Boundary conditions in FPM for LIQUID solver

1. Free Surface BC

1.1. Standard Boundary Condition

The conditions at a free surface can be given by

$$\begin{aligned} \mathbf{a}^T \cdot \mathbf{S} \cdot \mathbf{n} &= \mathrm{Q_a} \\ \mathbf{b}^T \cdot \mathbf{S} \cdot \mathbf{n} &= \mathrm{Q_b} \\ \mathbf{n}^T \cdot \mathbf{S} \cdot \mathbf{n} - \mathrm{p} &= -\mathrm{p_0} \end{aligned} \tag{1.1}$$

The third condition will be already fulfilled for the pressure Poisson equation, therefore we replace system (1.1) by

$$\begin{aligned} \mathbf{a}^T \cdot \mathbf{S} \cdot \mathbf{n} &= \mathrm{Q_a} \\ \mathbf{b}^T \cdot \mathbf{S} \cdot \mathbf{n} &= \mathrm{Q_b} \\ div(\mathbf{v}) &= D \end{aligned} \tag{1.2}$$

This can be rewritten by

$$\begin{aligned} \eta \cdot \left(\frac{\partial \left(\mathbf{a}^T \cdot \mathbf{v} \right)}{\partial n} + \frac{\partial \left(\mathbf{n}^T \cdot \mathbf{v} \right)}{\partial a} \right) &= \mathrm{Q_a} \\ \eta \cdot \left(\frac{\partial \left(\mathbf{b}^T \cdot \mathbf{v} \right)}{\partial n} + \frac{\partial \left(\mathbf{n}^T \cdot \mathbf{v} \right)}{\partial b} \right) &= \mathrm{Q_b} \\ \frac{\partial \left(\mathbf{n}^T \cdot \mathbf{v} \right)}{\partial n} + \frac{\partial \left(\mathbf{a}^T \cdot \mathbf{v} \right)}{\partial a} + \frac{\partial \left(\mathbf{b}^T \cdot \mathbf{v} \right)}{\partial b} &= D \end{aligned} \tag{1.3}$$

Here, the direction $\mathbf{n}$ is the inward pointing normal of the free surface and the directions $\mathbf{a}$ and $\mathbf{b}$ are perpendicular to $\mathbf{n}$ and to each other. Thus, $\mathbf{a}$ and $\mathbf{b}$ are local tangential directions to the free surface.

Our aim now is to isolate the term $\frac{\partial \mathbf{v}}{\partial n}$ in order to apply Neumann-like boundary conditions to the free surface. Let us first assume that the boundary is smooth an we can rewrite the system (1.3)

$$
\begin{aligned}
\mathbf{a}^T \cdot \frac{\partial \mathbf{v}}{\partial n} &+ \mathbf{n}^T \cdot \frac{\partial \mathbf{v}}{\partial a} = \frac{\mathrm{Q_a}}{\eta} = \bar{\mathrm{Q}}_\mathrm{a} \\
\mathbf{b}^T \cdot \frac{\partial \mathbf{v}}{\partial n} &+ \mathbf{n}^T \cdot \frac{\partial \mathbf{v}}{\partial b} = \frac{\mathrm{Q_b}}{\eta} = \bar{\mathrm{Q}}_\mathrm{b} \\
\mathbf{n}^T \cdot \frac{\partial \mathbf{v}}{\partial n} &+ \mathbf{a}^T \cdot \frac{\partial \mathbf{v}}{\partial a} + \mathbf{b}^T \cdot \frac{\partial \mathbf{v}}{\partial b} = D
\end{aligned}
\tag{1.4}
$$

