Reliable Simulation Techniques in Solid Mechanics
Development of Non-standard Discretization Methods, Mechanical and Mathematical Analysis

J. Schröder, N. Viebahn & M. Igelbücher

Challenges in discretization techniques in solid mechanics
Novel mixed Finite-Elements for the large deformation framework
Least-Squares FEM - a unifying discretization technique?
A novel Kirchhoff-Love shell formulation
Challenges in Discretization Techniques in Solid Mechanics

Displacements based low order Finite Element formulations tend to behave suspiciously stiff in various situations (e.g. incompressibility, bending dominated problems, anisotropy, thin structures).

.. and their stress approximation suffers due to oscillations, especially in the incompressible regime.

Non-standard discretization methods may improve the results tremendously.
Kinematics; Deformation and Stress Measures

Deformation gradient

\[ F(X) := \text{Grad}\varphi_t(X) = \text{Grad}x \]

Right & left Cauchy-Green tensor; Green-Lagrange strain tensor

\[ C := F^T F ; \quad b = FF^T ; \quad E := \frac{1}{2}(C - 1) ; \quad \text{Lin}[E] =: \varepsilon \]

Piola transformation (\(\sigma\) - Cauchy stresses, \(P\) - 1\(^{\text{st}}\) Piola-Kirchhoff stresses)

\[ t\ da = t_0\ dA : \quad \sigma n\ da = \sigma\ \text{Cof}F\ dA = P\ dA \rightarrow P = \sigma\ \text{Cof}F = J\sigma F^{-T} \]

Kirchhoff stress tensor \(\tau = J\sigma\), 2\(^{\text{nd}}\) Piola-Kirchhoff stresses \(S := F^{-1}P\)
Some keystones in Mixed FEM for Solid Mechanics

Reissner [1950]
On a variational theorem in elasticity

Washizu [1955]
On the variational principles in elasticity

Veubeke [1965]
Displacement and equilibrium models

Zienkiewicz et al. [1971]
Reduced integration technique in general analysis of

Babuška [1973]
The FEM with Lagrangian Multipliers

Wilson [1973]
Incompatible Displacement Models

Nagtegaal et al. [1974]
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Brezzi [1974]
On the existence, uniqueness and ...

Simo & Rifai [1990]
A class of mixed assumed strain methods and ...

Pantuso & Bathe [1995]
A four-node quadrilateral mixed-interpolated element...

Wriggers & Reese [1996]
A note on enhanced strain methods for large deformations

Korelc et al. [2010]
An improved EAS brick element for finite deformations

Schröder et al. [2011]
A new mixed finite element based on different approximations of the...

Auricchio et al. [2013]
Approximation of incompressible large deformation elastic ...

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Mixed FEM in Solid Mechanics - a brief introduction

The terminus **Mixed** is used when different fields are introduced independently.

**„Classical“** problem of Linear Elasticity:

Find $\mathbf{u}$ such that: $\operatorname{Div}[\mathbf{C} : \nabla^s \mathbf{u}] + \mathbf{f} = 0$ on $\mathcal{B}$

**Mixed** two field problem of Linear Elasticity:

Find $(\sigma, \mathbf{u})$ such that:

\[
\begin{aligned}
\operatorname{Div} \sigma + \mathbf{f} &= 0 \quad \text{on } \mathcal{B} \\
\mathbf{C}^{-1} : \sigma &= \nabla^s \mathbf{u} \quad \text{on } \mathcal{B}
\end{aligned}
\]

**Mixed** three field problem of Linear Elasticity:

Find $(\varepsilon, \mathbf{u}, \sigma)$ such that:

\[
\begin{aligned}
\operatorname{Div} \sigma + \mathbf{f} &= 0 \quad \text{on } \mathcal{B} \\
\sigma &= \mathbf{C} : \varepsilon \quad \text{on } \mathcal{B} \\
\varepsilon &= \nabla^s \mathbf{u} \quad \text{on } \mathcal{B}
\end{aligned}
\]
Mixed FEM in Solid Mechanics - a brief introduction

Discretization of a Mixed-Galerkin approach results in an algebraic system of the general form

\[
\begin{bmatrix}
A & B^T \\
B & 0
\end{bmatrix}
\begin{bmatrix}
d_u \\
d_\sigma
\end{bmatrix}
= 
\begin{bmatrix}
f \\
g
\end{bmatrix}
\]

This saddle-point structure reveals the major challenge in the construction of mixed finite elements, because existence and uniqueness of a solution cannot be guaranteed in general.

The discretization of the individual field (dofs \(d_u\) and \(d_\sigma\)) have to be cautiously balanced, with regard of the conditions of well-posedness for mixed FE by Babuška [1973] and Brezzi [1974].

