# Computational Approach to Micromechanical Contacts

## Lecture 2.
## *Finite Element Method for Non-linear Materials*

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# Outline

# Non-linear material models

# Viscoelastic material

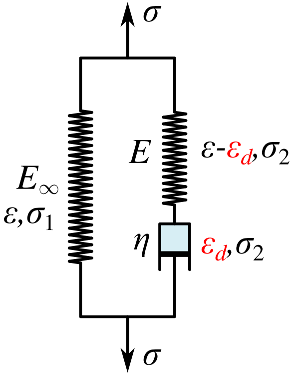
**One-dimensional constitutive equations**

- Applied stress $\sigma$
- In the left branch $\sigma_1 = E_\infty \varepsilon$
- In the dashpot $\sigma_2 = \eta \dot{\varepsilon}_d \quad (*)$
- In the right spring $\sigma_2 = E(\varepsilon - \varepsilon_d) \quad (**)$
- For the whole system $\sigma = \sigma_1 + \sigma_2$

$$\boxed{\sigma = (E_\infty + E)\varepsilon - E\varepsilon_d}$$

- From $(*)$ and $(**)$, and denoting $\tau = \eta/E$:

$$\boxed{\dot{\varepsilon}_d + \frac{\varepsilon_d}{\tau} = \frac{\varepsilon}{\tau},} \qquad \varepsilon_d \xrightarrow[t \to -\infty]{} 0$$

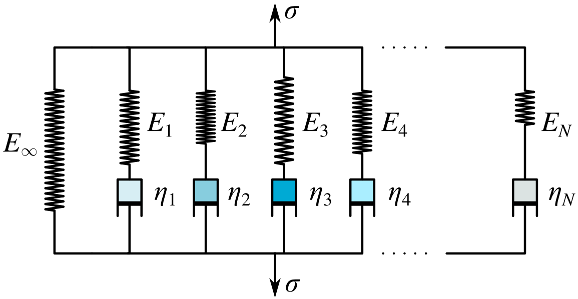


- Recall: 1D model

$$\sigma = (E_\infty + E)\varepsilon - E\varepsilon_d, \quad \dot\varepsilon_d + \frac{\varepsilon_d}{\tau} = \frac{\varepsilon}{\tau}, \quad \varepsilon_d \xrightarrow[t\to-\infty]{} 0$$

- Multiple dashpots in parallel

$$\sigma = \underbrace{(E_\infty + \sum_i E_i)\varepsilon}_{\text{elastic stress } \sigma_0} - \sum_i E_i\varepsilon_d^i, \quad \dot\varepsilon_d^i + \frac{\varepsilon_d^i}{\tau_i} = \frac{\varepsilon}{\tau_i}, \quad \varepsilon_d^i \xrightarrow[t\to-\infty]{} 0, \quad \tau_i = \frac{\eta_i}{E_i}$$



# • Three-dimensional viscoelastic model I

- Recall: 1D model

$$\sigma = (E_\infty + E)\varepsilon - E\varepsilon_d, \quad \dot\varepsilon_d + \frac{\varepsilon_d}{\tau} = \frac{\varepsilon}{\tau}, \quad \varepsilon_d \xrightarrow[t\to-\infty]{} 0$$

- Multiple dashpots in parallel

$$\sigma = \underbrace{(E_\infty + \sum_i E_i)\varepsilon}_{\text{elastic stress } \sigma_0} - \sum_i E_i\varepsilon_d^i, \quad \dot\varepsilon_d^i + \frac{\varepsilon_d^i}{\tau_i} = \frac{\varepsilon}{\tau_i}, \quad \varepsilon_d^i \xrightarrow[t\to-\infty]{} 0, \quad \tau_i = \frac{\eta_i}{E_i}$$

- Denote $E_0 = E_\infty + \sum_i E_i$, $\psi_i = E_i/E_0$, and $q_i = E_i\varepsilon_d^i$ we obtain

$$\sigma = E_0\varepsilon - \sum_i q_i, \quad \dot q_i + \frac{q_i}{\tau_i} = \frac{\psi_i}{\tau_i}\sigma_0, \quad \varepsilon_d^i \xrightarrow[t\to-\infty]{} 0$$

- By construction

$$\sum_i \psi_i + \frac{E_\infty}{E_0} = 1 \quad \Rightarrow \quad \sum_i \psi_i = 1 - \frac{E_\infty}{E_0}$$

# • Three-dimensional viscoelastic model II

- Linear elasticity:

$$\sigma = E_0\varepsilon - \sum_{i=1,N} q_i, \quad \dot q_i + \frac{q_i}{\tau_i} = \frac{\psi_i}{\tau_i}\sigma_0, \quad \varepsilon_d^i \xrightarrow[t\to-\infty]{} 0, \quad \sum_{i=1,N}\psi_i = 1 - \frac{E_\infty}{E_0}$$

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- Stored elastic energy $W(\varepsilon)$ (e.g., in linear elasticity $W = \frac{1}{2}E_0\varepsilon^2$ ) then

$$\sigma = \frac{\partial W}{\partial \varepsilon} - \sum_{i=1,N} q_i, \quad \dot{q}_i + \frac{q_i}{\tau_i} = \frac{\psi_i}{\tau_i}\frac{\partial W}{\partial \varepsilon}, \quad q_i \xrightarrow[t\to-\infty]{} 0, \quad \sum_{i=1,N} \psi_i = 1 - \frac{E_\infty}{E_0}$$

- This formulation is valid for non-linear elasticity, stored elastic energy $W$ should be a convex function.

# • Three-dimensional viscoelastic model III

- Decomposition of stress and strain tensors into deviatoric ( $\underline{\underline{s}}, \underline{\underline{e}}$ ) and spherical parts:

$$\underline{\underline{\sigma}} = \underline{\underline{s}} - p\underline{\underline{I}}, \quad \underline{\underline{\varepsilon}} = \underline{\underline{e}} + \frac{1}{3}\mathrm{tr}(\underline{\underline{\varepsilon}})\underline{\underline{I}} = \underline{\underline{e}} + \frac{1}{3}\theta\underline{\underline{I}}$$

- Linear isotropic elasticity:

$$\underline{\underline{\sigma}} = \lambda_0 \mathrm{tr}(\underline{\underline{\varepsilon}})\underline{\underline{I}} + 2G_0\underline{\underline{\varepsilon}} = \lambda_0\theta\underline{\underline{I}} + 2G_0\left(\underline{\underline{e}} + \frac{1}{3}\theta\underline{\underline{I}}\right) = \frac{3\lambda_0 + 2G_0}{3}\theta\underline{\underline{I}} + 2G_0\underline{\underline{e}} = K_0\theta\underline{\underline{I}} + 2G_0\underline{\underline{e}}$$

- Elastic energy: $W = \frac{1}{2}\underline{\underline{\sigma}} : \underline{\underline{\varepsilon}} = \frac{1}{2}K_0\theta^2 + G_0\underline{\underline{e}} : \underline{\underline{e}}$
- 3D formulation

$$\underline{\underline{\sigma}} = \frac{\partial W}{\partial \theta}\underline{\underline{I}} + \frac{\partial W}{\partial \underline{\underline{e}}} - \sum_{i=1,N} \underline{\underline{q}}_i \qquad (*)$$

$$\dot{\underline{\underline{q}}}_i + \frac{1}{\tau_i}\underline{\underline{q}}_i = \frac{\psi_i}{\tau_i}\frac{\partial W}{\partial \underline{\underline{e}}} \quad , \quad \underline{\underline{q}}_i \xrightarrow[t\to-\infty]{} 0, \quad \sum_{i=1,N}\psi_i = 1 - \psi_\infty$$

$$\psi_i \geq 0, \quad 0 \leq \psi_\infty \leq 1$$

# Three-dimensional viscoelastic model IV

- Integrate

$$\dot{\underline{\underline{q}}}_i + \frac{1}{\tau_i}\underline{\underline{q}}_i = \frac{\psi_i}{\tau_i}\frac{\partial W}{\partial \underline{\underline{e}}} \quad , \quad \underline{\underline{q}}_i \xrightarrow[t\to-\infty]{} 0$$

$$\underline{\underline{q}} = \frac{\psi_i}{\tau_i}\int\limits_{-\infty}^{t} \exp\left[-\frac{(t-t')}{\tau_i}\right]\frac{\partial W}{\partial \underline{\underline{e}}(t')}\,dt' \qquad (**)$$

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- Substitute $(**)$ in $(*)$

$$\underline{\underline{\sigma}} = \frac{\partial W}{\partial \theta}\underline{\underline{I}} + \frac{\partial W}{\partial \underline{\underline{e}}} - \sum_{i=1,N}\frac{\psi_i}{\tau_i}\int\limits_{-\infty}^{t}\exp\left[-\frac{(t-t')}{\tau_i}\right]\frac{\partial W}{\partial \underline{\underline{e}}(t')}\,dt'$$

# • Three-dimensional viscoelastic model IV

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$$\underline{\underline{\sigma}} = \frac{\partial W}{\partial \theta}\underline{\underline{I}} + \psi_\infty\frac{\partial W}{\partial \underline{\underline{e}}} + \sum_{i=1,N}\psi_i\int\limits_{-\infty}^{t}\exp\left[-\frac{(t-t')}{\tau_i}\right]\frac{d}{dt}\left\{\frac{\partial W}{\partial \underline{\underline{e}}(t')}\right\}dt'$$

| $\frac{d}{dt}[f\exp(t/\tau)] = \frac{df}{dt}\exp(t/\tau) + \frac{1}{\tau}f\exp(t/\tau)$ integrate $f\exp(t/\tau) = \int\limits_{-\infty}^{t}\left[\frac{df(t')}{dt'}\exp(t'/\tau) + \frac{1}{\tau}f(t')\exp(t'/\tau)\right]dt'$ |

| multiply by $\exp(-t/\tau)$ : $f = \int\limits_{-\infty}^{t}\left[\frac{df(t')}{dt'}\exp(-(t-t')/\tau) + \frac{1}{\tau}f(t')\exp(-(t-t')/\tau)\right]dt'$ |

| finally $\exp(-t/\tau)$ : $f - \frac{1}{\tau}\int\limits_{-\infty}^{t}\exp\left[-\frac{(t-t')}{\tau}\right]f(t')\,dt' = \int\limits_{-\infty}^{t}\exp\left[-\frac{(t-t')}{\tau}\right]\frac{df(t')}{dt'}\,dt'$ |