In matrix vector form, (1.4) looks

$$
\begin{pmatrix} \mathbf{a}^T \\ \mathbf{b}^T \\ \mathbf{n}^T \end{pmatrix} \cdot \frac{\partial \mathbf{v}}{\partial n} + \begin{pmatrix} \mathbf{n}^T \\ \mathbf{0} \\ \mathbf{a}^T \end{pmatrix} \cdot \frac{\partial \mathbf{v}}{\partial a} + \begin{pmatrix} \mathbf{0} \\ \mathbf{n}^T \\ \mathbf{b}^T \end{pmatrix} \cdot \frac{\partial \mathbf{v}}{\partial b} = \begin{pmatrix} \bar{\mathrm{Q}}_\mathrm{a} \\ \bar{\mathrm{Q}}_\mathrm{b} \\ D \end{pmatrix}
\tag{1.5}
$$

We multiply from left with the inverse of the leftmost matrix, i.e.

$$
\frac{\partial \mathbf{v}}{\partial n} + \begin{pmatrix} \mathbf{a} & \mathbf{b} & \mathbf{n} \end{pmatrix} \cdot \begin{pmatrix} \mathbf{n}^T \\ \mathbf{0} \\ \mathbf{a}^T \end{pmatrix} \cdot \frac{\partial \mathbf{v}}{\partial a} + \begin{pmatrix} \mathbf{a} & \mathbf{b} & \mathbf{n} \end{pmatrix} \cdot \begin{pmatrix} \mathbf{0} \\ \mathbf{n}^T \\ \mathbf{b}^T \end{pmatrix} \cdot \frac{\partial \mathbf{v}}{\partial b} = \begin{pmatrix} \mathbf{a} & \mathbf{b} & \mathbf{n} \end{pmatrix} \cdot \begin{pmatrix} \bar{\mathrm{Q}}_\mathrm{a} \\ \bar{\mathrm{Q}}_\mathrm{b} \\ D \end{pmatrix}
\tag{1.6}
$$

Equation (1.6) can be layed out a bit more simple by

$$
\frac{\partial \mathbf{v}}{\partial n} + \left(\mathbf{a}\mathbf{n}^T + \mathbf{n}\mathbf{a}^T\right) \cdot \frac{\partial \mathbf{v}}{\partial a} + \left(\mathbf{b}\mathbf{n}^T + \mathbf{n}\mathbf{b}^T\right) \cdot \frac{\partial \mathbf{v}}{\partial b} = \mathbf{a} \cdot \bar{\mathrm{Q}}_\mathrm{a} + \mathbf{b} \cdot \bar{\mathrm{Q}}_\mathrm{b} + \mathbf{n} \cdot D
\tag{1.7}
$$

1.2. BC including momentum balance, tangential direction

A more sophisticated ansatz for the free surfaces includes the momentum balance. Suppose we have a slice of material of thickness $\delta\mathrm{h}$ normal to the surface. The momentum balance taken in the tangential direction of $\mathbf{a}$ for this slice is

$$
\begin{aligned}
&\delta\mathrm{h} \cdot \mathrm{A} \cdot \rho \frac{d\mathbf{v}}{dt} + \delta\mathrm{h} \cdot \mathrm{A} \cdot \left(\mathbf{a}^T \cdot \nabla\varepsilon\right) = \\
&\quad \mathrm{A} \cdot \left(\mathbf{a}^T \cdot \mathbf{S} \cdot \mathbf{n} + \mathbf{a}^T \cdot \mathbf{Q}\right) + \delta\mathrm{h} \cdot \mathrm{A} \cdot \left(\mathbf{a}^T \cdot \mathbf{g}\right) - \delta\mathrm{h} \cdot \mathrm{A} \cdot \left(\mathbf{a}^T \cdot \nabla\mathrm{p}\right) - \delta\mathrm{h} \cdot \mathrm{A} \cdot \rho \cdot \beta \cdot \bar{\mathbf{B}} \cdot \left(\mathbf{v} - \mathbf{v}_0^{Darcy}\right)
\end{aligned}
\tag{1.8}
$$

$\mathbf{Q}$ is the tension acting on the surface from outside.

