SEPRAN

SEPRA ANALYSIS

Theoretical MANUAL

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Theoretical MANUAL

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Contents

1 Introduction

In this manual some theoretical background used by the SEPRAN package is given.
The same subdivision as in the manual Standard Problems is used.

2 Unknown

This chapter is under preparation

3 Second order elliptic and parabolic equations

This chapter is under preparation

4 Elements for lubrication theory

This chapter is under preparation

5 Mechanical elements

In this chapter some mechanical elements are described.
The following sections are available:

- 5.1 is devoted to standard linear elastic problems.
- 5.2 treats incompressible or nearly incompressible elasticity.
- 5.3 is devoted to non-linear elasticity problems.
- 5.4 deals with (thick) plates.

5.1 Linear elastic problems

This chapter is under preparation

5.2 Linear incompressible or nearly incompressible elastic problems

This chapter is under preparation

5.3 Nonlinear solid computation

Non-linear solid mechanics problems can be solved either by a Total Lagrange approach or an updated Lagrange approach. In SEPRAN elements for both types of equations are available.
Section (5.5) treats elements using the Total Lagrange approach.
Elements using the updated Lagrange approach are treated in Section (5.5.1).

5.4 Thick) plate elements

This chapter is under preparation

5.5 Nonlinear solid computation using a Total Lagrange approach

This chapter is under preparation

5.5.1 Nonlinear solid computation using an Updated Lagrange approach

Linearized weak form of the governing equations

As point of departure we take the equations of conservation of mass and momentum:

$$\begin{cases} \nabla \cdot \boldsymbol{\sigma} = \vec{0} & \text{in } \Omega(t) \quad (5.5.1.1a) \\ \det(\boldsymbol{F}) - 1 = 0 & \text{in } \Omega(t) \quad (5.5.1.1b) \end{cases}$$

The Cauchy stress can be written as:

$$\boldsymbol{\sigma} = -p\boldsymbol{I} + \boldsymbol{\tau} \tag{5.5.1.2}$$

We define weighting functions $\vec{w} \in \vec{W}$ and $q \in Q$ for the balance equations of mass and momentum, respectively. Here $\vec{W} = \{\vec{w} \in [H_0^1(\Omega)]^3\}$ with $H_0^1(\Omega)$ the Hilbert space satisfying the homogeneous version of the Dirichlet boundary conditions, and $Q = \{q \in L^2(\Omega); \int_\Omega q d\Omega = 0\}$. Then the weak form of (eq. 5.5.1.1b) is given by:

$$\begin{cases} \int\limits_{\Omega_t} (\text{grad}\, \vec{w})^T : \boldsymbol{\sigma} & = \int\limits_{\Gamma_t} \vec{w} \cdot (\boldsymbol{\sigma} \cdot \vec{n}) \\ \int\limits_{\Omega_t} q(J-1) & = 0 \end{cases} \tag{5.5.1.3}$$

where we used the abbreviation $J = \det \boldsymbol{F}$. To evaluate the integrals, they must be transformed from the current, unknown, configuration, to a known configuration. Following an updated Lagrange approach, we choose the last known configuration Ω_n as a reference and define:

$$\begin{aligned} \boldsymbol{F} &= \boldsymbol{F}_\Delta \cdot \boldsymbol{F}_n \\ \boldsymbol{F}_n &= (\text{grad}_0 \vec{x}_n)^T \\ \boldsymbol{F}_\Delta &= (\text{grad}_n \vec{x})^T \end{aligned} \tag{5.5.1.4}$$

where grad_n denotes the spatial gradient operator with respect to configuration Ω_n[1]:

$$\text{grad}_n = \boldsymbol{F}_\Delta^T \cdot \text{grad} \tag{5.5.1.5}$$

Transformation yields:

$$\begin{cases} \int\limits_{\Omega_n} (\text{grad}_n \vec{w})^T : \boldsymbol{F}_\Delta^{-1} \cdot \boldsymbol{\sigma} J_\Delta = \\ \qquad \int\limits_{\Gamma_n} n\vec{w} \cdot (\boldsymbol{\sigma} \cdot (\boldsymbol{F}_\Delta^{-T} \cdot \vec{n}_n)) J_\Delta \\ \int\limits_{\Omega_n} q(J-1) J_\Delta = 0 \end{cases} \tag{5.5.1.6}$$

Linearization

The nonlinear set of equations (5.5.1.6) is solved using Newton iterations. The (unknown) converged solution $(\vec{x}, p)$ on Ω is written as the sum of an estimate, $(\hat{\vec{x}}, \hat{p})$, and an error $(\delta\vec{x}, \delta p)$

$$\vec{x} = \hat{\vec{x}} + \delta\vec{x} \tag{5.5.1.7}$$

$$p = \hat{p} + \delta p \tag{5.5.1.8}$$

All other quantities in (5.5.1.6) can be written similarly, giving:

$$\boldsymbol{F}_\Delta = \hat{\boldsymbol{F}}_\Delta + \delta\boldsymbol{F}_\Delta \quad ; \quad \boldsymbol{\tau} = \hat{\boldsymbol{\tau}} + \delta\boldsymbol{\tau} \quad ; \quad J = \hat{J} + \delta J \tag{5.5.1.9}$$

[1] Use $\text{grad}\, \vec{x} = \boldsymbol{I} = \boldsymbol{F}_\Delta^{-T} \cdot \boldsymbol{F}_\Delta^T = \boldsymbol{F}_\Delta^{-T} \text{grad}_n \vec{x}$.

Substituting these expressions in (5.5.1.6) and neglecting the second order terms yields:

$$
\left\{
\begin{array}{l}
\int\limits_{\Omega_n} (\mathrm{grad}_n \vec{w})^T : \delta \boldsymbol{F}_\Delta^{-1} \cdot (-\hat{p}\boldsymbol{I} + \hat{\boldsymbol{\tau}})\hat{J}_\Delta + \\
\quad \int\limits_{\Omega_n} (\mathrm{grad}_n \vec{w})^T : \hat{\boldsymbol{F}}_\Delta^{-1} \cdot (-\delta p\boldsymbol{I} + \delta\boldsymbol{\tau})\hat{J}_\Delta + \\
\quad \int\limits_{\Omega_n} (\mathrm{grad}_n \vec{w})^T : \hat{\boldsymbol{F}}_\Delta^{-1} \cdot (-\hat{p}\boldsymbol{I} + \hat{\boldsymbol{\tau}})\delta J_\Delta - \\
\quad \int\limits_{\Gamma_n} n\vec{w} \cdot \left(\delta\boldsymbol{\sigma} \cdot \hat{\boldsymbol{F}}_\Delta^{-T} \cdot \vec{n}_n \hat{J}_\Delta + \hat{\boldsymbol{\sigma}} \cdot \delta\boldsymbol{F}_\Delta^{-T} \cdot \vec{n}_n \hat{J}_\Delta + \hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{F}}_\Delta^{-T} \cdot \vec{n}_n \delta J_\Delta \right) = \\
\quad - \int\limits_{\Omega_n} (\mathrm{grad}_n \vec{w})^T : \hat{\boldsymbol{F}}_\Delta^{-1} \cdot (-\hat{p}\boldsymbol{I} + \hat{\boldsymbol{\tau}})\hat{J}_\Delta + \\
\quad \int\limits_{\Gamma_n} n\vec{w} \cdot (\hat{\boldsymbol{\sigma}} \cdot (\hat{\boldsymbol{F}}_\Delta^{-T} \cdot \vec{n}_n))\hat{J}_\Delta \\
\int\limits_{\Omega_n} q \left((\hat{J} - 1)\delta J_\Delta + \delta J \hat{J}_\Delta \right) = - \int\limits_{\Omega_n} q(\hat{J} - 1)\hat{J}_\Delta
\end{array}
\right. \tag{5.5.1.10}
$$

Note that the right hand side of the first equation expresses the imbalance of momentum in the estimated configuration, as a consequence of the errors $\delta\boldsymbol{\tau}$, δp, $\delta\boldsymbol{F}_\Delta^{-1}$, δJ_Δ in the left hand side. This imbalance is used to iteratively reduce these errors. Commonly, in this iteration process the left hand side is approximated by neglecting the surface integral and the integral related to the error δJ_Δ. This might reduce convergence speed but will not influence the final solution, since no approximation is performed in the right hand side. Similarly, the right hand side of the second equation expresses the imbalance of mass, due to the errors δJ and δJ_Δ. Here, commonly the term with the error δJ_Δ is excluded in the iteration procedure.

If the error $\delta\vec{x}$ is sufficiently small, the errors $\delta\boldsymbol{F}_\Delta^{-1}$, δJ and $\delta\boldsymbol{\tau}$ can be written as (van de Vosse, 2003)[2]

$$
\begin{array}{rcl}
\delta\boldsymbol{F}_\Delta^{-1} & = & -\hat{\boldsymbol{F}}_\Delta^{-1} \cdot (\mathrm{grad}\, \delta\vec{x})^T \\
\delta J & = & \hat{J}(\mathrm{grad} \cdot \delta\vec{x}) \\
\delta J_\Delta & = & J_\Delta(\mathrm{grad} \cdot \delta\vec{x}) \\
\delta\boldsymbol{\tau} & = & {}^4\hat{\boldsymbol{M}} : (\mathrm{grad}\, \delta\vec{x})^T
\end{array} \tag{5.5.1.11}
$$

where the tensor ${}^4\hat{\boldsymbol{M}}$ is related to the stiffness of the material in the estimated configuration, and depends on the choice of the constitutive relation.

