Constitutive Driver using an Arc-Length Method

Andreas Seupel

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IMFD, TU Bergakademie Freiberg

1 Basics

We propose a testing environment for material routines for the following tasks:

- FE-program independent testing
- Reduction to the material point level
- 3D-analysis
- Test of different solving methods
- Test of the consistent tangent
- Parameter study and estimation for simple problems

Algebraic vectors are denoted by one underline; algebraic matrices have two underlines.

1.1 Test Problem

We consider the equilibrium equation at material point level in terms of the principle of virtual work

$$\delta W = \delta \underline{\boldsymbol{\varepsilon}}_{\text{log}}^{\text{T}} \left(\underline{\boldsymbol{\sigma}}_{\text{int}} \left(\underline{\boldsymbol{\varepsilon}}_{\text{log}} \right) - \chi \underline{\boldsymbol{\sigma}}_{\text{ext}} \right) = 0. \tag{1}$$

For non-vanishing entries in $\delta \underline{\boldsymbol{\varepsilon}}_{\text{log}}$ we find:

$$\underline{\boldsymbol{G}} = \underline{\boldsymbol{\sigma}}_{\text{int}} \left(\underline{\boldsymbol{\varepsilon}}_{\text{log}} \right) - \chi \underline{\boldsymbol{\sigma}}_{\text{ext}} = \underline{\boldsymbol{0}}. \tag{2}$$

The prescribed stress and the internal stress provided by the material are denoted as $\underline{\boldsymbol{\sigma}}_{\text{ext}}$ and $\underline{\boldsymbol{\sigma}}_{\text{int}} \left(\underline{\boldsymbol{\varepsilon}}_{\text{log}} \right)$, respectively. A dimensionless and unknown load parameter χ is introduced. The vector of virtual strains is denoted as $\delta \underline{\boldsymbol{\varepsilon}}_{\text{log}}$. We assume a strain $\underline{\boldsymbol{\varepsilon}}_{\text{log}}$, which is an unkown vector. The index „log“ shows the relation to the logarithmic strain in case of principle axis loadings.

The non-linear problem (2) is solved using an incremental loading. The loading parameter χ is arbitrary. Therefore an additional equation is needed. One possible option in case of rate-independent material behavior is the prescription of the so-called arc-length. This gives a constraint equation of type

$$l \left(\underline{\boldsymbol{\varepsilon}}_{\text{log}}, \chi \right) = 0, \tag{3}$$

which can be used to determine χ. An introduction to this topic can be found in Crisfield [1]. We like to use an *cylindrical arc-length method* which controls the maximum component of the strain increment, see Seupel [2]. The constraint equations should read

$$l = \Delta \underline{\boldsymbol{E}}^{\text{T}} \Delta \underline{\boldsymbol{E}} - \Delta \bar{s}^2 = 0. \tag{4}$$

1.1.1 Solving method

The computation within the load increment $n \to n+1$ is done using a NEWTON-RAPHSON-scheme. The solution is known at point n.

We linearize Eq. (2) to find a solution in an iterative manner. The linearized system of equations reads

$$\begin{bmatrix} \underline{\underline{\boldsymbol{K}}} & -\underline{\boldsymbol{\sigma}}_{\text{ext}} \end{bmatrix}_{n:k} \begin{bmatrix} \mathrm{d}\Delta\underline{\boldsymbol{E}} \\ \mathrm{d}\Delta\chi \end{bmatrix} = -\underline{\boldsymbol{G}} = -\left[\underline{\boldsymbol{\sigma}}_{\text{int}}\left(\underline{\boldsymbol{\varepsilon}}_{\log}\right) - \chi\underline{\boldsymbol{\sigma}}_{\text{ext}}\right]_{n:k}, \tag{5}$$

in iteration step k. The following definitions are used:

$$\Delta\underline{\boldsymbol{E}}_{k+1} = \Delta\underline{\boldsymbol{E}}_k + \mathrm{d}\Delta\underline{\boldsymbol{E}} \tag{6}$$

$$\Delta\chi_{k+1} = \Delta\chi_k + \mathrm{d}\Delta\chi \tag{7}$$

$$\underline{\underline{\boldsymbol{K}}}_{n:k} = \frac{\partial\underline{\boldsymbol{G}}}{\partial\Delta\underline{\boldsymbol{E}}} \tag{8}$$

$$\frac{\partial\underline{\boldsymbol{G}}}{\partial\Delta\chi} = -\underline{\boldsymbol{\sigma}}_{\text{ext}}. \tag{9}$$