Division by A yields

$$\delta h\cdot\rho\frac{d\mathbf{v}}{dt}+\delta h\cdot\rho\cdot\beta\cdot\bar{\mathbf{B}}\cdot\mathbf{v}+\delta h\cdot\left(\mathbf{a}^T\cdot\nabla\varepsilon\right)=\left(\mathbf{a}^T\cdot\mathbf{S}\cdot\mathbf{n}+\mathbf{a}^T\cdot\mathbf{Q}\right)+\delta h\cdot\rho\cdot\left(\mathbf{a}^T\cdot\mathbf{g}\right)-\delta h\cdot\left(\mathbf{a}^T\cdot\nabla p\right)+\delta h\cdot\rho\cdot\beta\cdot\bar{\mathbf{B}}\cdot\mathbf{v}_0^{Darcy} \tag{1.9}$$

which is equally

$$\begin{aligned}\delta h\cdot\rho\left(\frac{d\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{dt}+\beta\cdot\bar{\mathbf{B}}\cdot\mathbf{v}\right)+\delta h\cdot\left(\mathbf{a}^T\cdot\nabla\varepsilon\right)=\\ \eta\cdot\left(\frac{\partial\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial a}\right)+\mathbf{a}^T\cdot\mathbf{Q}+\delta h\cdot\rho\cdot\left(\mathbf{a}^T\cdot\mathbf{g}\right)-\delta h\cdot\left(\mathbf{a}^T\cdot\nabla p\right)+\delta h\cdot\rho\cdot\beta\cdot\bar{\mathbf{B}}\cdot\mathbf{v}_0^{Darcy}\end{aligned} \tag{1.10}$$

As a numerical scheme, it looks like

$$\begin{aligned}\delta h\cdot\rho\cdot\mathbf{a}^T\cdot\frac{\mathbf{v}-\mathbf{v}_0}{\Delta t}+\delta h\cdot\rho\cdot\beta\cdot\mathbf{a}^T\cdot\bar{\mathbf{B}}\cdot\mathbf{v}+\delta h\cdot\left(\mathbf{a}^T\cdot\tilde{\nabla}\varepsilon\right)=\\ \eta\cdot\left(\frac{\tilde{\partial}\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\tilde{\partial} n}+\frac{\tilde{\partial}\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\tilde{\partial} a}\right)+\mathbf{a}^T\cdot\mathbf{Q}+\delta h\cdot\rho\cdot\left(\mathbf{a}^T\cdot\mathbf{g}\right)-\delta h\cdot\left(\mathbf{a}^T\cdot\nabla p\right)+\delta h\cdot\rho\cdot\beta\cdot\bar{\mathbf{B}}\cdot\mathbf{v}_0^{Darcy}\end{aligned} \tag{1.11}$$

and we can put the unknown values on the left hand side and all the other ones on the right hand side.

$$\begin{aligned}\frac{\delta h\cdot\rho}{\Delta t}\mathbf{a}^T\cdot\left(\mathbf{I}+\Delta t\cdot\beta\cdot\bar{\mathbf{B}}\right)\cdot\mathbf{v}-\eta\cdot\left(\frac{\tilde{\partial}\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\tilde{\partial} n}+\frac{\tilde{\partial}\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\tilde{\partial} a}\right)+\delta h\cdot\left(\mathbf{a}^T\cdot\tilde{\nabla}\varepsilon\right)=\\ \frac{\delta h\cdot\rho}{\Delta t}\cdot\left(\mathbf{a}^T\cdot\mathbf{v}_0\right)+\mathbf{a}^T\cdot\mathbf{Q}+\delta h\cdot\rho\cdot\left(\mathbf{a}^T\cdot\mathbf{g}\right)-\delta h\cdot\left(\mathbf{a}^T\cdot\nabla p\right)+\delta h\cdot\rho\cdot\beta\cdot\bar{\mathbf{B}}\cdot\mathbf{v}_0^{Darcy}\end{aligned} \tag{1.12}$$