Neglecting the left hand side terms, discussed above, and using (5.5.1.5) and (5.5.1.11), equation (5.5.1.10) can be rewritten with respect to the estimated configuration $\hat{\Omega}$ as:

$$
\left\{
\begin{array}{l}
\int\limits_{\hat{\Omega}} (\widehat{\mathrm{grad}}\, \vec{w})^T : ({}^4\hat{\boldsymbol{M}} : (\widehat{\mathrm{grad}}\, \delta\vec{x})^T) - \\
\int\limits_{\hat{\Omega}} (\widehat{\mathrm{grad}}\, \vec{w})^T : (\widehat{\mathrm{grad}}\, \delta\vec{x})^T \cdot (-\hat{p}\boldsymbol{I} + \hat{\boldsymbol{\tau}}) + \\
\int\limits_{\hat{\Omega}} (\widehat{\mathrm{grad}}\, \vec{w})^T : (-\hat{p}\boldsymbol{I} + \hat{\boldsymbol{\tau}})(\mathrm{grad} \cdot \delta\vec{x}) + \\
\quad \int\limits_{\hat{\Omega}} (\widehat{\mathrm{grad}}\, \vec{w})^T : (-\delta p\boldsymbol{I}) = \\
\quad - \int\limits_{\hat{\Omega}} (\widehat{\mathrm{grad}}\, \vec{w})^T : (-\hat{p}\boldsymbol{I} + \hat{\boldsymbol{\tau}}) + \int\limits_{\Gamma_n} h\vec{w} \cdot (\hat{\boldsymbol{\sigma}} \cdot \hat{\vec{n}}) \\
\int\limits_{\hat{\Omega}} q\hat{J}(\mathrm{grad} \cdot \delta\vec{x}) = - \int\limits_{\hat{\Omega}} q(\hat{J} - 1)
\end{array}
\right. \tag{5.5.1.12}
$$

[2] Use $\boldsymbol{F}_\Delta^{-1} = (\hat{\boldsymbol{F}}_\Delta + \delta\boldsymbol{F}_\Delta)^{-1} = [\hat{\boldsymbol{F}}_\Delta \cdot (\boldsymbol{I} + \hat{\boldsymbol{F}}_\Delta^{-1} \cdot \delta\boldsymbol{F}_\Delta)]^{-1} = (\boldsymbol{I} + \hat{\boldsymbol{F}}_\Delta^{-1} \cdot \delta\boldsymbol{F}_\Delta)^{-1} \cdot \hat{\boldsymbol{F}}_\Delta^{-1} \approx (\boldsymbol{I} - \hat{\boldsymbol{F}}_\Delta^{-1} \cdot \delta\boldsymbol{F}_\Delta) \cdot \hat{\boldsymbol{F}}_\Delta^{-1} = \hat{\boldsymbol{F}}_\Delta^{-1} - \hat{\boldsymbol{F}}_\Delta^{-1} \cdot \delta\boldsymbol{F}_\Delta \cdot \hat{\boldsymbol{F}}_\Delta^{-1} = \hat{\boldsymbol{F}}_\Delta^{-1} - \hat{\boldsymbol{F}}_\Delta^{-1} \cdot (\hat{\boldsymbol{F}}_\Delta^{-T} \cdot \delta\boldsymbol{F}_\Delta^T)^T = \hat{\boldsymbol{F}}_\Delta^{-1} - \hat{\boldsymbol{F}}_\Delta^{-1} \cdot (\hat{\boldsymbol{F}}_\Delta^{-T} \cdot \mathrm{grad}_n \delta\vec{x})^T = \hat{\boldsymbol{F}}_\Delta^{-1} - \hat{\boldsymbol{F}}_\Delta^{-1} \cdot (\mathrm{grad}\, \delta\vec{x})^T$; $J = \det(\boldsymbol{F}) = \det(\hat{\boldsymbol{F}} + \delta\boldsymbol{F}) = \det((\boldsymbol{I} \cdot (\delta\boldsymbol{F} \cdot \hat{\boldsymbol{F}}^{-1}) \cdot \hat{\boldsymbol{F}}) = \det(\boldsymbol{I} \cdot \delta\boldsymbol{F} \cdot \hat{\boldsymbol{F}}^{-1}) \det(\hat{\boldsymbol{F}}) \approx \hat{J}(1 + \mathrm{tr}\,(\delta\boldsymbol{F} \cdot \hat{\boldsymbol{F}}^{-1})) = \hat{J} + \hat{J}\mathrm{tr}\,((\hat{\boldsymbol{F}}^{-T} \cdot \delta\boldsymbol{F}^T)^T) = \hat{J} + \hat{J}\mathrm{tr}\,((\hat{\boldsymbol{F}}^{-T} \cdot \mathrm{grad}_0 \delta\vec{x})^T) = \hat{J} + \hat{J}\mathrm{tr}\,((\mathrm{grad}\, \delta\vec{x})^T) = \hat{J} + \hat{J}(\mathrm{grad} \cdot \delta\vec{x})$.

Elaboration of the linearized weighted residual formulation

We will now transform the coordinate free equation (5.5.1.12) into a matrix formulation with respect to a Cartesian basis in 3D space. For clarity, we omit the indication that all quantities are taken with respect to the estimated configuration $\hat{\Omega}$.

First we store the components of the tensor grad $\vec{w}$ in a column $\underset{\sim}{H}_w$:

$$\begin{aligned} \underset{\sim}{H}_w &= \begin{bmatrix} \frac{\partial\partial w_1}{\partial\partial x_1} & \frac{\partial\partial w_2}{\partial\partial x_2} & \frac{\partial\partial w_3}{\partial\partial x_3} & \frac{\partial\partial w_2}{\partial\partial x_1} & \frac{\partial\partial w_3}{\partial\partial x_2} & \frac{\partial\partial w_1}{\partial\partial x_3} & \frac{\partial\partial w_1}{\partial\partial x_2} & \frac{\partial\partial w_2}{\partial\partial x_3} & \frac{\partial\partial w_3}{\partial\partial x_1} \end{bmatrix}^T \\ &= [H_{w11}\ H_{w22}\ H_{w33}\ H_{w12}\ H_{w23}\ H_{w31}\ H_{w21}\ H_{w32}\ H_{w13}]^T \end{aligned} \tag{5.5.1.13}$$

Similarly, the components of grad $\delta\vec{x}$ are stored as:

$$\begin{aligned} \underset{\sim}{H}_{\delta x} &= \begin{bmatrix} \frac{\partial\partial\delta x_1}{\partial\partial x_1} & \frac{\partial\partial\delta x_2}{\partial\partial x_2} & \frac{\partial\partial\delta x_3}{\partial\partial x_3} & \frac{\partial\partial\delta x_2}{\partial\partial x_1} & \frac{\partial\partial\delta x_3}{\partial\partial x_2} & \frac{\partial\partial\delta x_1}{\partial\partial x_3} & \frac{\partial\partial\delta x_1}{\partial\partial x_2} & \frac{\partial\partial\delta x_2}{\partial\partial x_3} & \frac{\partial\partial\delta x_3}{\partial\partial x_1} \end{bmatrix}^T \\ &= [H_{\delta x11}\ H_{\delta x22}\ H_{\delta x33}\ H_{\delta x12}\ H_{\delta x23}\ H_{\delta x31}\ H_{\delta x21}\ H_{\delta x32}\ H_{\delta x13}]^T \end{aligned} \tag{5.5.1.14}$$

Next, because equation (5.5.1.12) contains terms $(\text{grad}\,\vec{w})^T : \boldsymbol{A}$, we evaluate the double dot product:

$$\begin{aligned} (\text{grad}\,\vec{w})^T : \boldsymbol{A} &= \boldsymbol{H}_w : \boldsymbol{A} \\ &= H_{w11}A_{11} + H_{w22}A_{22} + H_{w33}A_{33} + \\ &\quad H_{w12}A_{21} + H_{w23}A_{32} + H_{w31}A_{13} + \\ &\quad H_{w21}A_{12} + H_{w32}A_{23} + H_{w13}A_{31} \\ &= \underset{\sim}{H}_w^T \underset{\approx}{A} \end{aligned} \tag{5.5.1.15}$$

which defines how the components of $\boldsymbol{A}$ are stored in $\underset{\approx}{A}$:

$$\underset{\approx}{A} = [A_{11} \quad A_{22} \quad A_{33} \quad A_{21} \quad A_{32} \quad A_{13} \quad A_{12} \quad A_{23} \quad A_{31}]^T \tag{5.5.1.16}$$

Note that the storage of components of $\boldsymbol{A}$ in $\underset{\approx}{A}$ differs from the storage of components of $\boldsymbol{H}_w$ in $\underset{\sim}{H}_w$. Now we consider the first term in (5.5.1.12), which is transformed as:

$$\int\limits_{\Omega_t} (\text{grad}\,\vec{w})^T : ({}^4\boldsymbol{M} : (\text{grad}\,\delta\vec{x})^T)\, d\Omega_t = \int\limits_{\Omega_t} \underset{\sim}{H}_w^T \underset{=}{D}_T \underset{\sim}{H}_{\delta x}\, d\Omega_t \tag{5.5.1.17}$$

Comparison with equation (5.5.1.15) shows that the term ${}^4\boldsymbol{M} : (\text{grad}\,\delta\vec{x})^T$, which in fact represents the error in $\boldsymbol{\tau}$ must regarded as an example of a tensor $\boldsymbol{A}$. Thus the components of $\delta\boldsymbol{\tau}$ must be stored in a column $\delta\underset{\approx}{\tau}$ according to sequence in equation (5.5.1.16). In combination with equation (5.5.1.14) this defines how the components of ${}^4\boldsymbol{M}$ are stored in $\underset{=}{D}_T$. In section 5.5.1 some examples of $\underset{=}{D}_T$ will be elaborated.