However, the immediate calculation of the field of interests (e.g. stresses, pressure, ..) often worth the additional efforts.
Assumed Stress Elements in Linear Elasticity

The solution of the elasticity problem with body $B \in \mathbb{R}^3$, with $\varepsilon(u) = \nabla^s u$

$$
div \sigma + f = 0 \quad \text{on } B
$$

$$
C^{-1} : \sigma = \varepsilon(u) \quad \text{on } B
$$

$$
u = 0 \quad \text{on } \partial B_u
$$

$$
\sigma n = \bar{t} \quad \text{on } \partial B_\sigma
$$

is equivalent to the Hellinger-Reissner principle (satisfying the displacement boundary conditions a priori) which seeks a saddle-point $(\sigma, u) \in L^2(B) \times H^1_0(B)$

$$
\Pi^{HR}(\sigma, u) = \int_B \left( -\frac{1}{2} \sigma : C^{-1} : \sigma + \sigma : \varepsilon(u) \right) \, dV - \int_{\partial B_\sigma} u \cdot \bar{t} \, dA
$$

$$
\delta_u \Pi^{HR} = \int_B \varepsilon(\delta u) : \sigma \, dV - \int_{\partial B_\sigma} \delta u \cdot \bar{t} \, dA = 0 \quad \forall \delta u \in H^1_0(B)
$$

$$
\delta_\sigma \Pi^{HR} = \int_B \delta \sigma : (\varepsilon(u) - C^{-1} : \sigma) \, dV = 0 \quad \forall \delta \sigma \in L^2(B)
$$
The displacements and stresses defined on the isoparametric space are

\[ \mathbf{u} = \mathbf{N} \mathbf{d} \quad \text{and} \quad \mathbf{\epsilon} = \mathbf{B} \mathbf{d} \]

\[ \mathbf{\hat{\sigma}} = (\mathbf{\hat{\sigma}}_{11}, \mathbf{\hat{\sigma}}_{22}, \mathbf{\hat{\sigma}}_{12})^T = \mathbf{\hat{L}}(\xi) \mathbf{\hat{\beta}}, \]

where \( \mathbf{N} \) contains the bilinear shape functions, \( \mathbf{B} \) its spatial derivatives, \( \mathbf{d} \) the nodal displacements, \( \mathbf{\hat{\beta}} \) the element-wise stress unknowns and \( \mathbf{\hat{L}} \) the corresponding interpolation functions with the structure

\[ \mathbf{\hat{L}} = \text{diag}(\hat{L}_{11}, \hat{L}_{22}, \hat{L}_{12}) \].

5-parameter based interpolation, proposed by PIAN & SUMIHARA [1984]

\[ \hat{L}_{11} = (1, \eta), \quad \hat{L}_{22} = (1, \xi), \quad \hat{L}_{12} = (1). \]

Uniform convergence has been proven by YU, XIE & CARSTENSEN [2011]
Boundary Value Problem Hyperelasticity

Let the second Piola Kirchhoff stress $\mathbf{S}$ and the displacements $\mathbf{u}$ be independent quantities. Then the BVP can be given with $\mathcal{B} \in \mathbb{R}^3$, $\mathbf{F} = \mathbf{I} + \nabla \chi \mathbf{u}$, $\mathbf{C} = \mathbf{F}^T \mathbf{F}$, $\mathbf{E} = \frac{1}{2}(\mathbf{C} - \mathbf{I})$ and $\mathbf{P} = \mathbf{F} \mathbf{S}$

\[
\text{Div} \mathbf{P} + \mathbf{f} = 0 \quad \text{on} \; \mathcal{B}
\]

\[
\frac{\partial \chi(\mathbf{S})}{\partial \mathbf{S}} = \mathbf{E} \quad \text{on} \; \mathcal{B}
\]

\[
\mathbf{u} = \mathbf{u} \quad \text{on} \; \partial \mathcal{B}_{\mathbf{u}}
\]

\[
\mathbf{P} \mathbf{N} = \mathbf{t} \quad \text{on} \; \partial \mathcal{B}_{\mathbf{\sigma}}
\]

where $\chi(\mathbf{S})$ is a complementary stored energy. St. Venant type nonlinear elasticity

\[
\chi(\mathbf{S}) = \frac{1}{2} \mathbf{S} : \mathbf{C}^{-1} : \mathbf{S}.
\]

Unfortunately, such explicit complementary functions only exist for special cases.
Weak Form / Linearization

Assume that \( \chi(S) \) exists. The corresponding potential is given by

\[
\Pi^{HR}(S, u) = \int_B (S : \mathbf{E} - \chi(S)) \, dV + \Pi^{ext}.
\]

and the weak forms follow by

\[
\delta_u \Pi = \int_B \delta \mathbf{E} : S \, dV + \delta_u \Pi^{ext} = 0
\]

\[
\delta_S \Pi = \int_B \delta S : (\mathbf{E} - \partial_S \chi(S)) \, dV = 0
\]