# • Three-dimensional viscoelastic model V

- Finally

$$\underline{\underline{\sigma}} = \frac{\partial W}{\partial \theta}\underline{\underline{I}} + \psi_\infty \frac{\partial W}{\partial \underline{\underline{e}}} + \sum_{i=1,N} \psi_i \int\limits_{-\infty}^{t} \exp\left[-\frac{(t-t')}{\tau_i}\right] \frac{d}{dt}\left\{\frac{\partial W}{\partial \underline{\underline{e}}(t')}\right\} dt'$$

- For linear isotropic elasticity:

$$\underline{\underline{\sigma}} = K\theta\underline{\underline{I}} + 2\psi_\infty G_0 \underline{\underline{e}} + 2G_0 \sum_{i=1,N} \psi_i \int\limits_{-\infty}^{t} \exp\left[-\frac{(t-t')}{\tau_i}\right] \dot{\underline{\underline{e}}}(t')\, dt'$$

- Denote $G_\infty = \psi_\infty G_0$, recall $\sum_{i=1,N} \psi_i = 1 - \psi_\infty$
- Alternatively one can replace $G_0$ by $G_0 - G_\infty$ and put $\sum_{i=1,N} \psi_i = 1$
- Finally

$$\underline{\underline{\sigma}} = K\theta\underline{\underline{I}} + 2G_\infty \underline{\underline{e}} + 2(G_0 - G_\infty) \sum_{i=1,N} \psi_i \int\limits_{-\infty}^{t} \exp\left[-\frac{(t-t')}{\tau_i}\right] \dot{\underline{\underline{e}}}(t')\, dt'$$

# • Three-dimensional viscoelastic model

Linear viscoelastic (generalized Maxwell model, standard solid)

- Stress-strain relation:

$$\underline{\underline{\sigma}}(t) = K\theta\underline{\underline{I}} + \int\limits_{-\infty}^{t} G(t-\tau)\underline{\underline{\dot{e}}}(\tau)d\tau,$$

- Kernel $G(\tau)$ is given by:

$$G(\tau) = 2G_\infty + 2(G_0 - G_\infty)\Psi(\tau) \text{ with } \Psi(\tau) = \sum_{i=1}^{n} \psi_i \exp(-\tau/\tau_i)$$

  - $G_\infty, G_0$ are the slow/fast loading shear moduli, respectively, such that $G_\infty \le G_0$;
  - $K$ is the bulk modulus, and for elastomers/polymers $K/G_0 \gg 1$;
  - $\psi_i$ are the influence coefficients, such that $\sum_{i=1}^{n} \psi_i = 1$;
  - $\tau_i$ are the respective relaxation times.

# • Material model: *storage* and loss moduli

- Consider a harmonic (rigid) loading: $\underline{e}(t) = \underline{e}_0 \exp(i\omega t)$
- Split the kernel: $G(t) = 2G_\infty + \tilde{G}(t)$
- Then, the storage modulus (general case):

$$G'(\omega) = 2G_\infty + \omega \int\limits_0^\infty \tilde{G}(\tau)\sin(\omega\tau)\,d\tau$$

- The storage modulus in the framework of the generalized Maxwell model:

$$G'(\omega) = 2G_\infty + 2\omega(G_0 - G_\infty)\sum_{i=1}^{n}\psi_i \int\limits_0^\infty \exp(-\tau/\tau_i)\sin(\omega\tau)\,d\tau$$

$$G'(\omega) = 2G_\infty + 2(G_0 - G_\infty)\sum_{i=1}^{n}\frac{\psi_i\omega^2\tau_i^2}{1+\omega^2\tau_i^2}$$

- Remark:

$$\int \exp(cx)\sin(bx)\,dx = \frac{\exp(cx)}{c^2+b^2}[c\sin(bx) - b\cos(bx)]$$

# • Material model: storage and *loss* moduli

- The loss modulus (general case):

$$G''(\omega) = \omega \int\limits_0^\infty \tilde{G}(\tau)\cos(\omega\tau)\,d\tau$$

- The loss modulus in the framework of the generalized Maxwell model:

$$G''(\omega) = 2\omega(G_0 - G_\infty)\sum_{i=1}^{n}\psi_i \int\limits_0^\infty \exp(-\tau/\tau_i)\cos(\omega\tau)\,d\tau$$

$$G''(\omega) = 2(G_0 - G_\infty)\sum_{i=1}^{n}\frac{\psi_i\omega\tau_i}{1+\omega^2\tau_i^2}.$$

- Remark:

$$\int \exp(cx)\cos(bx)\,dx = \frac{\exp(cx)}{c^2+b^2}[c\cos(bx) + b\sin(bx)]$$

# • Material model: example

- Material parameters: $G_0 = 1.1$ MPa, $G_\infty = 50$ kPa
- Single relaxation time: $\tau_0 = 10^{-7}$ s
- Quasi-incompressible material: $K/G_0 = 10^6 \gg 1$
- Uniaxial (rigid) loading: $\varepsilon_{xx} = A\sin(\omega t)$, $\sigma_{yy} = \sigma_{zz} = 0$, $\varepsilon_{yy} = \varepsilon_{zz} \approx -0.5\varepsilon_{xx}$
- Spherical and deviatoric parts: $\underline{\epsilon} \approx A(1-2\nu)\sin(\omega t)\underline{\boldsymbol{I}}$, $\underline{\boldsymbol{e}} \approx \underline{\boldsymbol{\varepsilon}}$
- Stress-strain relation:

$$\underline{\boldsymbol{\sigma}}(t) = \int\limits_{-\infty}^{t} 2(G_0 - G_\infty)\exp[-(t-\tau)/\tau_0]\underline{\dot{\boldsymbol{e}}}(\tau)d\tau + 2G_\infty\underline{\boldsymbol{e}} + K\underline{\boldsymbol{\epsilon}},$$

- Axial and radial stress components:

$$\sigma_{xx} = 2G_\infty\varepsilon_{xx} + K(\varepsilon_{xx} + 2\varepsilon_{yy}) + \int\limits_{-\infty}^{t} 2(G_0 - G_\infty)\exp[-(t-\tau)/\tau_0]\dot{\varepsilon}_{xx}(\tau)d\tau$$

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$$\sigma_{yy} = 0$$

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$$\sigma_{yy} = 0 = 2G_\infty\varepsilon_{yy} + K(\varepsilon_{xx} + 2\varepsilon_{yy}) + \int\limits_{-\infty}^{t} 2(G_0 - G_\infty)\exp[-(t-\tau)/\tau_0]\dot{\varepsilon}_{yy}(\tau)d\tau$$

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$$\sigma_{yy} = 0 = 2G_\infty\varepsilon_{yy} + K(\varepsilon_{xx} + 2\varepsilon_{yy}) + \int\limits_{-\infty}^{t} 2(G_0 - G_\infty)\exp[-(t-\tau)/\tau_0]\dot{\varepsilon}_{yy}(\tau)d\tau$$

$$\boxed{\sigma_{xx} = 3G_\infty\varepsilon_{xx} + \int\limits_{-\infty}^{t} 3(G_0 - G_\infty)\exp[-(t-\tau)/\tau_0]\dot{\varepsilon}_{xx}(\tau)d\tau}$$

# • Material model: example II

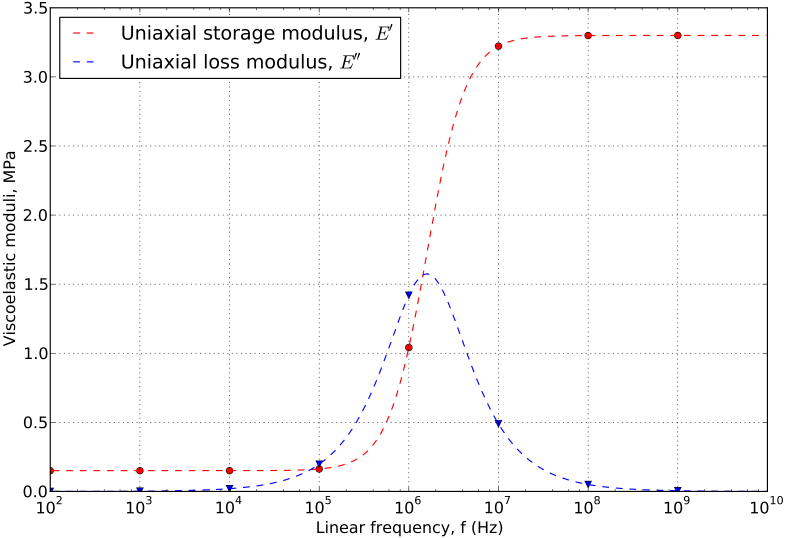
- Uniaxial storage modulus:

$$E'(\omega) = 3G_\infty + 3(G_0 - G_\infty)\frac{\omega^2\tau_0^2}{1+\omega^2\tau_0^2}$$