The second term in (5.5.1.12) is transformed as:

$$-\int\limits_{\Omega_t} (\text{grad}\,\vec{w})^T : (\text{grad}\,\delta\vec{x})^T \cdot \boldsymbol{\sigma}\, d\Omega_t = \int\limits_{\Omega_t} \underset{\sim}{H}_w^T \underset{=}{D}_F \underset{\sim}{H}_{\delta x}\, d\Omega_t \tag{5.5.1.18}$$

The term $(\text{grad}\,\delta\vec{x})^T \cdot \boldsymbol{\sigma}$ is transformed into $\underline{D}_F \underset{\sim}{H}_{\delta x}$ as follows:

$$
\begin{aligned}
& -(\text{grad}\,\delta\vec{x})^T \cdot \boldsymbol{\sigma} = \\
& - \begin{bmatrix} H_{\delta x11} & H_{\delta x12} & H_{\delta x13} \\ H_{\delta x21} & H_{\delta x22} & H_{\delta x23} \\ H_{\delta x31} & H_{\delta x32} & H_{\delta x33} \end{bmatrix} \quad \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} \\
= \; & - \begin{bmatrix}
\sigma_{11} & 0 & 0 & \sigma_{12} & 0 & 0 & 0 & 0 & \sigma_{31} \\
0 & \sigma_{22} & 0 & 0 & \sigma_{23} & 0 & \sigma_{12} & 0 & 0 \\
0 & 0 & \sigma_{33} & 0 & 0 & \sigma_{31} & 0 & \sigma_{23} & 0 \\
0 & \sigma_{12} & 0 & 0 & \sigma_{31} & 0 & \sigma_{11} & 0 & 0 \\
0 & 0 & \sigma_{23} & 0 & 0 & \sigma_{12} & 0 & \sigma_{22} & 0 \\
\sigma_{31} & 0 & 0 & \sigma_{23} & 0 & 0 & 0 & 0 & \sigma_{33} \\
\sigma_{12} & 0 & 0 & \sigma_{22} & 0 & 0 & 0 & 0 & \sigma_{23} \\
0 & \sigma_{23} & 0 & 0 & \sigma_{33} & 0 & \sigma_{32} & 0 & 0 \\
0 & 0 & \sigma_{31} & 0 & 0 & \sigma_{11} & 0 & \sigma_{12} & 0
\end{bmatrix}
\begin{bmatrix} H_{\delta x11} \\ H_{\delta x22} \\ H_{\delta x33} \\ H_{\delta x12} \\ H_{\delta x23} \\ H_{\delta x31} \\ H_{\delta x21} \\ H_{\delta x32} \quad H_{\delta x13} \end{bmatrix} \\
= \; & \underline{D}_F \underset{\sim}{H}_{\delta x}
\end{aligned}
\tag{5.5.1.19}
$$

which defines the matrix $\underline{D}_F$.

The third term in (5.5.1.12) is transformed as:

$$
\int_{\hat{\Omega}} (\text{grad}\,\vec{w})^T : \boldsymbol{\sigma}(\text{grad} \cdot \delta\vec{x}) = \int_{\Omega_t} \underset{\sim}{H}_w^T \underline{D}_J \underset{\sim}{H}_{\delta x} \, d\Omega_t \tag{5.5.1.20}
$$

Here the term $\boldsymbol{\sigma}(\text{grad} \cdot \delta\vec{x})$ is elaborated as:

$$
\begin{aligned}
\boldsymbol{\sigma}(\text{grad} \cdot \delta\vec{x}) \; &= \; \text{tr}\,(\boldsymbol{H}_{\delta x})\boldsymbol{\sigma} \\
&= \; (H_{\delta x,11} + H_{\delta x,22} + H_{\delta x,33}) \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} \\
&= \; \begin{bmatrix}
\sigma_{11} & \sigma_{11} & \sigma_{11} & 0 & 0 & 0 & 0 & 0 & 0 \\
\sigma_{22} & \sigma_{22} & \sigma_{22} & 0 & 0 & 0 & 0 & 0 & 0 \\
\sigma_{33} & \sigma_{33} & \sigma_{33} & 0 & 0 & 0 & 0 & 0 & 0 \\
\sigma_{21} & \sigma_{21} & \sigma_{21} & 0 & 0 & 0 & 0 & 0 & 0 \\
\sigma_{32} & \sigma_{32} & \sigma_{32} & 0 & 0 & 0 & 0 & 0 & 0 \\
\sigma_{13} & \sigma_{13} & \sigma_{13} & 0 & 0 & 0 & 0 & 0 & 0 \\
\sigma_{12} & \sigma_{12} & \sigma_{12} & 0 & 0 & 0 & 0 & 0 & 0 \\
\sigma_{23} & \sigma_{23} & \sigma_{23} & 0 & 0 & 0 & 0 & 0 & 0 \\
\sigma_{31} & \sigma_{31} & \sigma_{31} & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\begin{bmatrix} H_{\delta x11} \\ H_{\delta x22} \\ H_{\delta x33} \\ H_{\delta x12} \\ H_{\delta x23} \\ H_{\delta x31} \\ H_{\delta x21} \\ H_{\delta x32} \\ H_{\delta x13} \end{bmatrix} \\
&= \; \underline{D}_J \underset{\sim}{H}_{\delta x}
\end{aligned}
\tag{5.5.1.21}
$$

which defines the matrix $\underline{D}_J$.

Summarizing, equation (5.5.1.12) can now be written as:

$$
\left\{
\begin{aligned}
& \int_{\Omega_t} \underset{\sim}{H}_w^T \left[\underline{D}_T + \underline{D}_F + \underline{D}_J\right] \underset{\sim}{H}_{\delta x} \, d\Omega_t - \int_{\Omega_t} \delta p \text{grad} \cdot \vec{w} \, d\Omega_t = \\
& \qquad - \int_{\Omega_t} \underset{\sim}{H}_w^T \underset{\sim}{\sigma} \, d\Omega_t + \int_{\Gamma_n} t\vec{w} \cdot (\boldsymbol{\sigma} \cdot \vec{n}) \\
& \int_{\Omega_t} qJ(\text{grad} \cdot \delta\vec{x}) \, d\Omega_t = - \int_{\Omega_t} q(J-1) \, d\Omega_t
\end{aligned}
\right.
\tag{5.5.1.22}
$$

where once more it is noted that the integrals are taken over the estimated configuration.

Finite element approximation

To obtain a discrete set of finite element equations, the domain Ω is subdivided into non overlapping sub domains Ω^e, called elements. The position field is described by three components (x_1, x_2, x_3).

Within each element the components of position field x_j^e and the pressure field p^e are approximated as interpolations between values at a limited number of nodal points:

$$x_j^e(\vec{x},t) = \sum_{i=1}^{n_x} \phi^i(\vec{x}) x_j^i(t) = \underset{\sim}{\phi}^T \underset{\sim}{x}_j{}^e \qquad \forall \vec{x} \in \Omega^e \tag{5.5.1.23}$$

$$p^e(\vec{x},t) = \sum_{i=1}^{n_p} \psi^i(\vec{x}) p^i(t) = \underset{\sim}{\psi}^T \underset{\sim}{p}^e \qquad \forall \vec{x} \in \Omega^e \tag{5.5.1.24}$$

where n_x and n_p are the number of nodes for the position and pressure field, respectively, $\underset{\sim}{\phi} = [\phi^1, \dots, \phi^{n_x}]^T$ and $\underset{\sim}{\psi} = [\psi^1, \dots, \psi^{n_p}]^T$ columns of shape functions for the position and pressure field, respectively, and $\underset{\sim}{\vec{x}}^e = [\vec{x}^1, \dots, \vec{x}^{n_x}]^T$ and $\underset{\sim}{p}^e = [p^1, \dots, p^{n_p}]^T$ columns of nodal positions and pressures, respectively.

The weighting functions $\vec{w}$, with components (w_1, w_2, w_3), and q are defined on the element level as well, and discretized according to Galerkins method as:

$$w_j^e(\vec{x},t) = \sum_{i=1}^{n_x} \phi^i(\vec{x}) w_j^i(t) = \underset{\sim}{\phi}^T \underset{\sim}{w}_j{}^e \qquad \forall \vec{x} \in \Omega^e \tag{5.5.1.25}$$

$$q^e(\vec{x},t) = \sum_{i=1}^{n_p} \psi^i(\vec{x}) q^i(t) = \underset{\sim}{\psi}^T \underset{\sim}{q}^e \qquad \forall \vec{x} \in \Omega^e \tag{5.5.1.26}$$

We now reconsider the column $\underset{\sim}{H}_w$, defined in equation (5.5.1.13), which is written as:

$$\begin{aligned}
\underset{\sim}{H}_w &= \begin{bmatrix} \frac{\partial\partial w_1}{\partial\partial x_1} & \frac{\partial\partial w_2}{\partial\partial x_2} & \frac{\partial\partial w_3}{\partial\partial x_3} & \frac{\partial\partial w_2}{\partial\partial x_1} & \frac{\partial\partial w_3}{\partial\partial x_2} & \frac{\partial\partial w_1}{\partial\partial x_3} & \frac{\partial\partial w_1}{\partial\partial x_2} & \frac{\partial\partial w_2}{\partial\partial x_3} & \frac{\partial\partial w_3}{\partial\partial x_1} \end{bmatrix}^T \\
&= \begin{bmatrix} \frac{\partial\partial \underset{\sim}{\phi}^T \underset{\sim}{w}_1^e}{\partial\partial x_1} & \frac{\partial\partial \underset{\sim}{\phi}^T \underset{\sim}{w}_2^e}{\partial\partial x_2} & \frac{\partial\partial \underset{\sim}{\phi}^T \underset{\sim}{w}_3^e}{\partial\partial x_3} & \frac{\partial\partial \underset{\sim}{\phi}^T \underset{\sim}{w}_2^e}{\partial\partial x_1} & \frac{\partial\partial \underset{\sim}{\phi}^T \underset{\sim}{w}_3^e}{\partial\partial x_2} & \frac{\partial\partial \underset{\sim}{\phi}^T \underset{\sim}{w}_1^e}{\partial\partial x_3} & \frac{\partial\partial \underset{\sim}{\phi}^T \underset{\sim}{w}_1^e}{\partial\partial x_2} & \frac{\partial\partial \underset{\sim}{\phi}^T \underset{\sim}{w}_2^e}{\partial\partial x_3} & \frac{\partial\partial \underset{\sim}{\phi}^T \underset{\sim}{w}_3^e}{\partial\partial x_1} \end{bmatrix}^T \\
&= \begin{bmatrix}
\frac{\partial\partial\phi^1}{\partial\partial x_1} & 0 & 0 & \frac{\partial\partial\phi^2}{\partial\partial x_2} & 0 & 0 & \dots & \frac{\partial\partial\phi^{n_x}}{\partial\partial x_1} & 0 & 0 \\
0 & \frac{\partial\partial\phi^1}{\partial\partial x_2} & 0 & 0 & \frac{\partial\partial\phi^2}{\partial\partial x_2} & 0 & \dots & 0 & \frac{\partial\partial\phi^{n_x}}{\partial\partial x_2} & 0 \\
0 & 0 & \frac{\partial\partial\phi^1}{\partial\partial x_3} & 0 & 0 & \frac{\partial\partial\phi^2}{\partial\partial x_3} & \dots & 0 & 0 & \frac{\partial\partial\phi^{n_x}}{\partial\partial x_3} \\
0 & \frac{\partial\partial\phi^1}{\partial\partial x_1} & 0 & 0 & \frac{\partial\partial\phi^2}{\partial\partial x_1} & 0 & \dots & 0 & \frac{\partial\partial\phi^{n_x}}{\partial\partial x_1} & 0 \\
0 & 0 & \frac{\partial\partial\phi^1}{\partial\partial x_2} & 0 & 0 & \frac{\partial\partial\phi^2}{\partial\partial x_2} & \dots & 0 & 0 & \frac{\partial\partial\phi^{n_x}}{\partial\partial x_2} \\
\frac{\partial\partial\phi^1}{\partial\partial x_3} & 0 & 0 & \frac{\partial\partial\phi^2}{\partial\partial x_3} & 0 & 0 & \dots & \frac{\partial\partial\phi^{n_x}}{\partial\partial x_3} & 0 & 0 \\
\frac{\partial\partial\phi^1}{\partial\partial x_2} & 0 & 0 & \frac{\partial\partial\phi^2}{\partial\partial x_2} & 0 & 0 & \dots & \frac{\partial\partial\phi^{n_x}}{\partial\partial x_2} & 0 & 0 \\
0 & \frac{\partial\partial\phi^1}{\partial\partial x_3} & 0 & 0 & \frac{\partial\partial\phi^2}{\partial\partial x_3} & 0 & \dots & 0 & \frac{\partial\partial\phi^{n_x}}{\partial\partial x_3} & 0 \\
0 & 0 & \frac{\partial\partial\phi^1}{\partial\partial x_1} & 0 & 0 & \frac{\partial\partial\phi^2}{\partial\partial x_1} & \dots & 0 & 0 & \frac{\partial\partial\phi^{n_x}}{\partial\partial x_1}
\end{bmatrix}
\begin{bmatrix} w_1^1 \\ w_2^1 \\ w_3^1 \\ w_1^2 \\ w_2^2 \\ w_3^2 \\ \vdots \\ w_1^{n_x} \\ w_2^{n_x} \\ w_3^{n_x} \end{bmatrix} \\
&= \underset{\sim}{B}_\phi \underset{\sim}{w}^e
\end{aligned} \tag{5.5.1.27}$$

which defines the matrix $\underset{\sim}{B}_\phi$ and the column $\underset{\sim}{w}^e$. Similarly, we can write:

$$\underset{\sim}{H}_{\delta x} = \underset{\sim}{B}_\phi \delta \underset{\sim}{x}^e \tag{5.5.1.28}$$

where

$$\delta \underset{\sim}{x}^e = \begin{bmatrix} \delta x_1^1 & \delta x_2^1 & \delta x_3^1 & \delta x_1^2 & \delta x_2^2 & \delta x_3^2 & \dots & \delta x_1^{n_x} & \delta x_2^{n_x} & \delta x_3^{n_x} \end{bmatrix}^T \tag{5.5.1.29}$$

The dot product grad $\cdot\, \vec{w}$ is written as:

$$\begin{aligned}
\text{grad} \cdot \vec{w} &= \frac{\partial\partial w_1}{\partial\partial x_1} + \frac{\partial\partial w_2}{\partial\partial x_2} + \frac{\partial\partial w_3}{\partial\partial x_3} \\
&= \frac{\partial\partial \underset{\sim}{\phi}^e \underset{\sim}{w}_1^e}{\partial\partial x_1} + \frac{\partial\partial \underset{\sim}{\phi}^e \underset{\sim}{w}_2^e}{\partial\partial x_2} + \frac{\partial\partial \underset{\sim}{\phi}^e \underset{\sim}{w}_3^e}{\partial\partial x_3} \\
&= \begin{bmatrix} \frac{\partial\partial\phi^1}{\partial\partial x_1} & \frac{\partial\partial\phi^1}{\partial\partial x_2} & \frac{\partial\partial\phi^1}{\partial\partial x_3} & \frac{\partial\partial\phi^2}{\partial\partial x_1} & \frac{\partial\partial\phi^2}{\partial\partial x_2} & \frac{\partial\partial\phi^2}{\partial\partial x_3} & \dots & \frac{\partial\partial\phi^{n_x}}{\partial\partial x_1} & \frac{\partial\partial\phi^{n_x}}{\partial\partial x_2} & \frac{\partial\partial\phi^{n_x}}{\partial\partial x_3} \end{bmatrix} \underset{\sim}{w}_e \\
&= \underset{\sim}{b}_\phi^T \underset{\sim}{w}^e
\end{aligned} \tag{5.5.1.30}$$

which defines the column $\underset{\sim}{b}_\phi$. With this definition, we can also write:

$$\text{grad} \cdot \delta\vec{x} = \underset{\sim}{b}_\phi^T \delta\underset{\sim}{x}^e \tag{5.5.1.31}$$

Finally, we elaborate the integrand of the surface integral as:

$$\begin{aligned} \vec{w}\cdot(\boldsymbol{\sigma}\cdot\vec{n}) &= \vec{w}\cdot\vec{t} \\ &= w_1 t_1 + w_2 t_2 + w_3 t_3 && (5.5.1.32) \\ &= (\underset{\sim}{\Phi}\underset{\sim}{w}^e)^T \underset{\sim}{\Phi}\underset{\sim}{t}^e && (5.5.1.33) \end{aligned}$$

where the components of the surface traction vector $\vec{t}$ are stored in the column $\underset{\sim}{t}^e$ according to equation (5.5.1.27), and $\underset{\sim}{\Phi}$ contains the basis functions ϕ^i.

Substitution of the above expressions in equation (5.5.1.22) yields:

$$\left\{ \begin{array}{l} \sum_1^{n_{el}} \left(\int\limits_{\Omega_t^e} (\underline{B}_\phi \underset{\sim}{w}^e)^T \left[\underline{D}_T + \underline{D}_F + \underline{D}_J\right] \underline{B}_\phi \delta\underset{\sim}{x}^e \, d\Omega_t^e - \int\limits_{\Omega_t^e} \underset{\sim}{\psi}^T \delta\underset{\sim}{p}^e \underset{\sim}{b}_\phi^T \underset{\sim}{w}^e \, d\Omega_t^e \right) = \\ \qquad \sum_1^{n_{el}} \left(-\int\limits_{\Omega_t^e} (\underline{B}_\phi \underset{\sim}{w}^e)^T \underset{\sim}{\sigma} \, d\Omega_t^e + \int\limits_{\Gamma_n} te(\underset{\sim}{\Phi}\underset{\sim}{w}^e)^T \underset{\sim}{\Phi}\underset{\sim}{t}^e \right) \\ \sum_1^{n_{el}} \left(\int\limits_{\Omega_t^e} \underset{\sim}{\psi}^T \underset{\sim}{q}^e \underset{\sim}{b}_\phi \delta\underset{\sim}{x}^e \, d\Omega_t^e \right) = \sum_1^{n_{el}} \left(-\int\limits_{\Omega_t^e} \underset{\sim}{\psi}^T \underset{\sim}{q}^e \frac{\partial J - 1}{\partial J} \, d\Omega_t^e \right) \end{array} \right. \tag{5.5.1.34}$$

where it must be noted that, to eventually get a symmetric stiffness matrix, in the second equation all terms were divided by J. Now, since the columns $\underset{\sim}{w}^e$, $\underset{\sim}{q}^e$, $\delta\underset{\sim}{x}^e$ and $\delta\underset{\sim}{p}^e$ are constants, they can be taken outside the integrals, and we can write:

$$\left\{ \begin{array}{l} \sum_1^{n_{el}} \left((\underset{\sim}{w}^e)^T \underline{K}^e \delta\underset{\sim}{x}^e - (\underset{\sim}{w}^e)^T (\underline{P}^e)^T \delta\underset{\sim}{p}^e \right) = \sum_1^{n_{el}} \left((\underset{\sim}{w}^e)^T \underset{\sim}{r}_x^e \right) \\ \sum_1^{n_{el}} \left((\underset{\sim}{q}^e)^T \underline{P}^e \delta\underset{\sim}{x}^e \right) = \sum_1^{n_{el}} \left(-(\underset{\sim}{q}^e)^T \underset{\sim}{r}_p^e \right) \end{array} \right. \tag{5.5.1.35}$$

where we introduced:

$$\underline{K}^e = \int\limits_{\Omega_t^e} (\underline{B}_\phi)^T \left[\underline{D}_T + \underline{D}_F + \underline{D}_J\right] \underline{B}_\phi \, d\Omega_t^e \tag{5.5.1.36}$$

$$\underline{P}^e = \int\limits_{\Omega_t^e} \underset{\sim}{b}_\phi^T \underset{\sim}{\psi} \, d\Omega_t^e \tag{5.5.1.37}$$

$$\underset{\sim}{r}_x^e = \int\limits_{\Omega_t^e} (\underline{B}_\phi)^T \underset{\sim}{\sigma} \, d\Omega_t^e + \int\limits_{\Gamma_n} te(\underset{\sim}{\Phi})^T \underset{\sim}{\Phi}\underset{\sim}{t}^e \tag{5.5.1.38}$$

$$\underset{\sim}{r}_p^e = \int\limits_{\Omega_t^e} \underset{\sim}{\psi} \frac{\partial J - 1}{\partial J} \, d\Omega_t^e \tag{5.5.1.39}$$