In cases where no complementary stored energy is known, the partial derivative \( \partial_S \chi(S) := \mathbf{E}^{\text{cons}} \) can be computed iteratively in each integration point at fixed \( S \):

\[
r(\mathbf{E}^{\text{cons}}) = S - \partial_E \psi(\mathbf{E})|_{\mathbf{E}^{\text{cons}}} \approx 0
\]

we have to update (until convergence)

\[
\mathbf{E}^{\text{cons}} \leftarrow \mathbf{E}^{\text{cons}} + \left[ \partial^2_{EE} \psi(\mathbf{E})|_{\mathbf{E}^{\text{cons}}} \right]^{-1} r(\mathbf{E}^{\text{cons}}) =: \mathbf{D}
\]
Cook’s Membrane Problem

Neo-Hookean free energy: \( \psi = \frac{\Lambda}{4} (J^2 - 1) - \left( \frac{\Lambda}{2} + \mu \right) \ln J + \frac{\mu}{2} (\text{tr}C - 3) \)

Material parameter: \( E = 200, \nu = 0.4999 \)

Displacement convergence:

Necessary load steps:

Boundary Conditions:
\( x = 0 \):
\( u_1 = 0 \)
\( u_2 = 0 \)
\( x = 48 \):
\( \bar{t} = (0, 10)^T \)

Q1-EAS: EAS Element with 4 Parameters; Simo & Rifai [1990]

Q1-FBar: Selective reduced integration technique of shape functions; Simo, Taylor, Pister [1985]

Implementation in AceGen/AceFEM
Cook’s Membrane Problem

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Cook’s Membrane

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Material parameter: \( E = 200, \nu = 0.4999 \)

Boundary Conditions:

\begin{align*}
  x = 0 : & \quad u_1 = 0 \\
  u_2 = 0 \\
  u_3 = 0 \\
  x = 48 : & \quad \bar{t} = (0, 10, 0)^T
\end{align*}

Q1-EAS: EAS Element with 4 Parameters; Simo & Rifai [1990]

Q1-FBar: Selective reduced integration technique of shape functions; Simo, Taylor, Pister [1985]

Implementation in AceGen/AceFEM

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Compression Block

Neo-Hookean free energy: $\psi = \frac{\Lambda}{4}(J^2 - 1) - \left(\frac{\Lambda}{2} + \mu\right) \ln J + \frac{\mu}{2}(\text{tr}C - 3)$

Material parameter: $E = 4.82926, \nu = 0.498393$

Displacement convergence:

Necessary load steps:

Q1-EAS: EAS Element with 4 Parameters; Simo & Rifai [1990]

Q1-FBar: Selective reduced integration technique of shape functions; Simo, Taylor, Pister [1985]

Implementation in AceGen/AceFEM
Pinched Cylinder with rigid ends

\[ \psi = \frac{\Lambda}{4} (J^2 - 1) - \left( \frac{\Lambda}{2} + \mu \right) \ln J + \frac{\mu}{2} (\text{tr} C - 3) \]

Geometrical Data: \( R = 100, \ L = 200, \ h = 1 \)

Material Data: \( E = 3 \cdot 10^4, \ \nu = 0.3 \)

Load: \( F = 1200 \)

Number of elements (per height): \( 48 \times 48 \times 1 \)
Novel Approach: SKA - Simplified Kinematics for Anisotropy

Considering an additively decoupled strain energy

$$\psi = \psi_{\text{isotropic\_part}}(\bullet) + \psi_{\text{anisotropic\_part}}(C)$$

where we have the following alternative for the modeling of $\psi_{\text{isotropic\_part}}$:

- **Standard approximation of the deformation gradient $C$**

  $$\psi^{\text{i\_p}} = \psi^{\text{i\_p}}(C)$$

- **Volumetric-isochoric split of the free energy, $\tilde{C} = \tilde{F}^T \tilde{F} = J^{-2/3} C$**

  $$\psi^{\text{i\_p}} = \psi^{\text{vol}}(J) + \psi^{\text{unimodular}}(\tilde{C})$$

- **Modified deformation gradient with constant volume dilatation $\theta$**

  $$\psi^{\text{i\_p}} = \psi(\theta^{2/3} \tilde{C})$$

→ Different approximations for $\theta$, $C$ and $C$ can be investigated

→ The introduced kinematic-like field has to be controlled

J. Schröder, N. Viebahn, D. Balzani, P. Wriggers [2016], A novel mixed finite element for finite anisotropic elasticity; the SKA-element Simplified Kinematics for Anisotropy, CMAME [2016]