We define $\bar{\mathbf{a}}^T=\frac{1}{\left(1+\Delta t\cdot\beta\right)}\mathbf{a}^T\cdot\left(\mathbf{I}+\Delta t\cdot\beta\cdot\bar{\mathbf{B}}\right)=\frac{1}{\bar{\beta}}\mathbf{a}^T\cdot\left(\mathbf{I}+\Delta t\cdot\beta\cdot\bar{\mathbf{B}}\right)$, which helps to rewrite (1.12) as

$$\begin{aligned}\frac{\delta h\cdot\rho}{\Delta t}\cdot\bar{\beta}\cdot\left(\bar{\mathbf{a}}^T\cdot\mathbf{v}\right)-\eta\cdot\left(\frac{\tilde{\partial}\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\tilde{\partial} n}+\frac{\tilde{\partial}\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\tilde{\partial} a}\right)+\delta h\cdot\left(\mathbf{a}^T\cdot\tilde{\nabla}\varepsilon\right)=\\ \frac{\delta h\cdot\rho}{\Delta t}\cdot\left(\mathbf{a}^T\cdot\mathbf{v}_0\right)+\mathbf{a}^T\cdot\mathbf{Q}+\delta h\cdot\rho\cdot\left(\mathbf{a}^T\cdot\mathbf{g}\right)-\delta h\cdot\left(\mathbf{a}^T\cdot\nabla p\right)+\delta h\cdot\rho\cdot\beta\cdot\bar{\mathbf{B}}\cdot\mathbf{v}_0^{Darcy}\end{aligned} \tag{1.13}$$

Let us also divide by a non-dimensionalizing term N

$$\frac{\delta h\cdot\rho}{\Delta t\cdot N}\cdot\bar{\beta}\cdot\left(\bar{\mathbf{a}}^T\cdot\mathbf{v}\right)-\frac{\eta}{N}\cdot\left(\frac{\tilde{\partial}\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\tilde{\partial}n}+\frac{\tilde{\partial}\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\tilde{\partial}a}\right)+\frac{\delta h}{N}\cdot\left(\mathbf{a}^T\cdot\tilde{\nabla}\varepsilon\right)=$$

$$\frac{\delta h\cdot\rho}{\Delta t\cdot N}\cdot\left(\mathbf{a}^T\cdot\mathbf{v}_0\right)+\frac{1}{N}\cdot\left(\mathbf{a}^T\cdot\mathbf{Q}\right)+\frac{\delta h\cdot\rho}{N}\cdot\left(\mathbf{a}^T\cdot\mathbf{g}\right)-\frac{\delta h}{N}\cdot\left(\mathbf{a}^T\cdot\nabla p\right)+\delta h\cdot\rho\cdot\beta\cdot\bar{\mathbf{B}}\cdot\mathbf{v}_0^{Darcy}$$

(1.14)

The choice of N is

$$N=\frac{\delta h\cdot\rho\cdot\bar{\beta}}{\Delta t}+\eta\cdot c^{diff} \tag{1.15}$$

N is chosen such that one of the terms on the right hand side has possibly order 1, the others less. In a simpler way, we can write

$$D_1\cdot\left(\bar{\mathbf{a}}^T\cdot\mathbf{v}\right)-D_2\cdot\left(\frac{\tilde{\partial}\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\tilde{\partial}n}+\frac{\tilde{\partial}\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\tilde{\partial}a}\right)+D_3\cdot\left(\mathbf{a}^T\cdot\tilde{\nabla}\varepsilon\right)=\mathbf{a}^T\cdot\mathbf{R} \tag{1.16}$$