Finally, is we assemble all element columns and matrices into columns and matrices at the global level, we obtain

$$\left\{ \begin{array}{l} \underset{\sim}{w}^T (\underline{K}\delta\underset{\sim}{x} - \underline{P}^T \delta\underset{\sim}{p}) = \underset{\sim}{w}^T \underset{\sim}{r}_x \\ \underset{\sim}{q}^T \underline{P}\delta\underset{\sim}{x} = \underset{\sim}{q}^T \underset{\sim}{r}_p \end{array} \right. \tag{5.5.1.40}$$

Since this equation must hold for all admissible weighting functions, it equivalent to the following set of linear equations:

$$\begin{bmatrix} \underline{K} & \underline{P}^T \\ \underline{P} & \underline{0} \end{bmatrix} \begin{bmatrix} \delta\underset{\sim}{x} \\ \delta\underset{\sim}{p} \end{bmatrix} = \begin{bmatrix} \underset{\sim}{r}_x \\ \underset{\sim}{r}_p \end{bmatrix} \tag{5.5.1.41}$$

which is the final finite element formulation of the governing equations.

Implementation of material behaviour

In this section the derivation of the material stiffness matrix $\underset{\sim}{D}_T$ is addressed for several material laws.

Incompressible Neo Hookean material

For an incompressible Neo Hookean material the following expression yields:

$$\boldsymbol{\tau} = G(\boldsymbol{B} - \boldsymbol{I}) \tag{5.5.1.42}$$

For the variation of $\boldsymbol{\tau}$ it holds:

$$\begin{aligned}
\delta\boldsymbol{\tau} &= G\delta\boldsymbol{B} \\
&= G\delta(\boldsymbol{F}\cdot\boldsymbol{F}^T) \\
&= G(\delta\boldsymbol{F}\cdot\boldsymbol{F}^T + \boldsymbol{F}\cdot\delta(\boldsymbol{F}^T)) \\
&= G((\mathrm{grad}_0\delta\vec{x})^T\cdot\boldsymbol{F}^T + \boldsymbol{F}\cdot(\mathrm{grad}_0\delta\vec{x})) \\
&= G((\boldsymbol{F}^T\cdot\mathrm{grad}\,\delta\vec{x})^T\cdot\boldsymbol{F}^T + \boldsymbol{F}\cdot(\boldsymbol{F}^T\cdot\mathrm{grad}\,\delta\vec{x})) \\
&= G((\mathrm{grad}\,\delta\vec{x})^T\cdot\boldsymbol{F}\cdot\boldsymbol{F}^T + \boldsymbol{F}\cdot\boldsymbol{F}^T\cdot(\mathrm{grad}\,\delta\vec{x})) \\
&= G(\boldsymbol{H}_{\delta x}\cdot\boldsymbol{B} + \boldsymbol{B}\cdot\boldsymbol{H}_{\delta x}^T)
\end{aligned} \tag{5.5.1.43}$$

The components of this tensor are stored in a column $\delta\underset{\approx}{\tau}$ according to the sequence of equation (5.5.1.16):

$$\delta\underset{\approx}{\tau} = [\delta\tau_{11}\ \delta\tau_{22}\ \delta\tau_{33}\ \delta\tau_{21}\ \delta\tau_{32}\ \delta\tau_{13}\ \delta\tau_{12}\ \delta\tau_{23}\ \delta\tau_{31}] \tag{5.5.1.44}$$

where a specific component $\delta\tau_{ij}$ is computed as:

$$\delta\tau_{ij} = G(H_{\delta x,ik}B_{ki} + B_{ik}H_{\delta x,jk}) \tag{5.5.1.45}$$

Then, for the matrix $\underset{\sim}{D}_T$ it holds:

$$\begin{aligned}
\delta\underset{\approx}{\tau} &= G\begin{bmatrix}
2B_{11} & 0 & 0 & 2B_{12} & 0 & 0 & 0 & 0 & 2B_{31} \\
0 & 2B_{22} & 0 & 0 & 2B_{23} & 0 & 2B_{12} & 0 & 0 \\
0 & 0 & 2B_{33} & 0 & 0 & 2B_{31} & 0 & 2B_{23} & 0 \\
B_{12} & B_{12} & 0 & B_{22} & B_{31} & 0 & B_{11} & 0 & B_{23} \\
0 & B_{23} & B_{23} & 0 & B_{33} & B_{12} & B_{31} & B_{22} & 0 \\
B_{31} & 0 & B_{31} & B_{23} & 0 & B_{11} & 0 & B_{12} & B_{33} \\
B_{12} & B_{12} & 0 & B_{22} & B_{31} & 0 & B_{11} & 0 & B_{23} \\
0 & B_{23} & B_{23} & 0 & B_{33} & B_{12} & B_{31} & B_{22} & 0 \\
B_{31} & 0 & B_{31} & B_{23} & 0 & B_{11} & 0 & B_{12} & B_{33}
\end{bmatrix}
\begin{bmatrix}
H_{\delta x11} \\ H_{\delta x22} \\ H_{\delta x33} \\ H_{\delta x12} \\ H_{\delta x23} \\ H_{\delta x31} \\ H_{\delta x21} \\ H_{\delta x32} \\ H_{\delta x13}
\end{bmatrix} \\
&= \underset{\sim}{D}_T\underset{\sim}{H}_{\delta x}
\end{aligned} \tag{5.5.1.46}$$

where symmetry of $\boldsymbol{B}$ was used. In SEPRAN, the matrix $\underset{\sim}{D}_T$ is computed in routine `elm200.f > elm8100.f > elm8200.f > el8302.f > el2730.f`.

Incompressible isotropic hyperelastic material

A more general example. In a compressible isotropic hyperelastic material, the stress can be derived from a strain energy function W_c:

$$W_c = W_c(I_1, I_2, I_3) \tag{5.5.1.47}$$

with invariants I_i defined as:

$$I_1 = \mathrm{tr}\,(\boldsymbol{C}) \tag{5.5.1.48}$$

$$I_2 = \partial\frac{1}{2}[\mathrm{tr}^2(\boldsymbol{C}) - \mathrm{tr}\,(\boldsymbol{C}^2)] \tag{5.5.1.49}$$

$$I_3 = \det(\boldsymbol{C}) = J^2 \tag{5.5.1.50}$$

where $J = \det(F)$ and the Cauchy-Green tensor $\boldsymbol{C}$ is defined as:

$$\boldsymbol{C} = \boldsymbol{F}^T \cdot \boldsymbol{F} \tag{5.5.1.51}$$

The Cauchy stress $\boldsymbol{\sigma}$ is related to W_c according to:

$$\boldsymbol{\sigma} = \frac{\partial 2}{\partial J}\boldsymbol{F} \cdot \frac{\partial dW_c}{\partial d\boldsymbol{C}} \cdot \boldsymbol{F}^T \tag{5.5.1.52}$$

If the material is incompressible, $I_3 = 1$, and the strain energy function W is a function of I_1 and I_2 only:

$$W = W(I_1, I_2) \tag{5.5.1.53}$$

Then the Cauchy stress is split according to equation (5.5.1.2) and the extra stress $\boldsymbol{\tau}$ is obtained from equation (5.5.1.52), yielding:

$$\boldsymbol{\tau} = 2\left[\frac{\partial\partial W}{\partial\partial I_1}\boldsymbol{B} - \frac{\partial\partial W}{\partial\partial I_2}\boldsymbol{B}^{-1}\right] = g_1(I_1, I_2)\boldsymbol{B} - g_2(I_1, I_2)\boldsymbol{B}^{-1} \tag{5.5.1.54}$$

which defines the functions g_1 and g_2. For the variation $\delta\boldsymbol{\tau}$ it holds (van Ooijen, 2003):

$$\begin{aligned}\delta\boldsymbol{\tau} \;&=\; \left(g_{11}\mathrm{tr}\,(\delta\boldsymbol{B}) + \partial\frac{1}{2}g_{12}(\mathrm{tr}\,(\boldsymbol{B})\mathrm{tr}\,(\delta\boldsymbol{B}) - \mathrm{tr}\,(\boldsymbol{B}\cdot\delta\boldsymbol{B}))\right)\boldsymbol{B} + g_1\delta\boldsymbol{B} + \\ &\left(g_{21}\mathrm{tr}\,(\delta\boldsymbol{B}) + \partial\frac{1}{2}g_{22}[(\mathrm{tr}\,(\boldsymbol{B})\mathrm{tr}\,(\delta\boldsymbol{B}) - \mathrm{tr}\,(\boldsymbol{B}\cdot\delta\boldsymbol{B}))\right)\boldsymbol{B}^{-1} + g_2\delta\boldsymbol{B}^{-1}\end{aligned} \tag{5.5.1.55}$$

with

$$g_{ij} = 2\frac{\partial\partial^2 W}{\partial\partial I_i \partial I_j} \tag{5.5.1.56}$$

and

$$\delta\boldsymbol{B} = \boldsymbol{H}_{\delta x}\cdot\boldsymbol{B} + \boldsymbol{B}\cdot\boldsymbol{H}_{\delta x}^T \tag{5.5.1.57}$$

$$\delta\boldsymbol{B}^{-1} = -\boldsymbol{H}_{\delta x}^T\cdot\boldsymbol{B}^{-1} - \boldsymbol{B}^{-1}\cdot\boldsymbol{H}_{\delta x} \tag{5.5.1.58}$$