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Hu-Washizu functional, Approximation of $C$

$$
\Pi(C, C, S) = \int_B \psi^{i-p}(C) \ dV + \int_B \psi^{a-p}(C) \ dV + \int_B \frac{1}{2} S : (C - C) \ dV + \Pi^{\text{ext}}(x)
$$

with $\Pi^{\text{ext}} = - \int_B x \cdot f \ dV - \int_{\partial B} x \cdot t_0 \ dA$

$$
\delta_u \Pi = \int_B \frac{1}{2} \delta C : (2 \partial_C \psi^{i-p} + S) \ dV - \int_B \delta u \cdot f \ dV - \int_{\partial B} \delta u \cdot t_0 \ dA
$$

$$
\delta_c \Pi = \int_B \delta C : (\partial_C \psi^{a-p} - \frac{1}{2} S) \ dV = 0
$$

$$
\delta_S \Pi = \int_B \frac{1}{2} \delta S : (C - C) \ dV = 0.
$$

The identified Euler-Lagrangian equations are

$$
\text{Div}(F (S^{i-p} + S)) + f = 0, \quad S = S^{a-p} \quad \text{and} \quad C = C.
$$
3D Artery - Boundary value problem

Material model (Balzani et al. [2006]):

\[ \psi_{i-p} = c_1 \left( \frac{I_1}{I_3^{1/3}} - 3 \right) + \varepsilon_1 (I_3^{e2} + I_3^{-e2} - 2) \]

\[ \psi_{a-p} = \sum_{a=1}^{2} \alpha_1 \langle I_1 + J_4^{(a)} - J_5^{(a)} - 2 \rangle^{\alpha_2} \]

Material parameter (Brands et al. [2008]):

<table>
<thead>
<tr>
<th></th>
<th>adv.</th>
<th>med.</th>
</tr>
</thead>
<tbody>
<tr>
<td>(c_1)</td>
<td>6.6</td>
<td>17.5</td>
</tr>
<tr>
<td>(\varepsilon_1)</td>
<td>23.9</td>
<td>499.8</td>
</tr>
<tr>
<td>(\varepsilon_2)</td>
<td>10.0</td>
<td>2.4</td>
</tr>
<tr>
<td>(\alpha_1)</td>
<td>1503.0</td>
<td>30001.9</td>
</tr>
<tr>
<td>(\alpha_2)</td>
<td>6.3</td>
<td>5.1</td>
</tr>
<tr>
<td>(\beta)</td>
<td>49.0</td>
<td>43.39</td>
</tr>
</tbody>
</table>

D. Brands, A. Klawonn, O. Rheinbach, J. Schröder [2008], Modelling and convergence in arterial wall simulations using a parallel FETI solution strategy, CMBBE, 569-583

3D Artery - Supra-physical pressure - Set 2

Deformed configurations for actual pressure: $p = 0$

Standard formulations

T$_2$

T$_2$P$_0$

Proposed formulations

SKA-T$_2$A$_0$

SKA-T$_2$P$_0$A$_0$
Deformed configurations for actual pressure: \( p = 5.82 \cdot 10^3 \)
Deformed configurations for actual pressure: $p = 2.19 \cdot 10^4$

Standard formulations

Proposed formulations

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Deformed configurations for actual pressure: \( p = 10^8 \)

Standard formulations

- \( T_2 \)
- \( T_2P_0 \)

Proposed formulations

- \( \text{SKA}-T_2A_0 \)
- \( \text{SKA}-T_2P_0A_0 \)
Motivation for Least-squares FEM

The advantage of using conform mixed $(\sigma, u)$-based methods lies in the stress approximation, here with Raviart-Thomas functions in $H(\text{div})$, which yields continuous stress distributions in contrast to standard displacement methods (StDM).

Advantages of the classical Least-Squares Method:
- LS functional leads to a minimization problem
- Not restricted by the LBB condition
- Symmetric and positive definite matrices
- A posteriori error estimator is provided

Disadvantages of the classical Least-Squares Method:
- Lower order elements have a poor performance
- Weighting of the individual residuals is questionable
General construction of a Least-Squares Functional

To define the minimization problem, we apply the squared $L^2(\mathcal{B})$-norm to a first-order system of $n$ differential equations, see e.g. Cai & Starke [2004],

$$
\mathcal{F}(u, \sigma) = \frac{1}{2} \left( \| \omega_1(\text{div} \sigma + f) \|^2_{L^2(\mathcal{B})} + \| \omega_2(\sigma - C : \nabla^s u) \|^2_{L^2(\mathcal{B})} \right) \to \text{minimize}.
$$

with $\delta_{\sigma, u} \mathcal{F} = 0$. Requirements for approximation spaces $(V, X)$ and finite element spaces $RT_m P_k$ with

$$
V = \{ u \in H^1(\mathcal{B})^d \} \supseteq V_h^k = \{ u \in H^1(\mathcal{B})^d : u|_{\mathcal{B}_e} \in P_k(\mathcal{B}_e)^d \ \forall \ \mathcal{B}_e \},
$$

and furthermore

$$
X = \{ \sigma \in H(\text{div}, \mathcal{B})^d \} \supseteq X_h^m = \{ \sigma \in H(\text{div}, \mathcal{B})^d : \sigma|_{\mathcal{B}_e} \in RT_m(\mathcal{B}_e)^d \ \forall \ \mathcal{B}_e \}.
$$
Remarks on least-squares finite element methods