Similarly, for the second tangential vector, we have

$$D_1\cdot\left(\bar{\mathbf{b}}^T\cdot\mathbf{v}\right)-D_2\cdot\left(\frac{\tilde{\partial}\left(\mathbf{b}^T\cdot\mathbf{v}\right)}{\tilde{\partial}n}+\frac{\tilde{\partial}\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\tilde{\partial}b}\right)+D_3\cdot\left(\mathbf{b}^T\cdot\tilde{\nabla}\varepsilon\right)=\mathbf{b}^T\cdot\mathbf{R} \tag{1.17}$$

The third condition is a linear combination of the momentum balance in the third direction $\mathbf{n}$:

$$D_1\cdot\left(\mathbf{n}^T\cdot\mathbf{v}\right)-D_2\cdot\left(\frac{\tilde{\partial}\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\tilde{\partial}n}+\frac{\tilde{\partial}\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\tilde{\partial}n}\right)+D_3\cdot\left(\mathbf{n}^T\cdot\tilde{\nabla}\varepsilon\right)=\mathbf{n}^T\cdot\mathbf{R} \tag{1.18}$$

and the requirement for the divergence of the velocity

$$\frac{\partial\rho}{\partial p}\cdot\frac{1}{\rho\cdot\Delta t}\cdot\varepsilon+\left(\frac{\tilde{\partial}\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\tilde{\partial}n}+\frac{\tilde{\partial}\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\tilde{\partial}a}+\frac{\tilde{\partial}\left(\mathbf{b}^T\cdot\mathbf{v}\right)}{\tilde{\partial}b}\right)=\overline{\nabla^T\mathbf{v}} \tag{1.19}$$

Where ε is the pressure change within the time cycle and $D\equiv\overline{\nabla^T\mathbf{v}}$ the requested "outer" compression/expansion of the fluid.

For incorporation of (1.18) and (1.19) (both valid boundary conditions), we scale them with the weighting factors x and D_4, respectively.

Written in matrix vector formulation we obtain

$$
\begin{aligned}
& D_1 \begin{pmatrix} \bar{\mathbf{a}}^T \\ \bar{\mathbf{b}}^T \\ x \cdot \mathbf{n}^T \end{pmatrix} \cdot \mathbf{v} - \begin{pmatrix} D_2 \mathbf{a}^T \\ D_2 \mathbf{b}^T \\ \left(D_4 + 2xD_2\right)\mathbf{n}^T \end{pmatrix} \cdot \frac{\partial \mathbf{v}}{\partial n} - \begin{pmatrix} D_2 \mathbf{n}^T \\ \mathbf{0} \\ D_4 \mathbf{a}^T \end{pmatrix} \cdot \frac{\partial \mathbf{v}}{\partial a} - \begin{pmatrix} \mathbf{0} \\ D_2 \mathbf{n}^T \\ D_4 \mathbf{b}^T \end{pmatrix} \cdot \frac{\partial \mathbf{v}}{\partial b} \\
& + \begin{pmatrix} D_3 \cdot \frac{\partial \varepsilon}{\partial a} \\ D_3 \cdot \frac{\partial \varepsilon}{\partial b} \\ xD_3 \cdot \frac{\partial \varepsilon}{\partial n} \end{pmatrix} - \begin{pmatrix} 0 \\ 0 \\ D_4 \cdot D_5 \cdot \varepsilon \end{pmatrix} = \begin{pmatrix} \mathbf{a}^T \cdot \mathbf{R} \\ \mathbf{b}^T \cdot \mathbf{R} \\ x\mathbf{n}^T \cdot \mathbf{R} - D_4 \cdot D \end{pmatrix}
\end{aligned}
\tag{1.20}
$$

In fact, we have $D_5 = \frac{\partial \rho}{\partial p} \cdot \frac{1}{\rho \cdot \Delta t}$, if some compressibility is given, otherwise, this term is zero.