The iteration stops if

$$\left\|\underline{\boldsymbol{\sigma}}_{\text{int}}\left(\Delta\underline{\boldsymbol{E}}_{n:k+1}\right) - \chi_{n:k+1}\underline{\boldsymbol{\sigma}}_{\text{ext}}\right\| < \epsilon \cap \|\mathrm{d}\Delta\underline{\boldsymbol{E}}\| < \epsilon\ , \epsilon \ll 1 \tag{10}$$

is fulfilled. In case of convergence, we update

$$\underline{\boldsymbol{\varepsilon}}_{\log,n+1} = \underline{\boldsymbol{\varepsilon}}_{\log,n} + \Delta\underline{\boldsymbol{E}} \tag{11}$$

$$\chi_{n+1} = \chi_n + \Delta\chi. \tag{12}$$

The improvement $\mathrm{d}\Delta\underline{\boldsymbol{E}}$ can be determined from Eq. (5):

$$\mathrm{d}\Delta\underline{\boldsymbol{E}} = \underbrace{-\underline{\underline{\boldsymbol{K}}}_{n:k}^{-1}\underline{\boldsymbol{G}}}_{\mathrm{d}\Delta\underline{\boldsymbol{U}}_{\text{G}}} + \underbrace{\underline{\underline{\boldsymbol{K}}}_{n:k}^{-1}\underline{\boldsymbol{\sigma}}_{\text{ext}}}_{\mathrm{d}\Delta\underline{\boldsymbol{U}}_{\text{F}}}\mathrm{d}\Delta\chi. \tag{13}$$

The unknown value of $\mathrm{d}\Delta\chi$ can be directly found as explained within the next section. The parts $\mathrm{d}\Delta\underline{\boldsymbol{U}}_{\text{G}}$ und $\mathrm{d}\Delta\underline{\boldsymbol{U}}_{\text{F}}$ can be computed by solving

$$\underline{\underline{\boldsymbol{K}}}_{n:k}\,\mathrm{d}\Delta\underline{\boldsymbol{U}}_{\text{G}} = -\underline{\boldsymbol{G}}_{n:k} \tag{14}$$

$$\underline{\underline{\boldsymbol{K}}}_{n:k}\,\mathrm{d}\Delta\underline{\boldsymbol{U}}_{\text{F}} = \underline{\boldsymbol{\sigma}}_{\text{ext}}. \tag{15}$$

1.1.2 Cylindrical Arc-Length method

The improvement $\mathrm{d}\Delta\chi$ can be found by direct solving Eq. (4). During iteration the constrained equation reads

$$l = \left(\Delta\underline{\boldsymbol{E}}_{k+1}\right)^{\text{T}}\Delta\underline{\boldsymbol{E}}_{k+1} - \Delta\bar{s}_{n+1}^2 = 0. \tag{16}$$

The arc-length $\Delta\bar{s}_{n+1}$ is a prescribed parameter. Using Eq. (6) and the improvement $\mathrm{d}\Delta\underline{\boldsymbol{E}}$ given by Eq. (13) yields

$$\left(\Delta\underline{\boldsymbol{E}}_k + \mathrm{d}\Delta\underline{\boldsymbol{U}}_{\text{G}} + \mathrm{d}\Delta\underline{\boldsymbol{U}}_{\text{F}}\mathrm{d}\Delta\chi\right)^{\text{T}}\left(\Delta\underline{\boldsymbol{E}}_k + \mathrm{d}\Delta\underline{\boldsymbol{U}}_{\text{G}} + \mathrm{d}\Delta\underline{\boldsymbol{U}}_{\text{F}}\mathrm{d}\Delta\chi\right) - \Delta\bar{s}_{n+1}^2 = 0. \tag{17}$$