Stress-displacement LSFEM with use of Raviart-Thomas approximation functions

\[
\mathcal{F}(\sigma, u) = \frac{1}{2} \| \omega_m (\text{div } \sigma + f) \|^2_{L^2(B)} + \frac{1}{2} \| \omega_c (\sigma - \mathbf{C} : \nabla^s u) \|^2_{L^2(B)}
\]

and

\[
\mathcal{F}(\sigma, u) = \frac{1}{2} \| \omega_m (\text{div } \sigma + f) \|^2_{L^2(B)} + \frac{1}{2} \| \omega_c (\sigma - \mathbf{C} : \nabla^s u) \|^2_{L^2(B)} + \frac{1}{2} \| \omega_a ((x - x_0) \times (\text{div } \sigma + f) + \mathbf{a} \mathbf{1}[\sigma - \sigma^T]) \|^2_{L^2(B)}.
\]

\[
\psi_0^1 = \begin{pmatrix} \xi \\ \eta - 1 \end{pmatrix}, \\
\psi_0^2 = \begin{pmatrix} \xi \\ \eta \end{pmatrix}, \\
\psi_0^3 = \begin{pmatrix} \xi - 1 \\ \eta \end{pmatrix}
\]

\(RT_0 P_1\) dof for 2D (left) and exemplarily basis function for lower edge (right)
Approximation of reaction force for a cantilever beam

\[ E = 70 \]
\[ \nu = 0.34 \]
\[ \sigma \cdot n = (0, 0.1)^T \]

standard disp.: \[
H = \sum_{I \in \partial B_u} F^I_{x_1} \\
V = \sum_{I \in \partial B_u} F^I_{x_2} \\
M = \sum_{I \in \partial B_u} F^I_{x_1} \cdot x^I_{2}
\]

LSFEM: \[
H = \int_{\partial B_u} \sigma_{11} \, dx_2 \\
V = \int_{\partial B_u} \sigma_{21} \, dx_2 \\
M = \int_{\partial B_u} \sigma_{11} \cdot \hat{x}_2 \, dx_2 \\
\hat{x}_2 = x_2 - x_M
\]

Reaction forces compared to analytical results \((\sum H = 0, \sum V = 0.1, \sum M = 0.5)\):
Least-squares functional for finite strain elasticity

Extending the formulation by adding a mathematically redundant residual cf. [3], [4], given by a stress symmetry condition, here in terms of the 2nd Piola-Kirchhoff stresses $S = F^{-1} P$; $R_3 = S - S^T$. The resulting least-squares functional yields

$$
F = \frac{1}{2} \int_B \omega_1^2 (\text{Div} \ P + f) \cdot (\text{Div} \ P + f) \, dV \\
+ \frac{1}{2} \int_B \omega_2^2 (P - \rho_0 \partial_F \psi(C)) : (P - \rho_0 \partial_F \psi(C)) \, dV \\
+ \frac{1}{2} \int_B \omega_3^2 (F^{-1} P - (F^{-1} P)^T) : (F^{-1} P - (F^{-1} P)^T) \, dV ,
$$

based on a Neo-Hookean type free energy function $\psi(C)$ in terms of $C = F^T F$

$$
\psi(C) = \frac{\mu}{2}(I_1 - 3) + \frac{\Lambda}{4}(J^2 - 1) - \left( \frac{\Lambda}{2} + \mu \right) \ln J
$$

with the principal invariant $I_1 = \text{tr} \ C$, $J = \text{det} \ F$ and $\rho_0 = 1 \frac{\text{kg}}{\text{m}^3}$.


