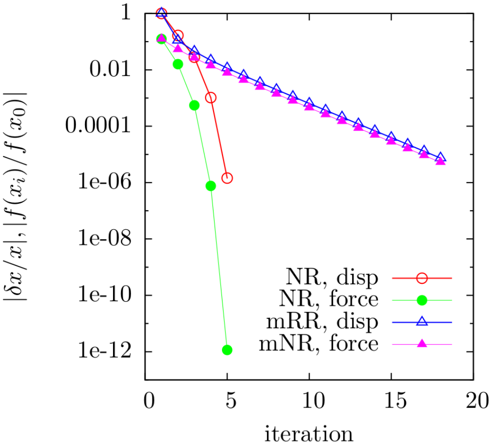
```
IT X DX F 1 2.5000E+00 2.5000E+00 -6.2500E+00
IT X DX F 2 3.0000E+00 5.0000E-01 -8.0000E-01
IT X DX F 3 3.0870E+00 8.6956E-02 -2.7484E-02
IT X DX F 4 3.0902E+00 3.2089E-03 -3.8145E-05
IT X DX F 5 3.0902E+00 4.4661E-06 -5.7383E-11
```

Chord Newton (modified Newton)

```
IT X DX F 1 2.5000E+00 2.5000E+00 -6.2500E+00
IT X DX F 2 2.8125E+00 3.1250E-01 -2.6489E+00
IT X DX F 3 2.9449E+00 1.3245E-01 -1.3173E+00
IT X DX F 4 3.0108E+00 6.5867E-02 -7.0094E-01
IT X DX F 5 3.0459E+00 3.5047E-02 -3.8570E-01
```

...

```
IT X DX F 14 3.0899E+00 2.1268E-04 -2.4365E-03
IT X DX F 15 3.0900E+00 1.2183E-04 -1.3958E-03
IT X DX F 16 3.0901E+00 6.9790E-05 -7.9966E-04
IT X DX F 17 3.0901E+00 3.9983E-05 -4.5814E-04
IT X DX F 18 3.0901E+00 2.2907E-05 -2.6248E-04
```



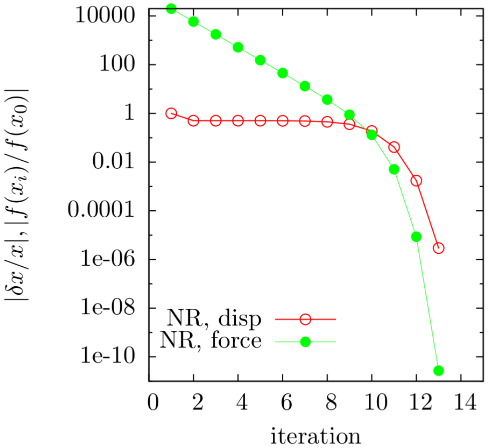
Example 1 - Hardening spring, results

$\epsilon_{\mathrm{r}} = 10^{-5}, \epsilon_{\mathrm{a}} = 10^{-10}$.

Full Newton

```
 IT X DX F 1 1.0000E+02 1.0000E+02 2.0000E+06
 IT X DX F 2 6.6667E+01 -3.3333E+01 5.9257E+05
 IT X DX F 3 4.4447E+01 -2.2220E+01 1.7556E+05
 IT X DX F 4 2.9637E+01 -1.4810E+01 5.1994E+04
 IT X DX F 5 1.9773E+01 -9.8638E+00 1.5382E+04
 IT X DX F 6 1.3219E+01 -6.5541E+00 4.5333E+03
 IT X DX F 7 8.8997E+00 -4.3195E+00 1.3187E+03
 IT X DX F 8 6.1307E+00 -2.7690E+00 3.6697E+02
 IT X DX F 9 4.5105E+00 -1.6201E+00 8.8045E+01
 IT X DX F 10 3.7951E+00 -7.1540E-01 1.3119E+01
 IT X DX F 11 3.6451E+00 -1.5007E-01 5.0606E-01
 IT X DX F 12 3.6388E+00 -6.2694E-03 8.5926E-04
 IT X DX F 13 3.6388E+00 -1.0681E-05 2.7241E-09
```

What about chord Newton?



Non-linear system of equations

Newton's method is **locally convergent method**. It means that the initial value has to be sufficiently close to the solution.

Before detailed analysis of our example problem, consider Newton's method for a system a non-linear equations.

The non-linear system of equation is briefly written as

$$\boldsymbol{f}(\boldsymbol{q}) = \boldsymbol{0}, \tag{3}$$

or written in component form

$$\begin{aligned} f_1(q_1, q_2, \ldots, q_n) &= 0, \\ f_2(q_1, q_2, \ldots, q_n) &= 0, \\ &\vdots \\ f_n(q_1, q_2, \ldots, q_n) &= 0, \end{aligned}$$

so, we have n equations $f_i = 0$ in n unknowns q_j.