With these expressions we derive:

$$\mathrm{tr}\,(\delta\boldsymbol{B}) = (\boldsymbol{B} + \boldsymbol{B}^T) : \boldsymbol{H}_{\delta x} \tag{5.5.1.59}$$

$$\mathrm{tr}\,(\boldsymbol{B}\cdot\delta\boldsymbol{B}) = (\boldsymbol{B}^2 + (\boldsymbol{B}^2)^T) : \boldsymbol{H}_{\delta x} \tag{5.5.1.60}$$

Substitution in equation (5.5.1.55) yields:

$$\begin{aligned}\delta\boldsymbol{\tau} \;=\;& g_1(\boldsymbol{H}_{\delta x}\cdot\boldsymbol{B} + \boldsymbol{B}\cdot\boldsymbol{H}_{\delta x}^T) - g_2(\boldsymbol{H}_{\delta x}^T\cdot\boldsymbol{B}^{-1} + \boldsymbol{B}^{-1}\cdot\boldsymbol{H}_{\delta x}) \\ &+\boldsymbol{V}_1(\boldsymbol{B}, \boldsymbol{B}^{-1})\boldsymbol{U}_1 : \boldsymbol{H}_{\delta x} + \boldsymbol{V}_2(\boldsymbol{B}, \boldsymbol{B}^{-1})\boldsymbol{U}_2 : \boldsymbol{H}_{\delta x}\end{aligned} \tag{5.5.1.61}$$

with:

$$\boldsymbol{V}_1 = (g_{11} + \partial\frac{1}{2}g_{12}\mathrm{tr}\,(\boldsymbol{B}))\boldsymbol{B} + (g_{21} + \partial\frac{1}{2}g_{22}\mathrm{tr}\,(\boldsymbol{B}))\boldsymbol{B}^{-1} \tag{5.5.1.62}$$

$$\boldsymbol{U}_1 = \boldsymbol{B} + \boldsymbol{B}^T \tag{5.5.1.63}$$

$$\boldsymbol{V}_2 = \partial\frac{1}{2}g_{12}\boldsymbol{B} + \partial\frac{1}{2}g_{22}\boldsymbol{B}^{-1} \tag{5.5.1.64}$$

$$\boldsymbol{U}_2 = \boldsymbol{B}^2 + (\boldsymbol{B}^2)^T \tag{5.5.1.65}$$

The general form of equation (5.5.1.61) is:

$$\delta\boldsymbol{\tau} = \boldsymbol{Q}\cdot\boldsymbol{H}_{\delta x} + \boldsymbol{R}\cdot\boldsymbol{H}_{\delta x}^T + \boldsymbol{H}_{\delta x}\cdot\boldsymbol{S} + \boldsymbol{H}_{\delta x}^T\cdot\boldsymbol{T} + \boldsymbol{V}(\boldsymbol{U} : \boldsymbol{H}_{\delta x}) \tag{5.5.1.66}$$

which is transformed into:

$$\begin{aligned}\delta\underset{\approx}{\tau} &= (\underset{\sim}{Q}+\underset{\sim}{R}+\underset{\sim}{S}+\underset{\sim}{T}+\underset{\approx}{V}\,\underset{\approx}{U}^T)\underset{\sim}{H}_{\delta x}\\ &= \underset{\sim}{D}_T\underset{\sim}{H}_{\delta x}\end{aligned} \tag{5.5.1.67}$$

where the components of $\delta\boldsymbol{\tau}$ are stored in $\delta\underset{\approx}{\tau}$ according to equation (5.5.1.44), and $\underset{\sim}{H}_{\delta x}$ was defined in equation (5.5.1.14). The matrices $\underset{\sim}{Q}$ through $\underset{\sim}{U}$ can be derived as:

$$\begin{aligned}\boldsymbol{Q}\cdot\boldsymbol{H}_{\delta x} &= \begin{bmatrix} Q_{11} & 0 & 0 & 0 & 0 & Q_{13} & Q_{12} & 0 & 0\\ 0 & Q_{22} & 0 & Q_{21} & 0 & 0 & 0 & Q_{23} & 0\\ 0 & 0 & Q_{33} & 0 & Q_{32} & 0 & 0 & 0 & Q_{31}\\ Q_{21} & 0 & 0 & 0 & 0 & Q_{23} & Q_{22} & 0 & 0\\ 0 & Q_{32} & 0 & Q_{31} & 0 & 0 & 0 & Q_{33} & 0\\ 0 & 0 & Q_{13} & 0 & Q_{12} & 0 & 0 & 0 & Q_{11}\\ 0 & Q_{12} & 0 & Q_{11} & 0 & 0 & 0 & Q_{13} & 0\\ 0 & 0 & Q_{23} & 0 & Q_{22} & 0 & 0 & 0 & Q_{21}\\ Q_{31} & 0 & 0 & 0 & 0 & Q_{33} & Q_{32} & 0 & 0 \end{bmatrix} \begin{bmatrix} H_{\delta x11}\\ H_{\delta x22}\\ H_{\delta x33}\\ H_{\delta x12}\\ H_{\delta x23}\\ H_{\delta x31}\\ H_{\delta x21}\\ H_{\delta x32}\\ H_{\delta x13} \end{bmatrix}\\ &= \underset{\sim}{Q}\underset{\sim}{H}_{\delta x}\end{aligned} \tag{5.5.1.68}$$

$$\begin{aligned}\boldsymbol{R}\cdot\boldsymbol{H}_{\delta x}^T &= \begin{bmatrix} R_{11} & 0 & 0 & R_{12} & 0 & 0 & 0 & 0 & R_{13}\\ 0 & R_{22} & 0 & 0 & R_{23} & 0 & R_{21} & 0 & 0\\ 0 & 0 & R_{33} & 0 & 0 & R_{31} & 0 & R_{32} & 0\\ R_{21} & 0 & 0 & R_{22} & 0 & 0 & 0 & 0 & R_{33}\\ 0 & R_{32} & 0 & 0 & R_{33} & 0 & R_{31} & 0 & 0\\ 0 & 0 & R_{13} & 0 & 0 & R_{11} & 0 & R_{12} & 0\\ 0 & R_{12} & 0 & 0 & R_{13} & 0 & R_{11} & 0 & 0\\ 0 & 0 & R_{23} & 0 & 0 & R_{21} & 0 & R_{22} & 0\\ R_{31} & 0 & 0 & R_{32} & 0 & 0 & 0 & 0 & R_{33} \end{bmatrix} \begin{bmatrix} H_{\delta x11}\\ H_{\delta x22}\\ H_{\delta x33}\\ H_{\delta x12}\\ H_{\delta x23}\\ H_{\delta x31}\\ H_{\delta x21}\\ H_{\delta x32}\\ H_{\delta x13} \end{bmatrix}\\ &= \underset{\sim}{R}\underset{\sim}{H}_{\delta x}\end{aligned} \tag{5.5.1.69}$$

$$\begin{aligned}\boldsymbol{H}_{\delta x}\cdot\boldsymbol{S} &= \begin{bmatrix} S_{11} & 0 & 0 & S_{21} & 0 & 0 & 0 & 0 & S_{31}\\ 0 & S_{22} & 0 & 0 & S_{32} & 0 & S_{12} & 0 & 0\\ 0 & 0 & S_{33} & 0 & 0 & S_{31} & 0 & S_{23} & 0\\ 0 & S_{21} & 0 & 0 & S_{13} & 0 & S_{11} & 0 & 0\\ 0 & 0 & S_{32} & 0 & 0 & S_{12} & 0 & S_{22} & 0\\ S_{13} & 0 & 0 & S_{23} & 0 & 0 & 0 & 0 & S_{33}\\ S_{12} & 0 & 0 & S_{22} & 0 & 0 & 0 & 0 & S_{32}\\ 0 & S_{23} & 0 & 0 & S_{33} & 0 & S_{13} & 0 & 0\\ 0 & 0 & S_{31} & 0 & 0 & S_{11} & 0 & S_{21} & 0 \end{bmatrix} \begin{bmatrix} H_{\delta x11}\\ H_{\delta x22}\\ H_{\delta x33}\\ H_{\delta x12}\\ H_{\delta x23}\\ H_{\delta x31}\\ H_{\delta x21}\\ H_{\delta x32}\\ H_{\delta x13} \end{bmatrix}\\ &= \underset{\sim}{S}\underset{\sim}{H}_{\delta x}\end{aligned} \tag{5.5.1.70}$$

$$\begin{aligned}\boldsymbol{H}_{\delta x}^T\cdot\boldsymbol{T} &= \begin{bmatrix} T_{11} & 0 & 0 & 0 & 0 & T_{31} & T_{21} & 0 & 0\\ 0 & T_{22} & 0 & T_{12} & 0 & 0 & 0 & T_{32} & 0\\ 0 & 0 & T_{33} & 0 & T_{23} & 0 & 0 & 0 & T_{13}\\ 0 & T_{21} & 0 & T_{11} & 0 & 0 & 0 & T_{31} & 0\\ 0 & 0 & T_{32} & 0 & T_{22} & 0 & 0 & 0 & T_{12}\\ T_{13} & 0 & 0 & 0 & 0 & T_{33} & T_{23} & 0 & 0\\ T_{12} & 0 & 0 & 0 & 0 & T_{32} & T_{22} & 0 & 0\\ 0 & T_{23} & 0 & T_{13} & 0 & 0 & 0 & T_{33} & 0\\ 0 & 0 & T_{31} & 0 & T_{21} & 0 & 0 & 0 & T_{11} \end{bmatrix} \begin{bmatrix} H_{\delta x11}\\ H_{\delta x22}\\ H_{\delta x33}\\ H_{\delta x12}\\ H_{\delta x23}\\ H_{\delta x31}\\ H_{\delta x21}\\ H_{\delta x32}\\ H_{\delta x13} \end{bmatrix}\\ &= \underset{\sim}{T}\underset{\sim}{H}_{\delta x}\end{aligned} \tag{5.5.1.71}$$