Cook’s membrane problem for finite strain elasticity

Left side: \( u = (0, 0)^T \)

Right face: \( P N = (0, 20)^T \)

\( \Lambda = 432.099, \, \nu = 185.185, \)

\( \omega_1 = 1, \, \omega_2 = 1/\mu \) and \( \omega_3 = 10/\mu \)

\( \sigma_{vM} \) distribution and convergence study at (48,60):
Cook’s membrane problem for finite strain elasticity

Left side: \( \mathbf{u} = (0, 0)^T \)

Right face: \( \mathbf{PN} = (0, 10)^T \)

\( \Lambda = (432.099, 750, 9260, 92600) \)

\( \nu = (0.35, 0.40099, 0.490197, 0.499002) \)

\( \omega_1 = 1, \omega_2 = 1/\mu \) and \( \omega_3 = 10/\mu \)

\( \sigma_{vM} \) distribution and locking behavior for \( RT_2P_3 \):
Perforated plate example for finite strain elasticity

Boundary conditions, material properties and system:

- Left side $u_1 = 0$, $P_{21} = 0$
- Lower side $u_2 = 0$, $P_{12} = 0$
- Right side $PN = (0, 0)^T$
- Upper side $PN = (0, 50)^T$
- $E = 200$, $\nu = 0.35$, $\omega_i = 1, 1/\mu, 1/\mu$

Convergence of $|F - F_h|$, order of convergence and $u_2$-displacement at (0,1):

<table>
<thead>
<tr>
<th></th>
<th>regular (rr)</th>
<th>adaptive (arD)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$RT_0P_1$</td>
<td>0.83355</td>
<td>1.07582</td>
</tr>
<tr>
<td>$RT_1P_2$</td>
<td>1.28705</td>
<td>1.80055</td>
</tr>
<tr>
<td>$RT_2P_3$</td>
<td>1.58372</td>
<td>3.21487</td>
</tr>
<tr>
<td>$RT_3P_4$</td>
<td>1.87417</td>
<td>3.92780</td>
</tr>
</tbody>
</table>
A simple triangular finite element for nonlinear thin shells - Statics, Dynamics and anisotropy

Acknowledgement: Paulo Pimenta

Based on the Kirchhoff-Love theory of plates, LOVE [1888].

Kinematic assumption: A straight normal of the reference mid-surface remains a straight normal of the deformed mid-surface.

Plane-stress and shear-rigid assumptions lead to a stress tensor, which is non-trivial only for the mid-plane of the shell, i.e. $\tau_{3i} = \tau_{i3} = 0$, whereas $e_1$ and $e_2$ span the mid-plane of the shell.

Assumptions are valid for “thin shells” with $h/L < 1/10$. 

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Kinematics

Based on Pimenta, Neto, Campello [2010] and using the assumption of initial flat reference elements.

Description of material point:
Point on middle Surface + **orthogonal** director

Reference configuration: \( \xi = \zeta + a^r \)
with \( \zeta = \xi_\alpha e^r_\alpha \) and \( a^r = \xi_3 e^r_3 \)

Current configuration: \( x = z + a \)
with \( z = u - \zeta \)

Orthogonal director: \( a = Q a^r \)
with rotation tensor \( Q = e_i \otimes e^r_i \)

Deformation gradient: \( F = \frac{\partial x}{\partial \xi_\alpha} \otimes e^r_\alpha + \frac{\partial x}{\partial \xi_3} \otimes e^r_3 \)
Enforcement of the $C^1$-Continuity

The $C^1$-continuity is asymptotically satisfied if $\beta$ does not change during the motion $\rightarrow \beta - \beta^r = 0$. This is enforced, using a penalty approach, by

$$\Pi^{\text{pen}} = \int_{\Gamma^r} \frac{1}{2} k (\sin \beta - \sin \beta^r)^2 d\Gamma^r,$$

with $\sin \beta^{(r)} = (e_{3,B}^{(r)} \times e_{3,A}^{(r)}) \cdot \tau_B^{(r)}$ and $k$ as a penalty parameter.

For this formulation no additional DOF is needed!

Alternatively the $C^1$-continuity could be enforced, using a Lagrange multiplier or the Augmented Lagrange method.
Enforcement of the $C^1$-Continuity

**Clamped Edges**

Clamping of free edges is enforced by minimization of

$$\Pi^{\text{pen},c} = - \int_{\Gamma^r} \frac{1}{2} k \left((e_{3,A}^r \times e_{3,A}^r) \cdot \tau_A^r\right)^2 d\Gamma^r.$$

**Branching shells**

Multiple branched shells are adopted by minimization of

$$\Pi^{\text{pen},b} = \int_{\Gamma^r} \frac{1}{2} k \left(\sin \beta_{AB} - \sin \beta_{AB}^r\right)^2 d\Gamma^r + \int_{\Gamma^r} \frac{1}{2} k \left(\sin \beta_{AC} - \sin \beta_{AC}^r\right)^2 d\Gamma^r.$$
Pinched Cylinder with rigid ends

\[ \psi = \frac{1}{4} \lambda ( (I_3 - 1) - \ln I_3 ) + \frac{1}{2} \mu (I_1 - 3 - \ln I_3) \]

Geometrical Data: \( r = 200, \ l = 400, \ h = 1 \)

Material Data: \( E = 3 \cdot 10^4, \ \nu = 0.3 \)