This last equation is a quadratic function in $\mathrm{d}\Delta\chi$. The roots read after some manipulations

$$\mathrm{d}\Delta\chi_{1,2} = -\frac{p}{2} \pm \sqrt{\frac{p^2}{4} - q}, \tag{18}$$

with the abbreviations

$$p = \frac{C_1}{C_2} \tag{19}$$

$$q = \frac{C_0}{C_2} \tag{20}$$

$$C_0 = \Delta\underline{\boldsymbol{E}}_k^{\text{T}}\Delta\underline{\boldsymbol{E}}_k + 2\Delta\underline{\boldsymbol{E}}_k^{\text{T}}\mathrm{d}\Delta\underline{\boldsymbol{U}}_{\text{G}} + \mathrm{d}\Delta\underline{\boldsymbol{U}}_{\text{G}}^{\text{T}}\mathrm{d}\Delta\underline{\boldsymbol{U}}_{\text{G}} - \triangle\bar{s}_{n+1}^2 \tag{21}$$

$$C_1 = 2\mathrm{d}\Delta \underline{\boldsymbol{U}}_{\mathrm{F}}^{\mathrm{T}} \left(\Delta \underline{\boldsymbol{E}}_k + \mathrm{d}\Delta \underline{\boldsymbol{U}}_{\mathrm{G}}\right) \tag{22}$$

$$C_2 = \mathrm{d}\Delta \underline{\boldsymbol{U}}_{\mathrm{F}}^{\mathrm{T}} \mathrm{d}\Delta \underline{\boldsymbol{U}}_{\mathrm{F}}. \tag{23}$$

The two possible roots in Eq. (18) can be physically interpreted. We are searching the solution which leads to an ongoing plastic-damage-loading [2]. One possibilty in the framework of elastic-plastic behavior is the elastic unloading branch. This solution should be avoided by the following method: The possible increments $\Delta \underline{\boldsymbol{E}}_{k+1,1}$ and $\Delta \underline{\boldsymbol{E}}_{k+1,2}$ are calculated with $\mathrm{d}\Delta\chi_{1,2}$, respectively. Afterwards, the dot product

$$g_i = \cos\left(\theta_i\right) = \Delta \underline{\boldsymbol{E}}_k^{\mathrm{T}} \Delta \underline{\boldsymbol{E}}_{k+1,i} \quad i = 1, 2. \tag{24}$$

is evaluated for each solution. We chose the loading increment $\mathrm{d}\Delta\chi_i$ with the highest cosine g_i. This stands for the smallest angle between the new prediction and the prediction of the last update. We follow the „tendency“ of the previous loading history.

1.1.3 Predictor Step

Before a new increment can start, a guess of $\Delta \underline{\boldsymbol{E}}_{k=1}$ and $\Delta\chi_{k=1}$ has to be made. For the first load step $n = 1$ we assume an elastic behavior. Therefore we use a (unscaled) predictor

$$\Delta \underline{\boldsymbol{E}}^* : \ \underline{\underline{\boldsymbol{K}}}_{n:0} \Delta \underline{\boldsymbol{E}}^* = \underline{\boldsymbol{\sigma}}_{\text{ext}}. \tag{25}$$

For all other steps we use the previous solution step $\Delta \underline{\boldsymbol{E}}^* = \underline{\boldsymbol{E}}_n - \underline{\boldsymbol{E}}_{n-1}$ as predictor. This method has been succesfully applied for *snap-back* problems, see Seupel [2]. The constrained equation (16) has to be fulfilled in the first iteration step. Therefore we have to scale the predictor with a factor

$$\alpha = \frac{\triangle \bar{s}_{n+1}^2}{\left(\Delta \underline{\boldsymbol{E}}^*\right)^{\mathrm{T}} \Delta \underline{\boldsymbol{E}}^*}. \tag{26}$$