- Uniaxial loss modulus:

$$E''(\omega) = 3(G_0 - G_\infty)\frac{\omega\tau}{1+\omega^2\tau_0^2}$$

# • Material model: example (FEA vs Analytics)



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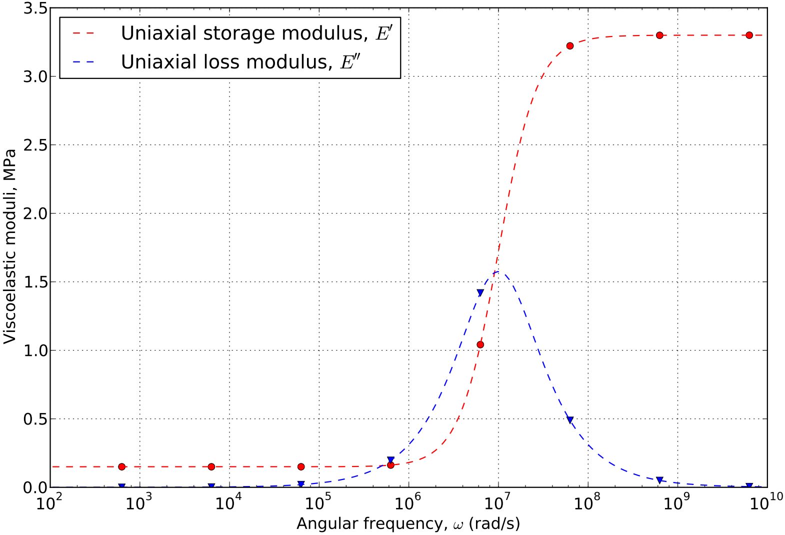

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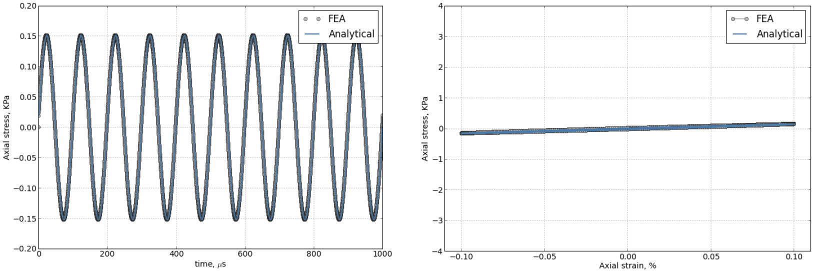
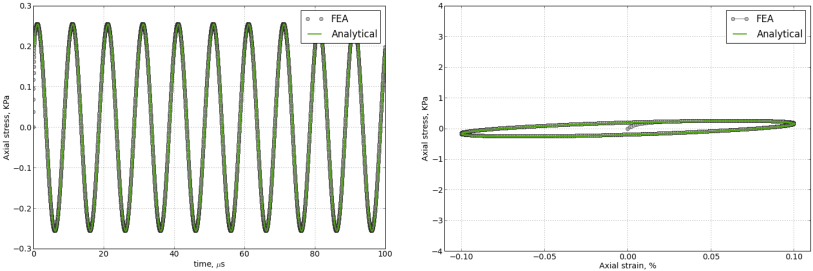


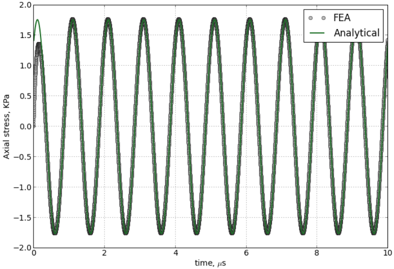

Linear frequency $f = 10^4$ Hz

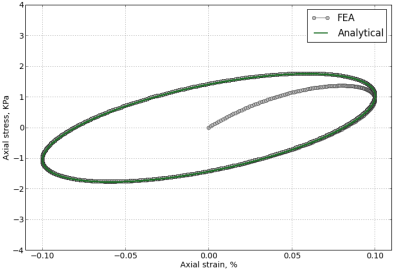
# • Material model: example (FEA vs Analytics)




Linear frequency $f = 10^5$ Hz

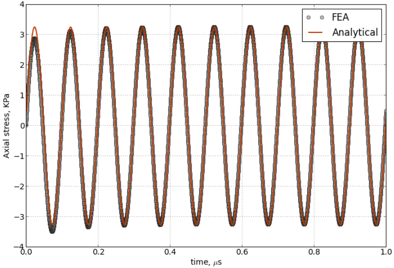
# • Material model: example (FEA vs Analytics)

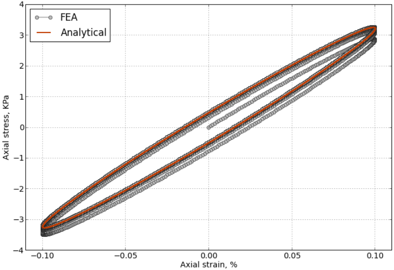



Linear frequency $f = 10^6$ Hz

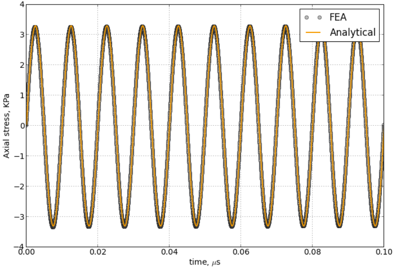
# • Material model: example (FEA vs Analytics)

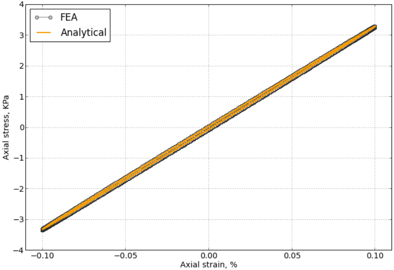



Linear frequency $f = 10^7$ Hz

# • Material model: example (FEA vs Analytics)




Linear frequency $f = 10^8$ Hz

# Numerical integration in time

# Motivation

- One-dimensional Maxwell model

$$\dot{\varepsilon}_d + \frac{\varepsilon_d}{\tau} = \frac{\varepsilon}{\tau}, \quad \varepsilon_d \xrightarrow[t\to-\infty]{} 0$$

- Three-dimensional generalized Maxwell models

$$\dot{\underline{\underline{q}}}_i + \frac{1}{\tau_i}\underline{\underline{q}}_i = \frac{\psi_i}{\tau_i}\frac{\partial W}{\partial \underline{\underline{e}}}, \quad \underline{\underline{q}}_i \xrightarrow[t\to-\infty]{} 0, \quad \sum_{i=1,N}\psi_i = 1 - \psi_\infty$$

- **Problem:** need to know $\underline{\underline{q}}(t^{k+1})$ at time step $t^{k+1}$ if we know it on previous time steps $t^i$ for $i = 0, k$.
- General problem of integration in time or *initial value problem* for the 1st-order linear differential equation (Cauchy problem):

$$\text{find } y(t) \text{ such that satisfies: } \begin{cases} \dot{y} = F(t, y), \\ y(0) = y_0 \end{cases}$$

# Numerical integration in time: explicit vs implicit

**Integration methods for** $\dot{y} = F(t, y) \quad (*)$

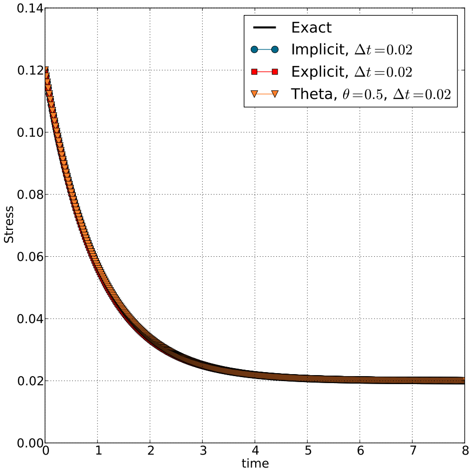
Replace $\dot{y} = \dfrac{y(t+\Delta t) - y(t)}{\Delta t}$

- **Explicit Euler**
  - Rewrite $(*)$ as $\dfrac{y(t+\Delta t) - y(t)}{\Delta t} = F(t, y(t))$
  - Obtain *result* $\boxed{y(t+\Delta t) = y(t) + \Delta t\, F(t, y(t))}$
  - Unstable for high $\Delta t$
- **Implicit Euler**
  - Rewrite $(*)$ as $\dfrac{y(t+\Delta t) - y(t)}{\Delta t} = F(t+\Delta t, y(t+\Delta t))$
  - Obtain *equation* $\boxed{y(t+\Delta t) = y(t) + \Delta t\, F(t+\Delta t, y(t+\Delta t))}$
  - Computationally more expensive
  - Very stable

# Comparison of methods

Relaxation test: apply $\varepsilon(t) = \varepsilon_0 H(t)$ with $H(t) = \begin{cases} 0, & t < 0 \\ 1, & t \geq 0 \end{cases}$

Parameters: $E = 1, E_\infty = 0.2, \tau = 1, t \in (0,8), \varepsilon_0 = 0.1$



# Comparison of methods

Relaxation test: apply $\varepsilon(t) = \varepsilon_0 H(t)$ with $H(t) = \begin{cases} 0, & t < 0 \\ 1, & t \ge 0 \end{cases}$

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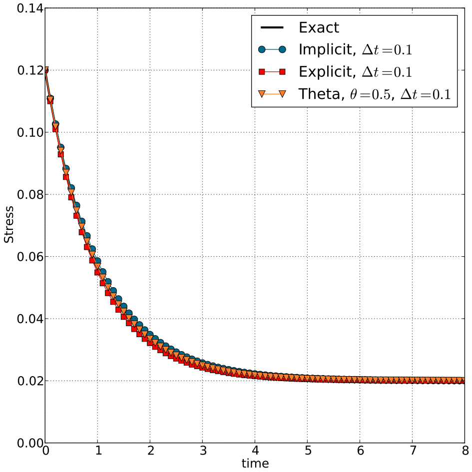