Penalty Parameter: \( k = \frac{E h^3}{12(1 - \nu^2)} \)

Boundary Conditions:
\( u_2(x_1 = 0) = 0, \ u_3(x_1 = 0) = 0 \)
\( u_2(x_1 = l) = 0, \ u_3(x_1 = l) = 0 \)

\( F = 5.4 \cdot 10^4 \)
Plate with stiffeners

Geometrical Data: \( l = 25.4 \), \( h = 0.254 \)
Stiffener: (b) \( h_s = 1.27 \), (c) \( h_s = 0.508 \)
Material Data: \( E = 117.25 \), \( \nu = 0.3 \)
Penalty Parameter: \( k = \frac{E h^3}{12(1 - \nu^2)} \)

Deformations scaled by factor 10.
Dynamic reversion of clamped dome

Geometrical Data: \( r = 0.05, h = 10^{-3} \)
Material Data: \( E = 10^5, \nu = 0.499, \rho = 1000 \)
Penalty Parameter: \( k = \frac{E h^3}{12(1 - \nu^2)} \)
Newmark Parameter: \( \beta = 0.3025, \gamma = 0.6 \)
Boundary Conditions: \( u(x_3 = 0) = 0, \quad u_3(x = (0, 0, r)) = -2r \)

movie
Thank you for your attention

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SPP 1748
Reliable Simulation Techniques in Solid Mechanics.
Development of Non-standard Discretization Methods,
Mechanical and Mathematical Analysis

Jože Korelc - For the deployment of AceGen and AceFEM
Korelc J., Automatic generation of finite-element code by simultaneous optimization of expressions,
Korelc J., Multi-language and Multi-environment Generation of Nonlinear Finite Element Codes,
Engineering with Computers, 2002, 18:312–327
Least-squares functional for finite strain elasto-plasticity

First-order system, based on the multiplicative split of \( F = F^e F^p \),
\[
b^e = F C^p F^T, \quad \psi(b^e) = \frac{A}{4} \det b^e + \frac{\mu}{2} \text{tr} b^e - \left( \frac{A}{2} + \mu \right) \ln \sqrt{\det b^e}:
\]
\[
F(P, u) = \frac{1}{2} \left( \|\omega_1(\text{Div} \, P + f)\|^2_0 + \|\omega_2(P F^T - 2 \frac{\partial \psi(b^e)}{\partial b^e} b^e)\|^2_0 + \|\omega_3(P F^T - FP^T)\|^2_0 \right).
\]

Principle of max. Dissipation; v. Mises criterion \( \Phi = \| \text{dev} \, \tau \| + \sqrt{\frac{2}{3}} (y_0 + \beta(\alpha)) \leq 0. \)
\[
L(\tau, \beta, \gamma) = -D_{\text{int}}(\tau, \beta) + \gamma \Phi(\tau, \beta) \rightarrow \text{stat.} \quad \text{with} \quad \gamma \geq 0
\]
\[
\partial_\tau L \Rightarrow \frac{1}{2} \mathcal{L}(b^e) b^e^{-1} = -\gamma n \quad \Rightarrow \quad C^p_{n+1} = F^{-1}_{n+1} \exp[-2\lambda_n] F_{n+1} C^p_{n},
\]
\[
\partial_\beta L \Rightarrow \dot{\alpha} = \gamma \sqrt{\frac{2}{3}} \quad \Rightarrow \quad \alpha_{n+1} = \alpha_n + \sqrt{\frac{2}{3}} \lambda,
\]
fulfilling the yield criterion at time \( t_{n+1} \) yields \( \lambda = \Delta t \gamma = \frac{3 \Phi^{\text{trial}}}{2 h} \).

Cook’s membrane problem for finite strain plasticity

Left side: \( \mathbf{u} = (0, 0, 0)^T \)

(a) Right face: \( \mathbf{P N} = (4.5, 0, 0)^T \)

(b) Right face: \( \mathbf{P N} = (0, 2.5, 0)^T \)

\( E = 2069, \nu = 0.29, \)

\( y_0 = 4.5, h = 15 \)

\( \omega_1 = 1, \omega_2 = 1/\mu \) and \( \omega_3 = 10/\mu \)

Convergence studies for load cases (a) and (b):

\( u_1 \) displacement at node (18,60,0)

\( u_2 \) displacement at node (18,60,0)
Cook’s membrane problem for finite strain plasticity

Plot of von Mises stress $\sigma_{vM}$ for $PN = (0, 2.5, 0)^T$:

Plot of equivalent plastic strains $\alpha$ for $PN = (0, 2.5, 0)^T$:
Hyperbolic shell (Balzani et al. [2008])

\[ \psi = c_1 \left( \frac{I_1}{I_3^{1/3}} - 3 \right) + \epsilon_1(I_3^{\epsilon_2} + I_3^{-\epsilon_2} - 2) + \alpha_1(I_1I_4 - I_5 - 2)^{\alpha_2} \]