Therewith, the guess of the strain increment and the load parameter yield

$$\Delta \underline{\boldsymbol{E}}_{k=1} = \sqrt{\alpha} \Delta \underline{\boldsymbol{E}}^*, \ \ \Delta\chi_{k=1} = \sqrt{\alpha}\Delta\chi^*. \tag{27}$$

1.1.4 Control of the Maxium Strain Component

We suggest a control of the absolute biggest entry of the strain component, see Seupel [2] . The predictor can be reformulated as

$$\alpha = \frac{\triangle \bar{s}_{n+1}^2}{\left(\Delta E_{\text{max}}^*\right)^2} \tag{28}$$

with

$$\Delta E_{\text{max}}^* = \max\left(\left|\Delta \underline{\boldsymbol{E}}^*\right|\right). \tag{29}$$

The index i_{max} of the component in $\Delta \underline{\boldsymbol{E}}^*$ containing ΔE_{max}^* is detected. For the following iteration steps the value i_{max} is kept:

$$\mathrm{d}\Delta U_{\mathrm{G}} = \mathrm{d}\Delta U_{\mathrm{G},i_{\text{max}}}, \mathrm{d}\Delta U_{\mathrm{F}} = \mathrm{d}\Delta U_{\mathrm{F},i_{\text{max}}}. \tag{30}$$

The constrained equation reads

$$l = \left(\Delta E_{\text{max}}\right)_{k+1}^2 - \Delta \bar{s}_{n+1}^2 = 0, \tag{31}$$

where $\Delta \bar{s}_{n+1}^2$ controls the maximum strain increment. The method is summarized in Scheme 1.

1.1.5 Remarks

The tangent $\underline{\underline{\boldsymbol{K}}}$ yields the consistent material tangent which is also needed within FEM-codes:

$$\underline{\underline{\boldsymbol{K}}} = \frac{\partial \underline{\boldsymbol{G}}}{\partial \Delta \underline{\boldsymbol{E}}} = \frac{\partial \underline{\boldsymbol{\sigma}}_{\text{int}}}{\partial \Delta \underline{\boldsymbol{E}}}. \tag{32}$$

Algorithm 1 Arc-length method following Seupel [2]

1. Predictor Step $(n,\ k=0)$**:**

1.1 if $n=1$:

$$\Delta\underline{\boldsymbol{E}}^{*}:\ \underline{\underline{\boldsymbol{K}}}_{n:0}\Delta\underline{\boldsymbol{E}}^{*}=\underline{\boldsymbol{\sigma}}_{\text{ext}}$$

else:

$$\Delta\underline{\boldsymbol{E}}^{*}=\underline{\boldsymbol{E}}_{n}-\underline{\boldsymbol{E}}_{n-1}$$

1.2 Scaling

$$\begin{aligned}
\Delta E^{*}_{\text{max}} &= \max\left(|\Delta\underline{\boldsymbol{E}}^{*}|\right)\\
\alpha &= \frac{\triangle\bar{s}^{2}_{n+1}}{\left(\Delta E^{*}_{\text{max}}\right)^{2}}\\
\Delta\underline{\boldsymbol{E}}_{1} &= \sqrt{\alpha}\Delta\underline{\boldsymbol{E}},^{*} && \Delta\chi_{1}=\sqrt{\alpha}\Delta\chi^{*}\\
k &= k+1
\end{aligned}$$