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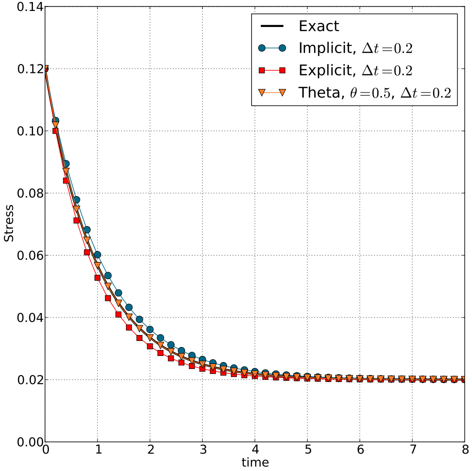

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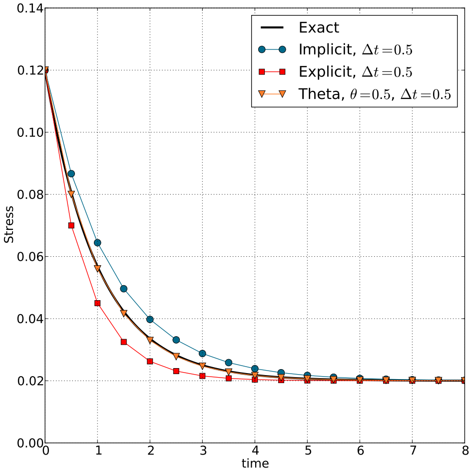

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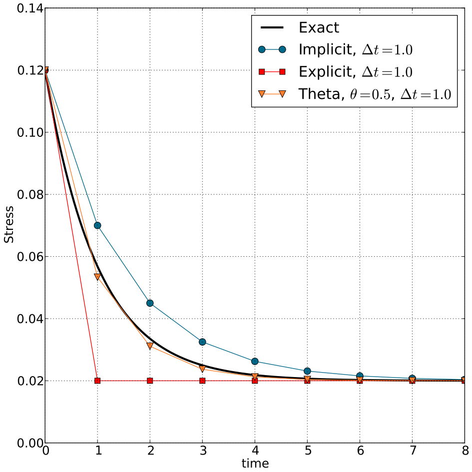

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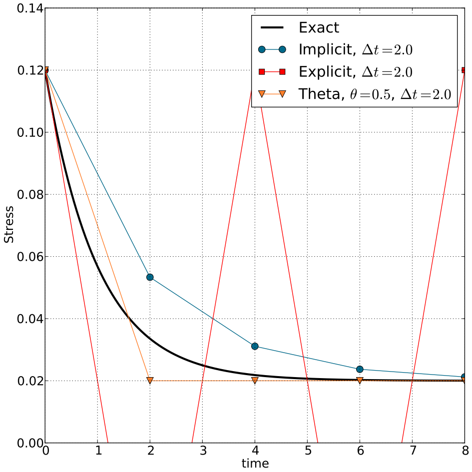

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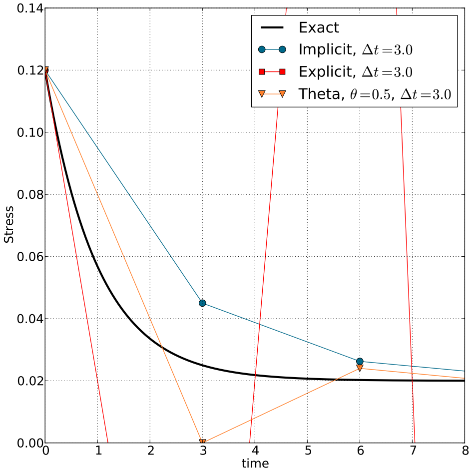


# Numerical integration in time: $\theta$-method

**Integration methods for** $\dot y = F(t,y) \quad (*)$

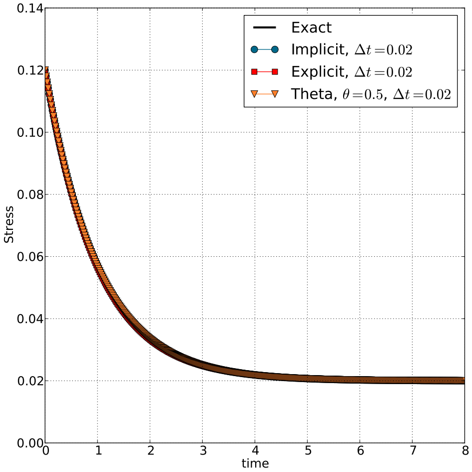
Replace $\dot y = \dfrac{y(t+\Delta t) - y(t)}{\Delta t}$

- Rewrite $(*)$ as $\dfrac{y(t+\Delta t) - y(t)}{\Delta t} = F(t, \theta y(t+\Delta t) + (1-\theta) y(t))$
- Obtain *equation* $\boxed{y(t+\Delta t) = y(t) + \Delta t\, F(t+\Delta t, \theta y(t+\Delta t) + (1-\theta)y(t))}$
- **Remark:**
  - for $\theta = 1$ implicit,
  - for $\theta = 0$ explicit,
  - for $\theta = 0.5$ trapezoidal rule.
- Very stable (yet less than fully implicit method)

# Comparison of methods

Relaxation test: apply $\varepsilon(t) = \varepsilon_0 H(t)$ with $H(t) = \begin{cases} 0, & t < 0 \\ 1, & t \geq 0 \end{cases}$

Parameters: $E = 1, E_\infty = 0.2, \tau = 1, t \in (0, 8), \varepsilon_0 = 0.1$



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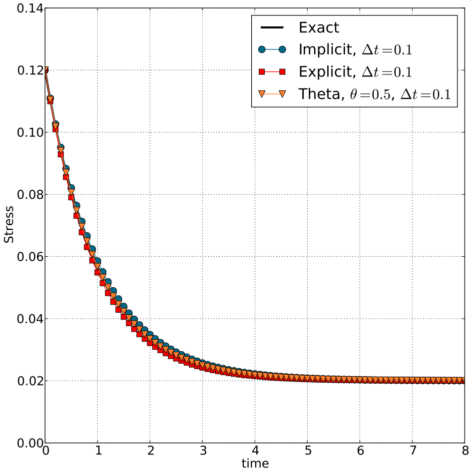

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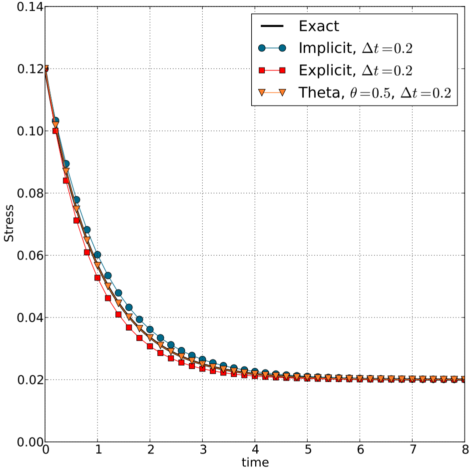

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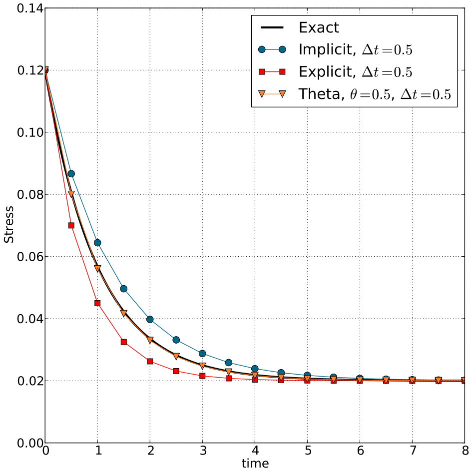

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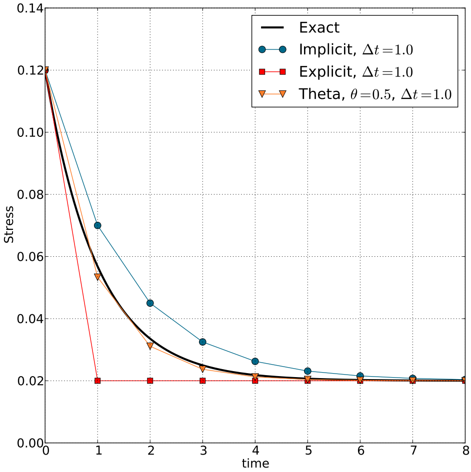

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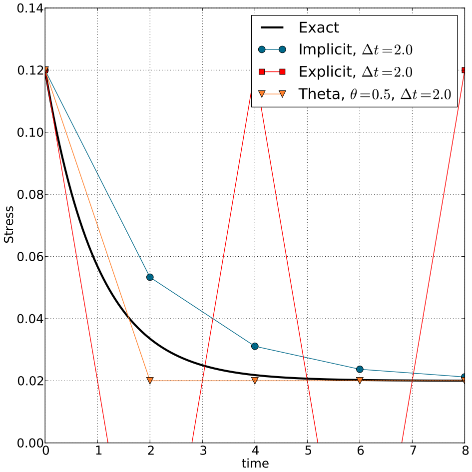

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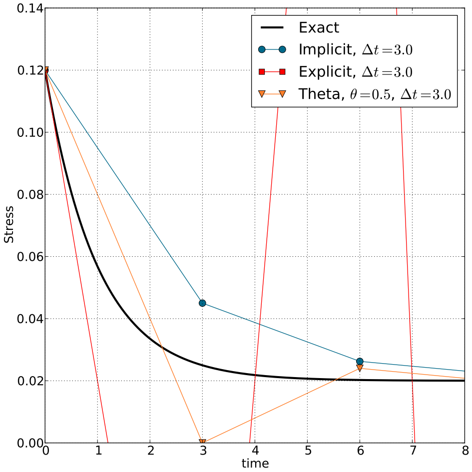