Geometrical Data: \( R_0 = 5, \ H = 12, \ h = 0.05 \)

Material Data: \( C_1 = 100, \ \epsilon_1 = 2000, \ \epsilon_2 = 10 \)

IF Tr. Iso.: \( \alpha_1 = 1000, \ \alpha_2 = 2.3 \)

Penalty Parameter: \( k = 10^4 \)
Algorithmic Treatment

ELEMENT LOOP

(1) Update displacements and stresses (Newton iteration k+1)
\[ d = d_n^{(k)} + \Delta d, \beta = \beta_n^{(k)} + \Delta \beta \]

INTEGRATION LOOP

(2) Compute stresses \( S \) and Green-Lagrange strain tensor \( E \) in each Gauss Point:
\[ S = L \beta, \quad E = B \cdot d, \]

Read from history: \( E^{\text{cons}} \)

CONSTITUTIVE LOOP

(3) Compute residuum:
\[ r(E^{\text{cons}}) = S - S^{\text{cons}} \]

with \( S^{\text{cons}} = \partial E^{\text{cons}} \psi(E^{\text{cons}}) \)

(4) Update:
\[ E^{\text{cons}} = E^{\text{cons}} + D : r(E^{\text{cons}}) \]

with \( D = (\partial E^{\text{cons}} S^{\text{cons}})^{-1} \)

(5) Check convergence

IF \[ \| D : r(E^{\text{cons}}) \|^2 \leq tol \]
THEN Update History \( E^{\text{cons}} \) and exit CONSTITUTIVE LOOP

(6) Check divergence

IF \( n_{\text{iter}} > n_{\text{tol}} \) THEN Stop Calculation

(7) Determine and export element stiffness and rhs-vector
Deformation of infinitesimal line element \[ dx = F \, dX \]

Deformation of vectorial area element \( dA \):
\[
d\mathbf{a} = (F \, d\mathbf{X}) \times (F \, d\mathbf{X}) = \text{Cof} \, F (d\mathbf{X} \times d\mathbf{X}) = \text{Cof} [F] \, dA
\]

Deformation of infinitesimal volume element
\[
dv = d\mathbf{a} \cdot F \, d\mathbf{X} = \text{Cof} [F] \, dA \cdot F \, d\mathbf{X} = J \, dA \cdot d\mathbf{X} = J \, dv
\]
Summary of Balance Equations in the Material Setting

Conservation of mass (densities $\rho_0 \in B_0$, $\rho \in B_t$)

$$\rho_0 = \rho J$$

Balance of linear momentum (body force $\rho_0 b$)

$$\text{Div } P + \rho_0 b = \rho_0 \ddot{x}$$

Balance of moment of momentum

$$PF^T = FP^T$$

Balance of energy (internal energy $e$, heat flux vector $q_0$ on $\partial B_0$)

$$\rho_0 \dot{e} = P \cdot \dot{F} - \text{Div } q_0 + \rho_0 r$$

Clausius-Duhem inequality (free energy $\psi$, entropy $\eta$, absolute temperature $\Theta$)

$$P \cdot \dot{F} - \rho_0 \left( \dot{\psi} + \dot{\Theta} \eta \right) - \frac{1}{\Theta} q_0 \cdot \text{Grad } \Theta \geq 0$$
Definition of Hyperelasticity

A material is termed hyperelastic if the existence of a free-energy $\psi$ is postulated.

Evaluating the Clausius-Duhem relation, neglecting thermal effects yields

$$P \cdot \dot{F} - \rho_0 \dot{\psi}(F) = 0 \quad \rightarrow \quad P = \rho_0 \frac{\partial \psi}{\partial F}$$

Internal work during quasi-static process in time interval $[t_0, t_1]$ for homogeneous deformation depends only on the values of $\psi$ at the initial and final placement:

$$\int_{t_0}^{t_1} P \cdot \dot{F} \, dt = \int_{t_0}^{t_1} \rho_0 \frac{\partial \psi}{\partial F} \cdot \dot{F} \, dt = \rho_0 \int_{t_0}^{t_1} \dot{\psi} \, dt = \rho_0 (\psi(F_1) - \psi(F_0))$$

Internal work during closed process is zero, i.e.

$$\rho_0 \int_{t_0}^{t_1} \dot{\psi} \, dt + \rho_0 \int_{t_1}^{t_2} \dot{\psi} \, dt = \rho_0 (\psi(F_1) - \psi(F_0)) + \rho_0 (\psi(F_0) - \psi(F_1)) = 0$$

where $F_0 = F(t_0)$, $F_1 = F(t_1)$, $F_2 = F(t_2) = F_0$