Newton's method for a systems of non-linear equations - linearization

As in the single uknown case, the Newton's method is based on linearization, starting with an initial value $\boldsymbol{q}^0$

$$\boldsymbol{f}(\boldsymbol{q}) \approx \boldsymbol{f}(\boldsymbol{q}^0) + \boldsymbol{f}'(\boldsymbol{q}^0)\delta\boldsymbol{q} = \boldsymbol{0}, \tag{4}$$

where

$$\boldsymbol{f}'(\boldsymbol{q}^0) = \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{q}}\Big|_{\boldsymbol{q}=\boldsymbol{q}^0} \tag{5}$$

is the **Jacobian matrix** of the non-linear system $\boldsymbol{f}$, written in component form

$$\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{q}} = \begin{bmatrix} \frac{\partial f_1}{\partial q_1} & \frac{\partial f_1}{\partial q_2} & \dots & \frac{\partial f_1}{\partial q_n} \\ \frac{\partial f_2}{\partial q_1} & \frac{\partial f_2}{\partial q_2} & \dots & \frac{\partial f_2}{\partial q_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial q_1} & \frac{\partial f_n}{\partial q_2} & \dots & \frac{\partial f_n}{\partial q_n} \end{bmatrix}. \tag{6}$$

Newton's method for a system of non-linear equations - algorithm

1. Select an initial value $\boldsymbol{q}^0$ and compute $r_0 = \|\boldsymbol{f}(\boldsymbol{q}^0)\|$
2. Set $i = 0$
3. Iterate until convergence
   - (i) Compute $\boldsymbol{f}'(\boldsymbol{q}^i)$
   - (ii) **Solve $\boldsymbol{f}'(\boldsymbol{q}^i)\delta\boldsymbol{q} = -\boldsymbol{f}(\boldsymbol{q}^i)$**
   - (iii) Update $\boldsymbol{q}^{i+1} = \boldsymbol{q}^i + \delta\boldsymbol{q}$
   - (iv) Set $i = i + 1$
   - (v) Compute $\boldsymbol{f}(\boldsymbol{q}^i)$
   - (vi) If $\|\boldsymbol{f}(\boldsymbol{q}^i)\| < \epsilon_{\rm r} r_0 + \epsilon_{\rm a}$ and $\|\delta\boldsymbol{q}\| > \epsilon_{\rm r}\|\boldsymbol{q}^i\| + \epsilon_{\rm a}$ converged

Computationally heavy part is the solution of the linearized system.

Convergence of the Newton's method

Newton attraction theorem. Local convergence of the Newton's iteration can be proved if:

1. $\boldsymbol{f}$ is continuously differentiable in an open convex domain $D \in \mathbb{R}^N$
2. there exists $\boldsymbol{q}^*$ and $r > 0$ such that $\mathcal{B}(\boldsymbol{q}^*, r) \in D$ and $\boldsymbol{f}(\boldsymbol{q}^*) = \boldsymbol{0}$
3. the Jacobian matrix $\boldsymbol{f}'$ is invertible at $\boldsymbol{q}^*$ and $\| \left[\boldsymbol{f}'(\boldsymbol{q}^*)\right]^{-1} \| \leq \beta$
4. the Jacobian matrix is Lipschitz continuous in $\mathcal{B}(\boldsymbol{q}^*, r)$, i.e.

$$\|\boldsymbol{f}'(\boldsymbol{q}) - \boldsymbol{f}'(\boldsymbol{y})\| \leq \gamma \|\boldsymbol{q} - \boldsymbol{y}\| \qquad \forall \boldsymbol{q}, \boldsymbol{y} \in \mathcal{B}(\boldsymbol{q}^*, r). \tag{7}$$

Then there exist $\epsilon > 0$ such that for all $\boldsymbol{q}^0 \in \mathcal{B}(\boldsymbol{q}^0, \epsilon)$ the sequence $\boldsymbol{q}^1, \boldsymbol{q}^2, \ldots$ generated by the Newton's iteration converges to $\boldsymbol{q}^*$ and obeys

$$\|\boldsymbol{q}^{k+1} - \boldsymbol{q}^*\| \leq \beta\gamma \|\boldsymbol{q}^k - \boldsymbol{q}^*\|^2. \tag{8}$$

Practically, this asymptotic result can be interpreted as doubling of the number of significant digits in $\boldsymbol{q}^k$ as an approximation to $\boldsymbol{q}^*$.

Kantorovich theorem

Assume that the Jacobian is nonsingular at the initial point $\boldsymbol{q}^0$, $\boldsymbol{f}'$ is Lipschitz continuous in a region containing $\boldsymbol{q}^0$, and the first step of Newton's method is sufficiently small, i.e.