Multiplication with the potential inverse matrix (at least with a regularizing matrix) yields

$$
\begin{aligned}
& D_1 \left(\mathbf{a} \quad \mathbf{b} \quad \mathbf{n}\right) \begin{pmatrix} \bar{\mathbf{a}}^T \\ \bar{\mathbf{b}}^T \\ x \cdot \mathbf{n}^T \end{pmatrix} \cdot \mathbf{v} - \left(\mathbf{a} \quad \mathbf{b} \quad \mathbf{n}\right) \begin{pmatrix} D_2 \mathbf{a}^T \\ D_2 \mathbf{b}^T \\ \left(D_4 + 2xD_2\right)\mathbf{n}^T \end{pmatrix} \cdot \frac{\partial \mathbf{v}}{\partial n} - \left(\mathbf{a} \quad \mathbf{b} \quad \mathbf{n}\right) \begin{pmatrix} D_2 \mathbf{n}^T \\ \mathbf{0} \\ D_4 \mathbf{a}^T \end{pmatrix} \cdot \frac{\partial \mathbf{v}}{\partial a} \\
& - \left(\mathbf{a} \quad \mathbf{b} \quad \mathbf{n}\right) \begin{pmatrix} \mathbf{0} \\ D_2 \mathbf{n}^T \\ D_4 \mathbf{b}^T \end{pmatrix} \cdot \frac{\partial \mathbf{v}}{\partial b} + \left(\mathbf{a} \quad \mathbf{b} \quad \mathbf{n}\right) \begin{pmatrix} D_3 \cdot \frac{\partial \varepsilon}{\partial a} \\ D_3 \cdot \frac{\partial \varepsilon}{\partial b} \\ xD_3 \cdot \frac{\partial \varepsilon}{\partial n} - D_4 \cdot D_5 \cdot \varepsilon \end{pmatrix} = \left(\mathbf{a} \quad \mathbf{b} \quad \mathbf{n}\right) \begin{pmatrix} \mathbf{a}^T \cdot \mathbf{R} \\ \mathbf{b}^T \cdot \mathbf{R} \\ x\mathbf{n}^T \cdot \mathbf{R} - D_4 \cdot D \end{pmatrix}
\end{aligned}
\tag{1.21}
$$

And finally

$$D_1\left(\mathbf{a}\bar{\mathbf{a}}^T+\mathbf{b}\bar{\mathbf{b}}^T+x\mathbf{n}\mathbf{n}^T\right)\cdot\mathbf{v}-\left(D_2\mathbf{a}\mathbf{a}^T+D_2\mathbf{b}\mathbf{b}^T+\left(D_4+2xD_2\right)\mathbf{n}\mathbf{n}^T\right)\cdot\frac{\partial\mathbf{v}}{\partial n}-\left(D_2\mathbf{a}\mathbf{n}^T+D_4\mathbf{n}\mathbf{a}^T\right)\cdot\frac{\partial\mathbf{v}}{\partial a}$$
$$-\left(D_2\mathbf{b}\mathbf{n}^T+D_4\mathbf{n}\mathbf{b}^T\right)\cdot\frac{\partial\mathbf{v}}{\partial b}+D_3\cdot\left(\mathbf{a}\frac{\partial\varepsilon}{\partial a}+\mathbf{b}\frac{\partial\varepsilon}{\partial b}+x\mathbf{n}\cdot\frac{\partial\varepsilon}{\partial n}\right)-D_4\cdot D_5\cdot\mathbf{n}\cdot\varepsilon= \qquad (1.22)$$
$$\mathbf{a}\left(\mathbf{a}^T\cdot\mathbf{R}\right)+\mathbf{b}\left(\mathbf{b}^T\cdot\mathbf{R}\right)+x\mathbf{n}\left(\mathbf{n}^T\cdot\mathbf{R}\right)+\mathbf{n}\left(-D_4\cdot D\right)$$

Remarks:

a) In the applications, $x=0$ turned out to be the optimal choice.
b) D_4 can be set freely in order to emphasize mass conservation at the free surface