$$
\begin{aligned}
\boldsymbol{V}(\boldsymbol{U}:\boldsymbol{H}_{\delta x}) &= \begin{bmatrix} V_{11} \\ V_{22} \\ V_{33} \\ V_{21} \\ V_{32} \\ V_{13} \\ V_{12} \\ V_{23} \\ V_{31} \end{bmatrix} \begin{bmatrix} U_{11} \\ U_{22} \\ U_{33} \\ U_{21} \\ U_{32} \\ U_{13} \\ U_{12} \\ U_{23} \\ U_{31} \end{bmatrix}^T \begin{bmatrix} H_{\delta x11} \\ H_{\delta x22} \\ H_{\delta x33} \\ H_{\delta x12} \\ H_{\delta x23} \\ H_{\delta x31} \\ H_{\delta x21} \\ H_{\delta x32} \\ H_{\delta x13} \end{bmatrix} \\
&= \underset{\approx}{V}\,\underset{\approx}{U}^T \underset{\sim}{H}_{\delta x}
\end{aligned}
\tag{5.5.1.72}
$$

Remark: This section is written by Tijmen Gunther and is compiled from work by Jurgen de Hart, Raoul van Loon, Chris van Ooijen, Marco Stijnen, Tijmen Gunther, Peter Bovendeerd and Frans van de Vosse of Eindhoven University.

6 Solidification problems

At this moment only the enthalpy method in Section 6.1 is described.

6.1 The enthalpy method

6.1.1 Problem description

The two-phase Stefan problem on a three-dimensional domain Ω with fixed outer boundary $\delta\Omega$ and moving boundary $\Gamma(t)$ is given by:

$$\begin{cases} \rho c \dfrac{\partial T(\boldsymbol{x},t)}{\partial t} = \nabla \cdot (\kappa \nabla T(\boldsymbol{x},t)) + Q(\boldsymbol{x},t) & \forall \boldsymbol{x} \in \Omega_{1,2}, t > 0 \qquad (6.1.1a) \\ +\rho L v_n = \left[\kappa \dfrac{\partial T}{\partial n}\right] & \text{for } \boldsymbol{x} = \Gamma(t), t > 0 \qquad (6.1.1b) \\ T(\boldsymbol{x},0) = \bar{T}_1(\boldsymbol{x}) & \forall \boldsymbol{x} \in \Omega_{1,2}, t > 0 \qquad (6.1.1c) \end{cases}$$

where we have set $t_0 = 0$, together with one or more of the following boundary conditions on the complementary parts $\delta\Omega_i, i = 1,2,3$ of the fixed outer boundary $\delta\Omega = \bigcup_{i=1}^{3} \delta\Omega_i$:

1. A Dirichlet condition on $\delta\Omega_1$:
$$T = \bar{T}_2(\boldsymbol{x}). \qquad (6.1.2)$$
2. A Neumann condition on $\delta\Omega_2$:
$$\kappa(T)\frac{\partial T}{\partial \boldsymbol{n}}(\boldsymbol{x}) = \bar{q}(\boldsymbol{x}), \qquad (6.1.3)$$
where $\mathbf{n}$ is the outward unit normal to the boundary surface, and $\bar{q}(\boldsymbol{x})$ a given normal heat flux.
3. A radiation-type boundary condition on $\delta\Omega_3$:
$$\kappa(T)\frac{\partial T}{\partial \boldsymbol{n}}(\boldsymbol{x}) = \bar{\alpha}(T), \qquad (6.1.4)$$
where $\bar{\alpha}(T)$ is a non-linear function of temperature.

In the enthalpy formulation the heat conduction equation and the Stefan condition are replaced by what is known as the enthalpy equation (in differential form):

$$H_t + \operatorname{div} \mathbf{q} = Q, \qquad (6.1.5)$$

where H is the enthalpy function. In this study we will mostly restrict ourselves to isothermal phase-change (that is, a melting point $T = T_m$, instead of a melting trajectory). Besides, we will consider only problems in which the physical parameters $\rho, c_s, c_l, \kappa_s, \kappa_l$ are constants. Subject to these assumptions, the enthalpy function is given by:

$$H = \begin{cases} \rho c_s (T - T_m), & T \leq T_m \\ \rho c_l (T - T_m) + \rho L, & T > T_m \end{cases} \qquad (6.1.6)$$

6.1.2 Employing the Kirchoff transform

According to Alexiades and Solomon (1993), p. 216, the Kirchoff temperature is "the best choice for the enthalpy scheme since it is consistent with the mushy nodes being treated as isothermal." Besides, "faster convergence is observed in the iterative scheme, making it more efficient", Alexiades and Solomon (1993), p. 224. Alexiades et al. present the enthalpy formulation, which could be referred to as "Voller's enthalpy formulation", in Alexiades and Solomon (1993), Chapter 4.3.E. Because of the inherent advantages of applying the Kirchoff transform, we next present the enthalpy formulation and consecutively the Elliott-Ockendon SOR scheme, in case the Kirchoff transformation is applied.

The normalized Kirchoff transformed temperature for constant κ_s, κ_l is given by

$$u = \begin{cases} \kappa_s(T - T_m) & T < T_m \\ 0 & T = T_m \\ \kappa_l(T - T_m) & T > T_m \end{cases}. \tag{6.1.1}$$

The corresponding enthalpy is

$$H = \begin{cases} \frac{\rho c_s u}{\kappa_s} & u \leq 0 \\ \frac{\rho c_l u}{\kappa_l} + \rho L & u > 0 \end{cases}. \tag{6.1.2}$$

The 1D finite volumes discretization of equation (6.1.5), using central differences in space and Euler backward in time, yields:

$$\frac{H_i^{n+1} - H_i^n}{\Delta t_n} - \frac{u_{i-1}^{n+1} - 2u_i^{n+1} + u_{i+1}^{n+1}}{\Delta x^2} = Q_i^{n+1}, \tag{6.1.3}$$

which after rearranging terms results in:

$$H_i^{n+1} + 2\frac{\Delta t}{\Delta x^2} u_i^{n+1} = \Delta t Q_i^{n+1} + H_i^n + \frac{\Delta t}{\Delta x^2}(u_{j-1}^{(p+1)} + u_{j+1}^{(p)}). \tag{6.1.4}$$

By giving names to the known terms, as in Alexiades and Solomon (1993):

$$C_j = 2\frac{\Delta t}{\Delta x^2}, \tag{6.1.5}$$

$$b_j^n = \Delta t Q_i^{n+1} + H_i^n, \tag{6.1.6}$$

$$z_j^{(p)} = b_j^n + \frac{\Delta t}{\Delta x^2}(u_{j-1}^{(p+1)} + u_{j+1}^{(p)}), \tag{6.1.7}$$

$$\tag{6.1.8}$$

where the superscript (p) denotes the iteration number, and n the previous time level, we have the following system of equations (Gauss-Seidel):

$$H_j^{(p+1)} + C_j u_j^{(p+1)} = z_j^{(p)}. \tag{6.1.9}$$

Consequently, the iteration process transforms into:

1. Compute C_j and $z_j^{(p)}$.
2. Compute $\tilde{u}_j^{(p+1)}$ from

$$\tilde{u}_j^{(p+1)} = \begin{cases} \frac{z_j^{(p)}}{\rho c_s/\kappa_s + C_j} & z_j^{(p)} \leq 0, \\ 0 & 0 < z_j^{(p)} < \rho L, \\ \frac{z_j^{(p)} - \rho L}{\rho c_l/\kappa_l + C_j} & z_j^{(p)} \geq \rho L \end{cases}. \tag{6.1.10}$$

3. Set $\hat{u}_j^{(p+1)} = u_j^{(p)} + \omega[\tilde{u}_j^{(p+1)} - u_j^{(p)}]$ (Over-relaxation).
4. Set

$$u_j^{(p+1)} = \begin{cases} \hat{u}_j^{(p+1)} & \text{if } \hat{u}_j^{(p+1)} \cdot u_j^{(p)} > 0, \\ \tilde{u}_j^{(p+1)} & \text{if } \tilde{u}_j^{(p+1)} \cdot u_j^{(p)} \leq 0 \end{cases}, \tag{6.1.11}$$

that is, only over-relax the nodes that have not just changed phase.

5. If a convergence criterion, say $\|u_j^{(p+1)} - u_j^{(p)}\| < tolerance$, is satisfied, then set $u_j^{n+1} = u_j^{(p+1)}$, hence

$$T_j^{n+1} = \begin{cases} T_m + u_j^{n+1}/\kappa_s & u_j^{n+1} < 0, \\ T_m & u_j^{n+1} = 0, , \\ T_m + u_j^{n+1}/\kappa_l & u_j^{n+1} > 0, \end{cases} \tag{6.1.12}$$

and $H_j^{n+1} = z_j^{(p)} - C_j \cdot u_j^{n+1}$.

6.1.3 Sepran implementation

The Sepran implementation of "Voller's method" in combination with Elliott-Ockendon SOR requires some adjustments to be made with concern to the solution algorithm. Next we present a short overview of the finite element equivalent to the previously described finite volume formulation.