# Numerical integration: explicit Runge-Kutta method

**Integration methods for** $\dot{y} = F(t, y) \quad (*)$

Replace $\dot{y} = \dfrac{y(t+\Delta t) - y(t)}{\Delta t}$

- Rewrite $(*)$ as $y(t+\Delta t) = y(t) + \Delta t \sum\limits_{i=1}^{S} b_i k_i$
- Where

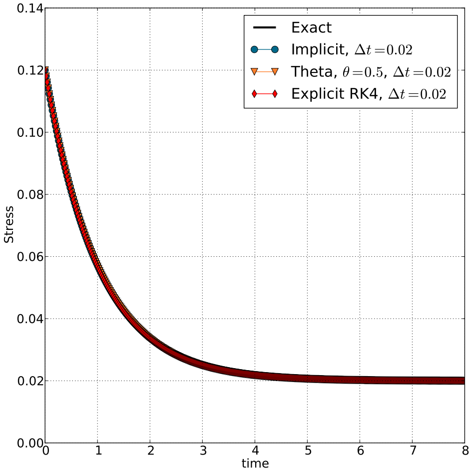
  $$k_1 = F(t,\ y(t))$$
  $$k_2 = F\left(t + c_2 \Delta t,\ y(t) + \Delta t (a_{21} k_1)\right)$$
  $$\ldots$$
  $$k_i = F\left(t + c_i \Delta t,\ y(t) + \Delta t \sum_{j=1}^{i-1} a_{ij} k_j\right)$$
- Coefficients $b_i, c_i, a_{ij}$ are tabulated for differen orders $S$
- For Runge-Kutta 4:

  $$b_1 = b_4 = 1/6, \quad b_2 = b_3 = 1/3$$
  $$c_2 = c_3 = 1/2, \quad c_4 = 1$$
  $$a_{21} = 1/2, \quad a_{31} = 0, \quad a_{32} = 1/2, \quad a_{41} = a_{42} = 0, \quad a_{43} = 1$$

# Comparison of methods

Relaxation test: apply $\varepsilon(t) = \varepsilon_0 H(t)$ with $H(t) = \begin{cases} 0, & t < 0 \\ 1, & t \geq 0 \end{cases}$

Parameters: $E = 1, E_\infty = 0.2, \tau = 1, t \in (0, 8), \varepsilon_0 = 0.1$



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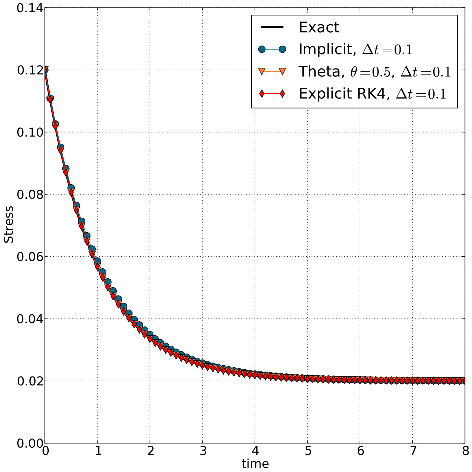

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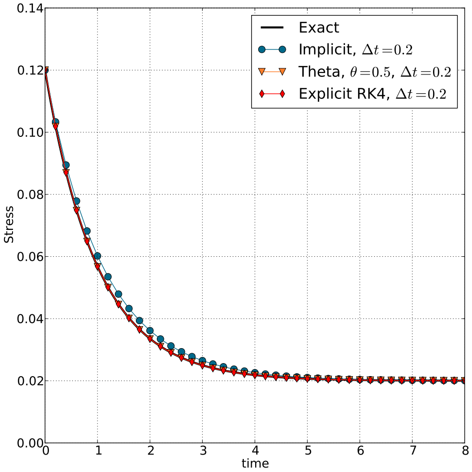

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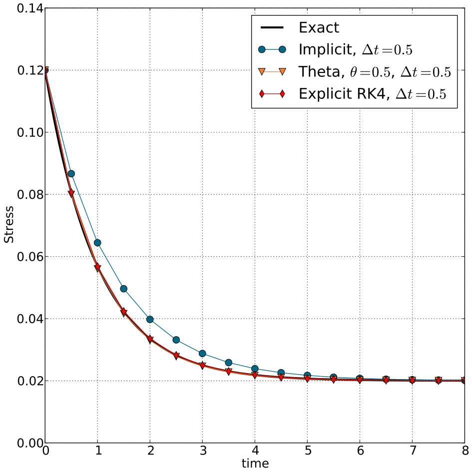

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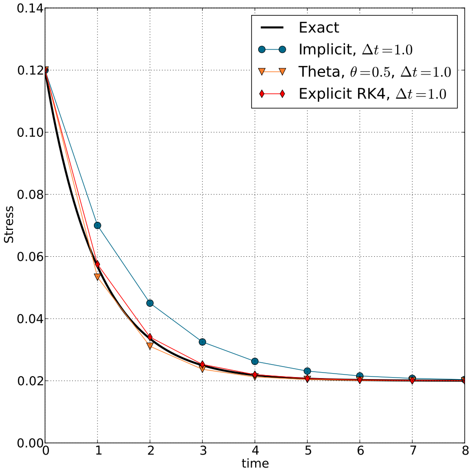

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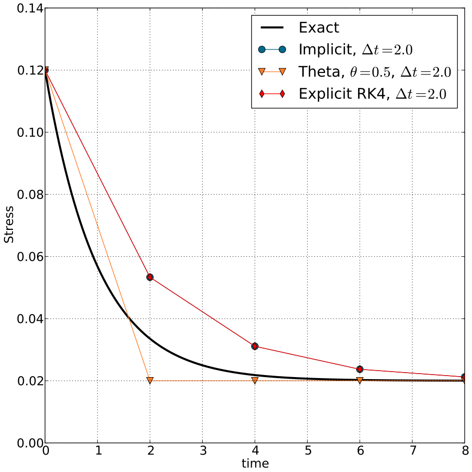

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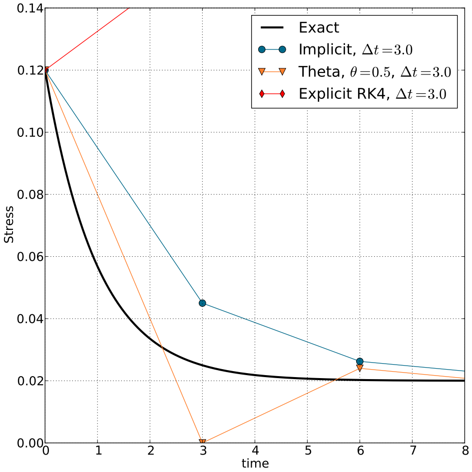


# Numerical integration: summary

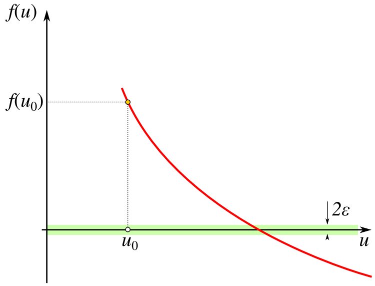
**List of integration methods**

- Theta-method ($0 < \theta < 1$)
- Implicit method ($\theta = 1$)
- Runge-Kutta method (RK4)
- **Remark:** explicit Euler method is rarely used.

# Non-linear finite element method

# Newton-Raphson method: how it works I

- Consider a problem: find $u$ such that $f(u) = 0$
- Start with an initial guess: $u = u_0$
  - Iteration $i$
  - Taylor expansion
    $f(u_i + \Delta u_i) \approx$
    $$f(u_i) + \left.\frac{\partial f}{\partial u}\right|_{u_i} \Delta u_i = 0$$
  - Increment
    $$\Delta u_i = -\left(\left.\frac{\partial f}{\partial u}\right|_{u_i}\right)^{-1} f(u_i)$$
  - Update $u_{i+1} = u_i + \Delta u_i$
  - Check convergence: if $\left|f(u_{i+1})\right| < \varepsilon$, then exit.



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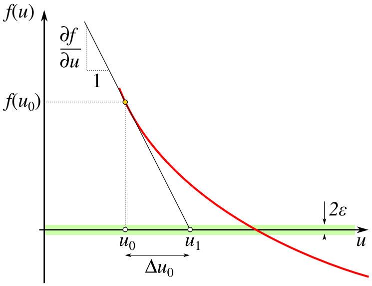

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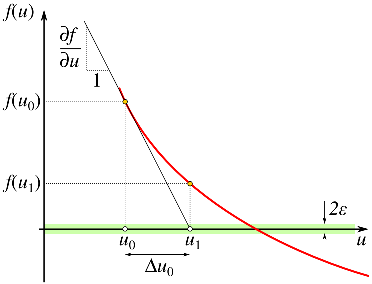

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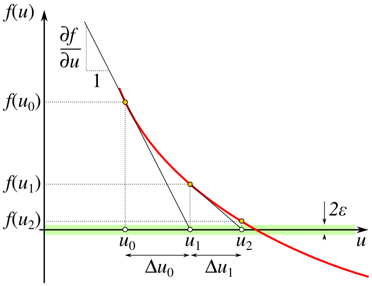

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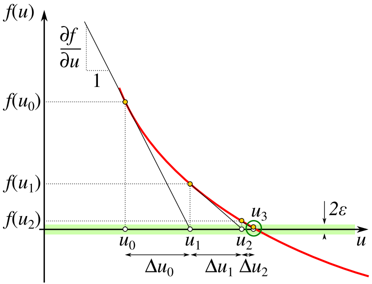