1.3. BC including momentum balance, normal direction

$$\delta\mathrm{h}\cdot\mathrm{A}\cdot\rho\frac{d\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{dt}+\mathrm{A}\cdot\left(\mathrm{p}+\varepsilon-\mathrm{p}_0\right)=\mathrm{A}\cdot\left(\mathbf{n}^T\cdot\mathbf{S}\cdot\mathbf{n}\right)+\delta\mathrm{h}\cdot\mathrm{A}\cdot\rho\cdot\left(\mathbf{n}^T\cdot\mathbf{g}\right) \qquad (1.23)$$

Equaly written as

$$\delta\mathrm{h}\cdot\rho\frac{d\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{dt}+\left(\mathrm{p}+\varepsilon-\mathrm{p}_0\right)=\left(\mathbf{n}^T\cdot\mathbf{S}\cdot\mathbf{n}\right)+\delta\mathrm{h}\cdot\rho\cdot\left(\mathbf{n}^T\cdot\mathbf{g}\right) \qquad (1.24)$$

As numerical scheme, it appears as

$$\frac{\delta\mathrm{h}\cdot\rho}{\Delta\mathrm{t}}\left(\mathbf{n}^T\cdot\mathbf{v}-\mathbf{n}^T\cdot\mathbf{v}_0\right)+\left(\mathrm{p}+\varepsilon-\mathrm{p}_0\right)=\hat{\eta}\left(2\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial n}-\frac{2}{3}D\right)+\left(\mathbf{n}^T\cdot\mathbf{S}_s\cdot\mathbf{n}\right)+\delta\mathrm{h}\cdot\rho\cdot\left(\mathbf{n}^T\cdot\mathbf{g}\right) \qquad (1.25)$$

After reordering of terms, we obtain

$$\frac{\delta\mathrm{h}\cdot\rho}{\Delta\mathrm{t}}\left(\mathbf{n}^T\cdot\mathbf{v}\right)-\eta\left(2\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial n}-\frac{2}{3}D\right)+\varepsilon=$$
$$\frac{\delta\mathrm{h}\cdot\rho}{\Delta\mathrm{t}}\left(\mathbf{n}^T\cdot\mathbf{v}_0\right)+\delta\mathrm{h}\cdot\rho\cdot\left(\mathbf{n}^T\cdot\mathbf{g}\right)+\mathrm{p}_0-\mathrm{p}_d-\mathrm{p}_h+\mathbf{n}^T\cdot\mathbf{S}_s\cdot\mathbf{n} \qquad (1.26)$$

Simplification yields

$$D_5\left(\mathbf{n}^T\cdot\mathbf{v}\right)-D_6\left(2\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial n}-\frac{2}{3}D\right)+\varepsilon=\mathrm{R} \qquad (1.27)$$

With $D = \nabla\mathbf{v}\big|_{soll} - \frac{\rho_p}{\rho \cdot \Delta t}\varepsilon$ we have

$$D_5\left(\mathbf{n}^T \cdot \mathbf{v}\right) - D_6\left(2\frac{\partial\left(\mathbf{n}^T \cdot \mathbf{v}\right)}{\partial n} - \frac{2}{3}\left(\nabla\mathbf{v}\big|_{soll} - \frac{\rho_p}{\rho \cdot \Delta t}\varepsilon\right)\right) + \varepsilon = \mathrm{R}$$

$$D_5\left(\mathbf{n}^T \cdot \mathbf{v}\right) - D_6 2\frac{\partial\left(\mathbf{n}^T \cdot \mathbf{v}\right)}{\partial n} + D_6\frac{2}{3}\nabla\mathbf{v}\big|_{soll} - D_6\frac{2}{3}\frac{\rho_p}{\rho \cdot \Delta t}\varepsilon + \varepsilon = \mathrm{R}$$