Starting point is the enthalpy equation:

$$\frac{\partial H}{\partial t} - \nabla(\kappa \nabla T) = Q, \tag{6.1.1}$$

subject to the boundary conditions on the disjunct boundaries $\partial\Omega_1, \partial\Omega_2$, $\partial\Omega_1 \cup \partial\Omega_2 = \partial\Omega$:

$$T = T_1, \qquad \text{for } x \in \partial\Omega_1, \tag{6.1.2}$$

$$\frac{\partial T}{\partial x} = 0, \qquad \text{for } x \in \partial\Omega_2. \tag{6.1.3}$$

Using the standard basis functions ϕ and the standard Galerkin approximations

$$T(t) = \sum_{j=1}^{N+N_b} T_j(t)\phi_j, \qquad H(t) = \sum_{j=1}^{N+N_b} H_j(t)\phi_j, \tag{6.1.4}$$

where N denotes the number of nodal points $\notin \partial\Omega_1$, the system of Galerkin equations is given by:

$$\sum_{j=1}^{N+N_b} \left\{ \frac{\partial H_j}{\partial t} \int_\Omega \phi_j \phi_i d\Omega + T_j \int_\Omega \kappa \nabla\phi_j \nabla\phi_i d\Omega \right\} = \int_\Omega Q_i \phi_i d\Omega, \tag{6.1.5}$$

for $i = 1, 2, \ldots, N$. Or in matrix-vector notation:

$$M\frac{\partial \mathbf{H}}{\partial t} + S\mathbf{T} = \mathbf{b}. \tag{6.1.6}$$

In case Euler backward is applied for the time integration, the final system is given by:

$$M\frac{\mathbf{H}^{n+1} - \mathbf{H}^n}{\Delta t} + S\mathbf{T}^{n+1} = \mathbf{b}^{n+1}. \tag{6.1.7}$$

If we let $\tilde{M}$ be the lumped version of the mass matrix M and D the diagonal of the stiffness matrix S, then for a Kirchoff transformed temperature u the third step of the iteration process as described in Section 6.1.2 is replaced by: Compute $\tilde{u}_j^{(p+1)}$ from

$$\tilde{u}_j^{(p+1)} = \begin{cases} \frac{z_j^{(p)}}{D_{jj}\Delta t + \tilde{M}_{jj}\rho c_s/\kappa_s} & z_j^{(p)} \leq 0, \\ 0 & 0 < z_j^{(p)} < \rho L, . \\ \frac{z_j^{(p)} - \tilde{M}_{jj}\rho L}{D_{jj}\Delta t + \tilde{M}_{jj}\rho c_l/\kappa_l} & z_j^{(p)} \geq \rho L \end{cases} \tag{6.1.8}$$

The enthalpy is updated according to:

$$H_j^{n+1} = (z_j^{(p)} - D_{jj}\Delta t \cdot u_j^{n+1})/\tilde{M}_{jj} \tag{6.1.9}$$

7 Flow problems

This chapter contains a description of the theory of the flow problems. At this moment only a part of Chapter 7 concerning incompressible flow has been written.

7.1 The isothermal laminar flow of incompressible or slightly compressible liquids

At this moment only a part of Section 7.1 concerning surface tension has been written.

7.1.1 Computation of the surface tension

The surface tension is an extra force acting on a surface. This tension is proportional to the curvature. The larger the local curvature the larger the surface tension. There are several ways to express the surface tension as part of the normal stress on the boundary. One way to express it is:

$$(\sigma_{ij}n_j)_{\text{surface\_tension}} = \frac{\gamma}{R}n_i \quad (R^2\text{only}) \tag{7.1.1.1}$$

or more general

$$(\sigma_{ij}n_j)_{\text{surface\_tension}} = 2\gamma H n_i \tag{7.1.1.2}$$

with γ the surface tension coefficient, σ_{ij} the components of the stress tensor and n_i the components of the outward normal.
H is the mean curvature defined by

$$H = \frac{1}{2}(\frac{1}{R_1} + \frac{1}{R_2}) \tag{7.1.1.3}$$

with R_1 and R_2 the radii corresponding to the principal curvatures. These curvatures can be taken in any set of orthogonal directions. Mark that in R^2 we have $R_2 = \infty$, so $2H = \frac{1}{R}$.
In some cases the curvature can be expressed explicitly in a formula like

- $R^2 \quad y = h(x)$ then $\frac{1}{R} = \frac{h_{xx}}{(1+h_x^2)^{\frac{3}{2}}}$
- R^2 axi-symmetric $\quad r = r(z)$ then $\frac{1}{R_1} = \frac{r_{zz}}{(1+r_z^2)^{\frac{3}{2}}}$; $\frac{1}{R_2} = -\frac{r_z}{r(1+r_z^2)^{\frac{1}{2}}}$
- $R^3 \quad z = h(x,y)$ then $H = \frac{(1+h_u^2)h_{uu} - 2h_u h_v h_{uv} + (1+h_u^2)h_{vv}}{(1+h_u^2+h_v^2)^{\frac{3}{2}}}$,
  with u and v coordinates along the free surface.

However, all these expressions are difficult to evaluate so it is easier to utilize the following expression:

$$2H = \text{div}\frac{\nabla s}{||\nabla s||} = -\text{div}(\mathbf{n}) \tag{7.1.1.4}$$

with $\mathbf{n}$ the outward normal and the free surface is given by $s(\mathbf{x}) = 0$.
Combination of (7.1.1.2) and (7.1.1.4) gives

$$(\sigma_{ij}n_j)_{\text{surface\_tension}} = -\gamma(n_{k,k})n_i \tag{7.1.1.5}$$

In some literature this term is written as

$$-(\gamma\nabla_s \cdot \mathbf{n})\mathbf{n} \tag{7.1.1.6}$$

where $\nabla_s \cdot \mathbf{n}$ denotes the curvature and ∇_s the surface gradient operator defined by

$$\nabla_s p = \frac{\partial p}{\partial s_1}\mathbf{t}_1 + \frac{\partial p}{\partial s_2}\mathbf{t}_2 \tag{7.1.1.7}$$

with $\mathbf{t}_1$ and $\mathbf{t}_2$ tangential vectors along the surfaces and s_1 and s_2 the coordinates along the corresponding coordinate directions.
These last expressions are important for the implementation in the finite element method. Consider for example momentum equations in case of the Stokes equation:

$$-\sigma_{ij,j} = \rho f_i \tag{7.1.1.8}$$

After constructing the weak formulation and the Galerkin method we get

$$\int_\Omega \sigma_{ij}(\phi_l)_{,j} d\Omega = \int_\Omega \rho f_i \phi_l d\Omega + \int_\Gamma \sigma_{ij} n_j \phi_l d\Gamma \tag{7.1.1.9}$$

So the surface tension part can be written as

$$\int_{\Gamma} 2\gamma H n_i \phi_l d\Gamma = -\gamma \int_{\Gamma} (n_{k,k}) n_i \phi_l d\Gamma \tag{7.1.1.10}$$

Expression (7.1.1.10) makes it natural to use integration by parts (Green's theorem on the surface) to get

$$-\gamma \int_{\Gamma} (n_{k,k}) n_i \phi_l d\Gamma = -\int_{\Gamma} (\gamma\phi_l)_{,i} d\Gamma + \int_{\partial\Gamma} \gamma \phi_l t_i ds \tag{7.1.1.11}$$

with $\partial\Gamma$ the boundary of Γ.
In R^2 the term on the boundary $\partial\Gamma$ is written as

$$\gamma [t_i \phi_l]_{l_1}^{l_2} = (\gamma t_i \phi_l)|_{l_2} - (\gamma t_i \phi_l)|_{l_1} \tag{7.1.1.12}$$

with l_1 and l_2 the begin and end point of the boundary $\partial\Gamma$. Mark that the last two terms can be prescribed by either prescribing the displacement of a point in which case the term vanishes, or by giving the contact angle. If the boundary is closed these terms obviously are not present.
In the axi-symmetric case we have to include both $\kappa_1 = \frac{1}{R_1}$ and $\kappa_2 = \frac{1}{R_2}$. The surface tension contribution in that case can be written as

$$2\pi \int_{\Gamma} \gamma(\kappa_1 + \kappa_2) n_i \phi_l r d\Gamma = 2\pi (\int_{\Gamma} \gamma \kappa_1 n_i \phi_l r d\Gamma + \int_{\Gamma} \gamma \kappa_2 n_i \phi_l r d\Gamma) \tag{7.1.1.13}$$

with Γ integration in the (r, z) plane. The first term in (7.1.1.13) can be written as (see 7.1.1.10):

$$2\pi \int_{\Gamma} \gamma \kappa_1 n_i \phi_l r d\Gamma = 2\pi \int_{\Gamma} \gamma \frac{dt_i}{ds} \phi_l r d\Gamma \tag{7.1.1.14}$$

Integration by parts gives:

$$2\pi \int_{\Gamma} \gamma \frac{dt_i}{ds} \phi_l r d\Gamma = -2\pi \int_{\Gamma} \gamma \frac{d\phi_l r}{ds} t_i d\Gamma + 2\pi\gamma [r t_i \phi_l]_{l_1}^{l_2} = -2\pi \int_{\Gamma} \gamma (r \frac{d\phi_l}{ds} + \phi_l \frac{dr}{ds}) t_i d\Gamma + 2\pi\gamma [r t_i \phi_l]_{l_1}^{l_2} \tag{7.1.1.15}$$

The second term in (7.1.1.13) can be written as

$$-2\pi \int_{\Gamma} \gamma \kappa_2 n_i \phi_l r d\Gamma = -2\pi \int_{\Gamma} \gamma \frac{r_z}{r(1+r_z^2)^{\frac{1}{2}}} \phi_l r d\Gamma = -2\pi (\int_{\Gamma} \gamma t_2 n_i \phi_l d\Gamma), \tag{7.1.1.16}$$

since

$$\mathbf{t} \;=\; \frac{1}{(1+r_z)^{\frac{1}{2}}} \begin{pmatrix} 1 \\ r_z \end{pmatrix} \tag{7.1.1.17}$$

8 Second order elliptic and parabolic equations using spectral elements

This chapter is under preparation

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