# Modified Newton-Raphson method

- Consider a problem: find $u$ such that $f(u) = 0$
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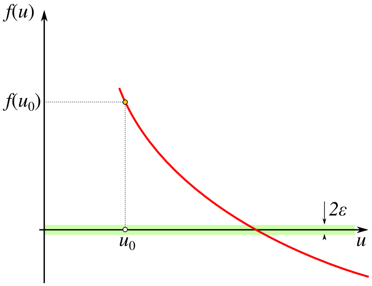
  - Update $u_{i+1} = u_i + \Delta u_i$
  - Check convergence: if $\left| f(u_{i+1}) \right| < \varepsilon$, then exit.
  - **Remark:** The tangent is computed only once



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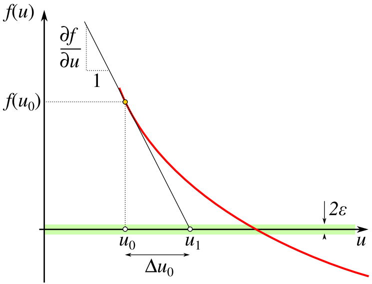

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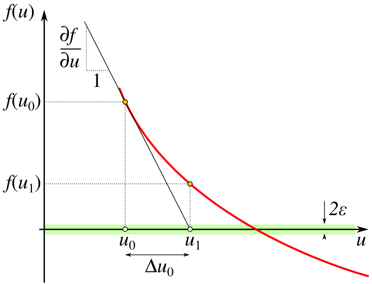

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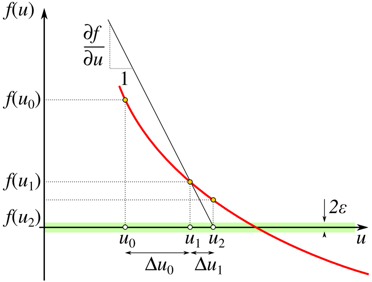

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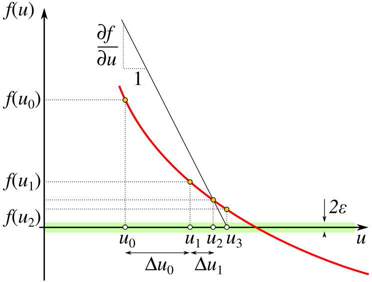

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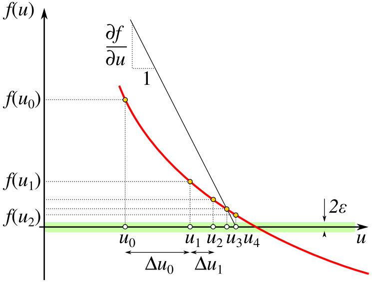
    $$\Delta u_i = -\left(\left.\frac{\partial f}{\partial u}\right|_{u_0}\right)^{-1} f(u_i)$$
  - Update $u_{i+1} = u_i + \Delta u_i$
  - Check convergence: if $\left|f(u_{i+1})\right| < \varepsilon$, then exit.
  - **Remark:** The tangent is computed only once



# Newton-Raphson method: how it works II

- Consider a system of non-linear equations $[\mathbf{f}([\mathbf{u}])] = 0$. Find vector $[\mathbf{u}]$.
- Start with an initial guess: $[\mathbf{u}] = [\mathbf{u}_0]$
  - Iteration $i$
  - Taylor expansion $[f([\mathbf{u}_\mathrm{i}] + \Delta[\mathbf{u}_\mathrm{i}])] \approx [\mathbf{f}([\mathbf{u}_\mathrm{i}])] + \left.\frac{\partial[\mathbf{f}]}{\partial[\mathbf{u}]}\right|_{[\mathbf{u}_\mathrm{i}]} \Delta[\mathbf{u}_\mathrm{i}] = 0$
  - System of linear equations: $\underbrace{\left[\left.\frac{\partial[\mathbf{f}]}{\partial[\mathbf{u}]}\right|_{[\mathbf{u}_\mathrm{i}]}\right]}_{\text{matrix }[\mathbf{K}]} \Delta[\mathbf{u}_\mathrm{i}] = -[\mathbf{f}([\mathbf{u}_\mathrm{i}])]$
  - Update $[\mathbf{u}_{\mathrm{i+1}}] = [\mathbf{u}_\mathrm{i}] + \Delta[\mathbf{u}_\mathrm{i}]$
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  - Update $[\mathbf{u_{i+1}}] = [\mathbf{u_i}] + \Delta[\mathbf{u_i}]$
  - Check convergence: if $\left\| f(u_{i+1}) \right\| < \varepsilon$, then exit.
  - **Example:** $\begin{bmatrix} f_1(x,y) \\ f_2(x,y) \end{bmatrix} = 0$, tangent matrix $[\mathbf{K}] = \begin{bmatrix} \frac{\partial f_1}{\partial x} & \frac{\partial f_1}{\partial y} \\ \frac{\partial f_2}{\partial x} & \frac{\partial f_2}{\partial y} \end{bmatrix}$
  - Start with $x_0, y_0$, giving the first increment
    $\begin{bmatrix} \Delta x_0 \\ \Delta y_0 \end{bmatrix} = -\left( [\mathbf{K}]\Big|_{x_0,y_0} \right)^{-1} \begin{bmatrix} f_1(x_0,y_0) \\ f_2(x_0,y_0) \end{bmatrix}$

# Newton-Raphson method: some theory

- To ensure quadratic convergence of the Newton-Raphson for any initial guess $u_0 \in \{\mathcal{I} \mid \forall u : |u - u_*| < \epsilon\}$, we require that

$$(1) \quad \forall u \in \mathcal{I} : \quad f(u) = f(u_*) + f'(u_*)(u-u_*) + \frac{1}{2} f''(u_*)(u-u_*)^2 + o((u-u_*)^3),$$

i.e. $f$ is well approximated by the truncated Taylor expansion everywhere in $\mathcal{I}$.

$$(2) \quad \forall u \in \mathcal{I} : \quad f \in C^2, \text{ i.e. second derivative is continuous.}$$

$$(3) \quad \forall u \in \mathcal{I} : \quad f'(u) \neq 0$$

$$(4) \quad \exists C < \infty, \forall u \in \mathcal{I} : \quad \left|\frac{f''(u)}{f'(u)}\right| < C \left|\frac{f''(u_*)}{f'(u_*)}\right|$$

$$(5) \quad C \left|\frac{f''(u_*)}{f'(u_*)}\right| < \frac{1}{2\epsilon}$$

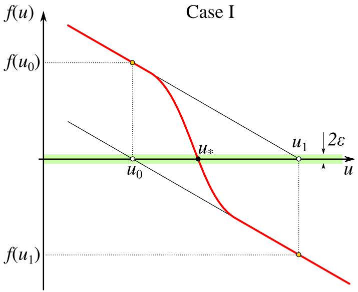
- **Remark:** normally in FEM we do not compute $f''$, so it is sometimes difficult to justify the convergence.

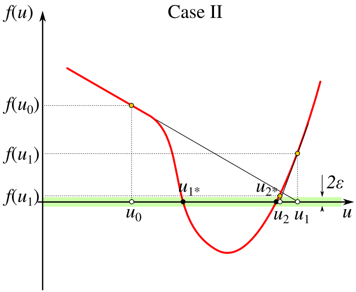
---

Where $f'(u_*) = \left.\frac{\partial f}{\partial u}\right|_{u=u_*}, f''(u_*) = \left.\frac{\partial^2 f}{\partial u^2}\right|_{u=u_*}$

# Newton-Raphson method: warning

- Cases which do not ensure convergence
- Case I: function $f$ is not well approximated in $\mathcal{I}$ by the three terms of Taylor expansion
- Case II: function has $\exists u \in \mathcal{I} \,:\, f'(u) = 0$



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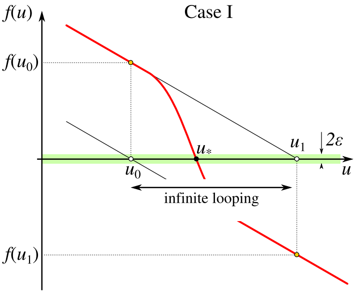
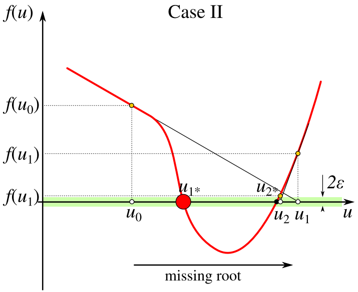
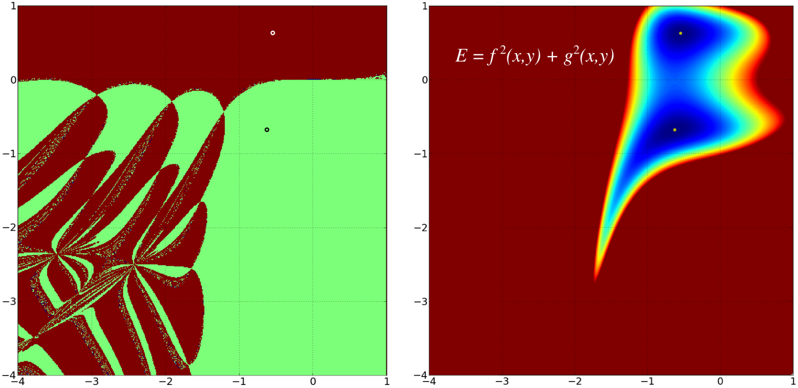


- Search for $x, y$ which solve $f(x,y) = x^3 + 2(x+2)y^2 - 1$, $g(x,y) = x^3 y + 2(x - y^2) + 2$
- Roots $\{-0.6286, -0.6746\}, \{-0.5474, 0.6330\}$
- Basins of attraction of these roots for different initial guess $x_0, y_0$