1. $\boldsymbol{f}$ is continuously differentiable in a ball $\mathcal{B}(\boldsymbol{q}^0, r), r > 0$,
2. the Jacobian matrix $\boldsymbol{f}'$ is nonsingular at $\boldsymbol{q}^0$ and $\| \left[\boldsymbol{f}'(\boldsymbol{q}^0)\right]^{-1} \| \leq \beta$
3. the Jacobian matrix is Lipschitz continuous in $\mathcal{B}(\boldsymbol{q}^0, r)$, see eq. (7), with Lipschitz constant γ,
4. the first Newton step is sufficently small: $\|[\boldsymbol{f}'(\boldsymbol{q}^0)]^{-1}\boldsymbol{f}(\boldsymbol{q}^0)\| \leq \eta$

then if $h_0 = \beta\gamma\eta < \frac{1}{2}$ the Newton sequence converges to a unique solution in $\mathcal{B}(\boldsymbol{q}^0, r_1)$, where $r_1 = \min(r, r_0)$

$$r_0 \equiv \frac{1 - \sqrt{1 - 2h_0}}{\beta\gamma}. \tag{9}$$

and

$$\|\boldsymbol{q}^k - \boldsymbol{q}^*\| \leq (2h_0)^{2^k} \frac{\eta}{h_0}, \qquad k = 0, 1, 2, \ldots \tag{10}$$

Example 1 - hardening spring, cause of failure

The equation to be solved was $f(x) = x + 2x^3 - 100 = 0$ and $f'(x) = 1 + 6x^2$ is clearly nonsingular for $x > 0$.

The Lipschitz constant γ can be estimated from the second derivative

$$\gamma < \max |f''(x)| \qquad x \in (0, r_0). \tag{11}$$

Now $f''(x) = 12x$ and thus $\gamma < 48$ when $x \in (0, 4)$, also $\beta \leq |[f'(0)]^{-1}| = 1$ and $\eta = 100$.

Now $h_0 = \beta\gamma\eta = 4800 \gg \frac{1}{2}$.

Globally convergent methods

Splitting the load in smaller steps, incremental loading. Mathematicians talk about homotopy methods.

It can also be called as a parametrized non-linear problem:

$$f(x, P) = k_1 x + k_3 x^3 - P. \tag{12}$$

Solve the following sequence of problems $0 < \lambda_1 P < \lambda_2 P < \cdots < \lambda_{n-1} P < \lambda_n P = P$

Thus, the system (12) can be denoted as

$$f(x, \lambda) = k_1 x + k_3 x^3 - \lambda P_{\text{ref}}. \tag{13}$$

Incremental procedure with Newton

Solution of system $\boldsymbol{f}(\boldsymbol{q}, \lambda) = \boldsymbol{0}$

1. Select an initial value $\boldsymbol{q}_1^0$, usually a zero vector if $\lambda_0 = 0$.
2. Increment load $\lambda_n = \lambda_{n-1} + \Delta\lambda$
3. Set $i = 0$, and $\Delta\boldsymbol{q}_n = \boldsymbol{0}$
   - (i) Iterate until convergence
   - (ii) Compute $\boldsymbol{f}'(\boldsymbol{q}_n^i)$
   - (iii) **Solve $\boldsymbol{f}'(\boldsymbol{q}_n^i)\delta\boldsymbol{q} = -\boldsymbol{f}(\boldsymbol{q}_n^i)$**
   - (iv) Update $\Delta\boldsymbol{q}_n^{i+1} = \Delta\boldsymbol{q}_n^i + \delta\boldsymbol{q}$
   - (v) Update $\boldsymbol{q}_n^{i+1} = \boldsymbol{q}_{n-1} + \Delta\boldsymbol{q}_n^{i+1}$
   - (vi) Set $i = i + 1$
   - (vii) Compute $\boldsymbol{f}(\boldsymbol{q}^i)$
   - (viii) If $\|\boldsymbol{f}(\boldsymbol{q}^i)\| < \epsilon_{\rm r} r_0 + \epsilon_{\rm a}$ and $\|\delta\boldsymbol{q}\| > \epsilon_{\rm r}\|\Delta\boldsymbol{q}^i\| + \epsilon_{\rm a}$ converged and proceed to a new step, go to 2.

Computing the Jacobian matrix

Numerical differentiation is one handy way:

```
DO J = 1, N
   DX = ABS(H*X(J))
   IF(DX.LT.H) DX = H
   XH = X
   XH(J) = XH(J) + DX
   CALL EQS(N,NPAR,XH,PAR,FH)
   DO I = 1, N
      DF(I,J) = (FH(I) - F(I))/DX
   END DO
END DO
```

Next

Exercises on Thursday at 2 PM in class FC112. Coding Newton's method for a scalar and vector valued cases.

Next lecture on non-linear continuum mechanics, kinematic, balance equations and stress measures.