2. Correction steps $(n,\ k=1,\ldots,k_{\textbf{limit}})$

2.1 Iteration step k

$$\begin{aligned}
\underline{\underline{\boldsymbol{K}}}_{n:k}\mathrm{d}\Delta\underline{\boldsymbol{U}}_{\text{G}} &= -\underline{\boldsymbol{G}}_{n:k}\\
\underline{\underline{\boldsymbol{K}}}_{n:k}\mathrm{d}\Delta\underline{\boldsymbol{U}}_{\text{F}} &= \underline{\boldsymbol{\sigma}}_{\text{ext}}\\
\Delta\left(E_{\text{max}}\right)_{k} &= \max\left(|\Delta E_{i,k}|\right)\rightarrow i_{\text{max}},\ i_{\text{max}}\in\left\{1,2,\ldots,\dim\left(\Delta\underline{\boldsymbol{E}}_{k}\right)\right\}\\
\mathrm{d}\Delta U_{\text{G}} &= \mathrm{d}\Delta U_{\text{G},i_{\text{max}}}\\
\mathrm{d}\Delta U_{\text{F}} &= \mathrm{d}\Delta U_{\text{F},i_{\text{max}}}\\
C_{0} &= \Delta\left(E_{\text{max}}\right)^{2}_{k}+2\Delta\left(E_{\text{max}}\right)_{k}\mathrm{d}\Delta U_{\text{G}}+\left(\mathrm{d}\Delta U_{\text{G}}\right)^{2}-\triangle\bar{s}^{2}_{n+1}\\
C_{1} &= 2\mathrm{d}\Delta U_{\text{F}}\left(\Delta\left(E_{\text{max}}\right)_{k}+\mathrm{d}\Delta U_{\text{G}}\right)\\
C_{2} &= \left(\mathrm{d}\Delta U_{\text{F}}\right)^{2}\\
p &= \frac{C_{1}}{C_{2}}\\
q &= \frac{C_{0}}{C_{2}}\\
\mathrm{d}\Delta\chi_{1,2} &= -\frac{p}{2}\pm\sqrt{\frac{p^{2}}{4}-q}\\
\Delta\underline{\boldsymbol{E}}_{k+1,i} &= \Delta\underline{\boldsymbol{E}}_{k}+\mathrm{d}\Delta\underline{\boldsymbol{U}}_{\text{G}}+\mathrm{d}\Delta\underline{\boldsymbol{U}}_{\text{F}}\mathrm{d}\Delta\chi_{i} && i=1,2\\
g_{i} &= \Delta\underline{\boldsymbol{E}}^{\text{T}}_{k}\Delta\underline{\boldsymbol{E}}_{k+1,i} && i=1,2
\end{aligned}$$

$$\max\left(g_{i}\right)\rightarrow i_{\text{chosen}}$$

2.2 Update($k\rightarrow k+1$)

$$\Delta\underline{\boldsymbol{E}}_{k+1}=\Delta\underline{\boldsymbol{E}}_{k}+\mathrm{d}\Delta\underline{\boldsymbol{E}}_{i_{\text{chosen}}},\qquad \Delta\chi_{k+1}=\Delta\chi_{k}+\mathrm{d}\Delta\chi_{i_{\text{chosen}}}$$

2.3 Tolerances satisfied?

$$\|\underline{\boldsymbol{\sigma}}_{\text{int}}\left(\Delta\underline{\boldsymbol{E}}_{n:k+1}\right)-\chi_{n:k+1}\underline{\boldsymbol{\sigma}}_{\text{ext}}\|<\epsilon\cap\|\mathrm{d}\Delta\underline{\boldsymbol{E}}\|<\epsilon$$

Yes: go to 3.
No: go to 2.1, $k=k+1$

3. Global Update $(n\rightarrow n+1)$

$$\underline{\boldsymbol{E}}_{n+1}=\underline{\boldsymbol{E}}_{n}+\Delta\underline{\boldsymbol{E}},\qquad \chi_{n+1}=\chi_{n}+\Delta\chi$$

References

[1] M. A. Crisfield. *Non-linear Finite Element Analysis of Solids and Structures*, volume 1: Essentials. John Wiley & Sons, 2000.

[2] A. Seupel. Numerische Untersuchungen eines schädigungsmechanischen Modells im Rahmen einer Gradiententheorie erster Ordnung anhand eindimensionaler Sonderfälle . Master's thesis, TU Bergakademie Freiberg, 2013.