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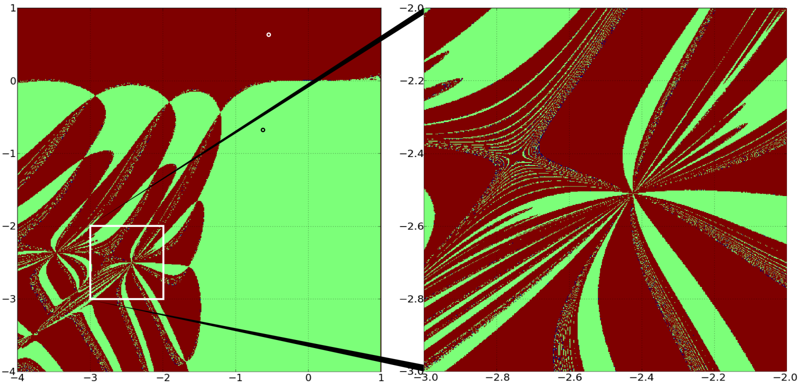

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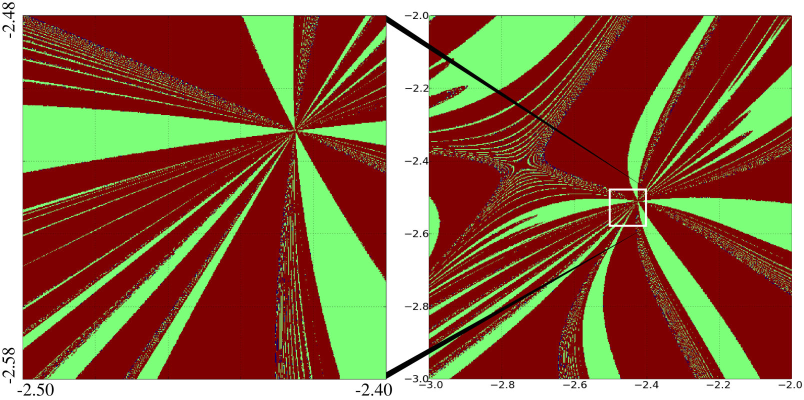

# Nonlinear weak form

- Let $\underline{\underline{\sigma}}$ be a non-linear function of strain, and $\underline{t}_0$ be a function of time

$$\int\limits_{\Omega} \underline{\underline{\sigma}}(\underline{\underline{\varepsilon}}) : \delta\underline{\underline{\varepsilon}}\, dV = \int\limits_{\Gamma_f} \underline{t}_0(t) \cdot \delta\underline{u}\, dS + \int\limits_{\Omega} \underline{f}_V \cdot \delta\underline{u}\, dV$$

- The equation (non-linear) to solve:

$$R(\underline{u}, t) = \int\limits_{\Omega} \underline{\underline{\sigma}}(\underline{\underline{\varepsilon}}) : \delta\underline{\underline{\varepsilon}}\, dV - \int\limits_{\Gamma_f} \underline{t}_0(t) \cdot \delta\underline{u}\, dS - \int\limits_{\Omega} \underline{f}_V \cdot \delta\underline{u}\, dV = 0$$

- Denote: $\underline{u}(t + \Delta t) = \underline{u}^{k+1}$
- Problem: find such field $u^{k+1}$ so that $R(\underline{u}^{k+1}, t^{k+1}) = 0$

# Newton-Raphson method: Step 1

- Initial guess: $\underline{u}^{k+1} = \underline{u}^k + \Delta\underline{u}_0$ with unknown $\Delta\underline{u}_0$
- Find such field $\Delta\underline{u}$ so that $R(\underline{u}^k + \Delta\underline{u}_0, t^{k+1}) = 0$
- Taylor expansion (zero-th iteration):

$$R(\underline{u}^k + \Delta\underline{u}_0, t^{k+1}) = \boxed{0 = R(\underline{u}^k, t^{k+1}) + \left.\frac{\partial R}{\partial \underline{u}}\right|_{u^k, t^{k+1}} \Delta\underline{u}_0} + o(\Delta\underline{u}_0^2)$$

$$R(\underline{u}^k, t^{k+1}) = \int\limits_{\Omega} \underline{\underline{\sigma}}(\underline{\underline{\varepsilon}}^k) : \delta\underline{\underline{\varepsilon}}\, dV - \int\limits_{\Gamma_f} \underline{t}_0(t^{k+1}) \cdot \delta\underline{u}\, dS - \int\limits_{\Omega} \underline{f}_V \cdot \delta\underline{u}\, dV$$

$$\left.\frac{\partial R}{\partial \underline{u}}\right|_{u^k, t^{k+1}} = \int\limits_{\Omega} \frac{\partial \underline{\underline{\sigma}}(\underline{\underline{\varepsilon}}^k)}{\partial \underline{u}} : \delta\underline{\underline{\varepsilon}}\, dV$$

- Solve boxed linear problem for $\Delta\underline{u}_0$ and update $\underline{u}_1^{k+1} = \underline{u}^k + \Delta\underline{u}_0$
- Construct new problem for $\underline{u}^{k+1} = \underline{u}_1^{k+1} + \Delta\underline{u}_1$, find $\Delta\underline{u}_1$, etc.

# Newton-Raphson method: Step 2

- New guess: $\underline{u}^{k+1} = \underline{u}^k + \Delta\underline{u}_0 + \Delta\underline{u}_1 = \underline{u}_1^k + \Delta\underline{u}_1$ with unknown $\Delta\underline{u}_1$
- Find such field $\Delta\underline{u}$ so that $R(\underline{u}_1^k + \Delta\underline{u}_1, t^{k+1}) = 0$
- Taylor expansion (zero-th iteration):

$$R(\underline{u}_1^k + \Delta\underline{u}_1, t^{k+1}) = \boxed{0 = R(\underline{u}_1^k, t^{k+1}) + \left.\frac{\partial R}{\partial \underline{u}}\right|_{u_1^k, t^{k+1}} \cdot \Delta\underline{u}_1} + o(\Delta\underline{u}_1^2)$$

$$R(\underline{u}_1^k, t^{k+1}) = \int\limits_\Omega \underline{\underline{\sigma}}(\underline{\underline{\varepsilon}}_1^k) : \delta\underline{\underline{\varepsilon}}\, dV - \int\limits_{\Gamma_f} \underline{t}_0(t^{k+1}) \cdot \delta\underline{u}\, dS - \int\limits_\Omega \underline{f}_V \cdot \delta\underline{u}\, dV$$

$$\left.\frac{\partial R}{\partial \underline{u}}\right|_{u_1^k, t^{k+1}} = \int\limits_\Omega \frac{\partial \underline{\underline{\sigma}}(\underline{\underline{\varepsilon}}_1^k)}{\partial \underline{u}} : \delta\underline{\underline{\varepsilon}}\, dV$$

- Solve boxed linear problem for $\Delta\underline{u}_1$ and update $\underline{u}_2^{k+1} = \underline{u}_1^k + \Delta\underline{u}_1$
- Construct new problem for $\underline{u}^{k+1} = \underline{u}_2^{k+1} + \Delta\underline{u}_1$, find $\Delta\underline{u}_2$, etc.

# Newton-Raphson method: Step 2

- New guess: $\underline{u}^{k+1} = \underline{u}^k + \Delta\underline{u}_0 + \Delta\underline{u}_1 = \underline{u}^k_1 + \Delta\underline{u}_1$ with unknown $\Delta\underline{u}_1$
- Find such field $\Delta\underline{u}$ so that $R(\underline{u}^k_1 + \Delta\underline{u}_1, t^{k+1}) = 0$
- Taylor expansion (zero-th iteration):

$$R(\underline{u}^k_1 + \Delta\underline{u}_1, t^{k+1}) = \boxed{0 = R(\underline{u}^k_1, t^{k+1}) + \left.\frac{\partial R}{\partial \underline{u}}\right|_{u^k_1, t^{k+1}} \cdot \Delta\underline{u}_1} + o(\Delta\underline{u}^2_1)$$

$$R(\underline{u}^k_1, t^{k+1}) = \int\limits_{\Omega} \underline{\underline{\sigma}}(\underline{\underline{\varepsilon}}^k_1) : \delta\underline{\underline{\varepsilon}}\, dV - \int\limits_{\Gamma_f} \underline{t}_0(t^{k+1}) \cdot \delta\underline{u}\, dS - \int\limits_{\Omega} \underline{f}_V \cdot \delta\underline{u}\, dV$$

$$\left.\frac{\partial R}{\partial \underline{u}}\right|_{u^k_1, t^{k+1}} = \int\limits_{\Omega} \frac{\partial \underline{\underline{\sigma}}(\underline{\underline{\varepsilon}}^k_1)}{\partial \underline{u}} : \delta\underline{\underline{\varepsilon}}\, dV$$

- Solve boxed linear problem for $\Delta\underline{u}_1$ and update $\underline{u}^{k+1}_2 = \underline{u}^k_1 + \Delta\underline{u}_1$
- Construct new problem for $\underline{u}^{k+1} = \underline{u}^{k+1}_2 + \Delta\underline{u}_1$, find $\Delta\underline{u}_2$, etc.
- And so on until convergence.

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$$\boxed{\left.\frac{\partial R}{\partial \underline{u}}\right|_{u^k_1, t^{k+1}} = \int\limits_\Omega \frac{\partial \underline{\underline{\sigma}}(\underline{\underline{\varepsilon}}^k_1)}{\partial \underline{u}} : \delta\underline{\underline{\varepsilon}}\, dV} \qquad (**)$$

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- And so on until convergence.

# Newton-Raphson method: residual vector

- Continuum residual:

$$R(\underline{u}_i^k, t^{k+1}) = \int\limits_{\Omega} \underline{\underline{\sigma}}(\underline{\underline{\varepsilon}}_i^k) : \delta\underline{\underline{\varepsilon}}\, dV - \int\limits_{\Gamma_f} \underline{t}_0(t^{k+1}) \cdot \delta\underline{u}\, dS - \int\limits_{\Omega} \underline{f}_V \cdot \delta\underline{u}\, dV \quad (*)$$

- Discretized residual:

$$R^h(\underline{u}_i^k, t^{k+1}) = \left( \sum_e \int\limits_{\Omega^e} \left\{ [\mathbf{S}([\mathbf{E_i^k}])][\mathbf{B}]^\intercal - \underbrace{[\mathbf{f_V}]^\intercal [\mathbf{N}]^\intercal}_{(\star)} \right\} \det[\,\mathbf{J}\,]\, d\xi d\eta - \underbrace{\int\limits_{\Gamma_f} [\mathbf{t_0}(t^{k+1})]^\intercal [\mathbf{N}]^\intercal\, dS}_{(\star\star)} \right) \delta[\mathbf{u}]$$

- Finally $R^h(\underline{u}_i^k, t^{k+1}) = [\mathbf{R}]^\intercal \delta[\mathbf{u}]$
- Assume that convergence is met if $\|\,[\mathbf{R}]\,\|_{\max} < \epsilon \,\|\,[\mathbf{t_0}]\,\|_{\max}$, where $\|\,[\mathbf{R}]\,\|_{\max} = \max\limits_i(|R_i|)$
- Terms $(\star)$ and $(\star\star)$ do not depend on $\underline{u}_i^k$ thus should be evaluated only once per load step
- If $\underline{f}_V$ and the mesh do not change during the simulation $(\star)$ should be evaluated only once at the first load step

# Newton-Raphson method: tangent stiffness matrix

- Continuum tangent:

$$\frac{\partial R}{\partial \underline{u}}\bigg|_{u_i^k, t^{k+1}} = \int_\Omega \frac{\partial \underline{\underline{\sigma}}(\underline{\underline{\varepsilon}}_i^k)}{\partial \underline{u}} : \delta \underline{\underline{\varepsilon}}\, dV = \int_\Omega \frac{\partial \underline{\underline{\varepsilon}}}{\partial \underline{u}} : \frac{\partial \underline{\underline{\sigma}}(\underline{\underline{\varepsilon}}_i^k)}{\partial \underline{\underline{\varepsilon}}} : \frac{\partial \underline{\underline{\varepsilon}}}{\partial \underline{u}} \cdot \delta \underline{u}\, dV \quad (**)$$

- Discretized tangent stiffness matrix:

$$[\mathbf{K}]\,(\underline{u}_i^k, t^{k+1}) = \sum_e \int_{\Omega^e} [\mathbf{B}]\,[\mathbf{D_T}]\,[\mathbf{B}]^\intercal \det[\,\mathbf{J}\,]\, d\xi d\eta$$

- Where $[\mathbf{D_T}] = \frac{\partial [\mathbf{S}]}{\partial [\mathbf{E}]}\bigg|_{u_i^k} \sim \frac{\partial \underline{\underline{\sigma}}(\underline{\underline{\varepsilon}}_i^k)}{\partial \underline{\underline{\varepsilon}}}$ is the tangent modulus (Voigt notations)
- **Remark I:** In case of linear elasticity $[\mathbf{D_T}] = [\mathbf{D}]$ is the elasticity tensor and we recover the linear FEM formulation
- **Remark II:** If there exists a stored-energy potential $W$ then $[\mathbf{D_T}] \sim \frac{\partial^2 W}{\partial \underline{\underline{\varepsilon}}^2}$:

  for example, for linear elasticity $W = \frac{1}{2}\,\underline{\underline{\varepsilon}} : {}^4\underline{\underline{C}} : \underline{\underline{\varepsilon}}$

# Newton-Raphson method: summary

- At every iteration $i$ we compute a linear system of equations:

$$[\mathbf{K_i}]\,\Delta[\mathbf{u_{i+1}}] = [\mathbf{R_i}]$$

  matrix $[\mathbf{K_i}]$ and residual $[\mathbf{R_i}]$ are computed in configuration determined by $[\mathbf{u_i}]$
- Displacement vector is updated $[\mathbf{u_{i+1}}] = [\mathbf{u_i}] + \Delta[\mathbf{u_{i+1}}]$
- The linear system is computed again with newly computed residual $[\mathbf{R_{i+1}}]$ and newly computed tangent stiffness matrix[1] $[\mathbf{K_{i+1}}]$

$$[\mathbf{K_{i+1}}]\,\Delta[\mathbf{u_{i+2}}] = [\mathbf{R_{i+1}}]$$

- And so on until convergence

[1] *If the full Newton-Raphson method is used, otherwise the tangent operator is computed only once on the first iteration (or on a few first iterations).*

# Example: elastic material

- Decomposition of stress and strain tensors into deviatoric ( $\underline{\underline{s}}, \underline{\underline{e}}$ ) and spherical parts:

$$\underline{\underline{\sigma}} = \underline{\underline{s}} - p\underline{\underline{I}}, \quad \underline{\underline{\varepsilon}} = \underline{\underline{e}} + \frac{1}{3}\theta\underline{\underline{I}}, \qquad \theta = \mathrm{tr}(\underline{\underline{\varepsilon}})$$

- Linear isotropic elasticity: $\underline{\underline{\sigma}} = K_0\theta\underline{\underline{I}} + 2G_0\underline{\underline{e}}$
- Tangent operator:

$$^4\underline{\underline{D}}_T = \frac{\partial\underline{\underline{\sigma}}}{\partial\underline{\underline{\varepsilon}}} = \frac{\partial\underline{\underline{\sigma}}}{\partial\theta} \otimes \frac{\partial\theta}{\partial\underline{\underline{\varepsilon}}} + \frac{\partial\underline{\underline{\sigma}}}{\partial\underline{\underline{e}}} : \frac{\partial\underline{\underline{e}}}{\partial\underline{\underline{\varepsilon}}}$$

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$$^4\underline{\underline{D}}_T = K_0\underline{\underline{I}} \otimes \underline{\underline{I}} + 2G_0\left({}^4\underline{\underline{I}} - \frac{1}{3}\underline{\underline{I}} \otimes \underline{\underline{I}}\right)$$

# Example: viscoelastic material

- 3D viscoelastic formulation

$$\underline{\underline{\sigma}} = K\theta \underline{\underline{I}} + 2G_0 \underline{\underline{e}} - \sum_{i=1,N} \underline{\underline{q}}_i$$

$$(*) \qquad \dot{\underline{\underline{q}}}_i + \frac{1}{\tau_i}\underline{\underline{q}}_i = 2G_0 \frac{\psi_i}{\tau_i}\underline{\underline{e}} \quad , \quad \underline{\underline{q}}_i \xrightarrow[t\to-\infty]{} 0, \quad \sum_{i=1,N} \psi_i = 1 - \psi_\infty$$

- Deviatoric part of the tangent operator:

$$\frac{\partial \underline{\underline{s}}}{\partial \underline{\underline{\varepsilon}}} = \frac{\partial \underline{\underline{s}}}{\partial \underline{\underline{e}}} : \left({}^4\underline{\underline{I}} - \frac{1}{3}\underline{\underline{I}} \otimes \underline{\underline{I}}\right) = \left(\frac{\partial \underline{\underline{s}}}{\partial \underline{\underline{e}}} + \sum_i \frac{\partial \underline{\underline{s}}}{\partial \underline{\underline{q}}_i} : \frac{\partial \underline{\underline{q}}_i}{\partial \underline{\underline{e}}}\right) : \left({}^4\underline{\underline{I}} - \frac{1}{3}\underline{\underline{I}} \otimes \underline{\underline{I}}\right)$$

- Use theta-rule to obtain $\partial \underline{\underline{q}}_i / \partial \underline{\underline{e}}$:

$$\underline{\underline{q}}_i(t+\Delta t) = \frac{1}{1 + \frac{\Delta t \theta}{\tau_i}} \left\{ \underline{\underline{q}}_i(t)\left(1 - (1-\theta)\frac{\Delta t}{\tau_i}\right) + \frac{2G_0\psi_i\Delta t}{\tau_i}\left[\theta \underline{\underline{e}}(t+\Delta t) + (1-\theta)\underline{\underline{e}}(t)\right]\right\}$$

$$\frac{\partial \underline{\underline{q}}_i}{\partial \underline{\underline{e}}} = \frac{2G_0\theta\psi_i\Delta t}{\tau_i + \theta\Delta t}\;{}^4\underline{\underline{I}}$$

# Example: viscoelastic material II

- Finally the deviatoric part turns:

$$\frac{\partial \underline{\underline{s}}}{\partial \underline{\underline{\varepsilon}}} = 2G_0 \left( 1 - \theta \Delta t \sum_i \frac{\psi_i}{\tau_i + \theta \Delta t} \right) : \left( {}^4\underline{\underline{I}} - \frac{1}{3} \underline{\underline{I}} \otimes \underline{\underline{I}} \right)$$

- The full tangent operator:

$${}^4\underline{\underline{D}}_T = \frac{\partial \underline{\underline{\sigma}}}{\partial \underline{\underline{\varepsilon}}} = K_0 \underline{\underline{I}} \otimes \underline{\underline{I}} + 2G_0 \left( 1 - \theta \Delta t \sum_i \frac{\psi_i}{\tau_i + \theta \Delta t} \right) \left( {}^4\underline{\underline{I}} - \frac{1}{3} \underline{\underline{I}} \otimes \underline{\underline{I}} \right)$$

- **Remark:** it does not depend on strain or stress, thus the Newton-Raphson procedure convergens in one iteration.

# Thank you for your attention!