And finally

$$D_5\left(\mathbf{n}^T \cdot \mathbf{v}\right) - D_6 2\frac{\partial\left(\mathbf{n}^T \cdot \mathbf{v}\right)}{\partial n} + \left(1 - D_6\frac{2}{3}\frac{\rho_p}{\rho \cdot \Delta t}\right)\varepsilon = \mathrm{R} - D_6\frac{2}{3}\nabla\mathbf{v}\big|_{soll}$$

However this will maybe lead to unstable configurations. It is better to rewrite this boundary condition as

$$D_5\left(\mathbf{n}^T \cdot \mathbf{v}\right) - D_6\left(2\frac{\partial\left(\mathbf{n}^T \cdot \mathbf{v}\right)}{\partial n} - \frac{2}{3}D\right) + \varepsilon = \mathrm{R}$$

$$D_5\left(\mathbf{n}^T \cdot \mathbf{v}\right) - D_6\left(2\left(D - \frac{\partial\left(\mathbf{a}^T \cdot \mathbf{v}\right)}{\partial a} - \frac{\partial\left(\mathbf{b}^T \cdot \mathbf{v}\right)}{\partial b}\right) - \frac{2}{3}D\right) + \varepsilon = \mathrm{R}$$

$$D_5\left(\mathbf{n}^T \cdot \mathbf{v}\right) - D_6\left(-2\left(\frac{\partial\left(\mathbf{a}^T \cdot \mathbf{v}\right)}{\partial a} - \frac{\partial\left(\mathbf{b}^T \cdot \mathbf{v}\right)}{\partial b}\right) + \frac{4}{3}D\right) + \varepsilon = \mathrm{R}$$

$$D_5\left(\mathbf{n}^T \cdot \mathbf{v}\right) + 2D_6\left(\frac{\partial\left(\mathbf{a}^T \cdot \mathbf{v}\right)}{\partial a} - \frac{\partial\left(\mathbf{b}^T \cdot \mathbf{v}\right)}{\partial b}\right) - \frac{4}{3}D_6 D + \varepsilon = \mathrm{R}$$

With $D = \nabla\mathbf{v}\big|_{soll} - \frac{\rho_p}{\rho \cdot \Delta t}\varepsilon$ we have

$$D_5\left(\mathbf{n}^T \cdot \mathbf{v}\right) + 2D_6\left(\frac{\partial\left(\mathbf{a}^T \cdot \mathbf{v}\right)}{\partial a} - \frac{\partial\left(\mathbf{b}^T \cdot \mathbf{v}\right)}{\partial b}\right) - \frac{4}{3}D_6\left(\nabla\mathbf{v}\big|_{soll} - \frac{\rho_p}{\rho \cdot \Delta t}\varepsilon\right) + \varepsilon = \mathrm{R}$$

And finally

$$D_5\left(\mathbf{n}^T\cdot\mathbf{v}\right)+2D_6\left(\frac{\partial\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\partial a}-\frac{\partial\left(\mathbf{b}^T\cdot\mathbf{v}\right)}{\partial b}\right)-\frac{4}{3}D_6\left(\nabla\mathbf{v}\big|_{soll}-\frac{\rho_p}{\rho\cdot\Delta t}\varepsilon\right)+\varepsilon=\mathrm{R}$$

$$D_5\left(\mathbf{n}^T\cdot\mathbf{v}\right)+2D_6\left(\frac{\partial\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\partial a}-\frac{\partial\left(\mathbf{b}^T\cdot\mathbf{v}\right)}{\partial b}\right)-\frac{4}{3}D_6\left(-\frac{\rho_p}{\rho\cdot\Delta t}\varepsilon\right)+\varepsilon=\mathrm{R}+\frac{4}{3}D_6\,\nabla\mathbf{v}\big|_{soll}$$

$$D_5\left(\mathbf{n}^T\cdot\mathbf{v}\right)+2D_6\left(\frac{\partial\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\partial a}-\frac{\partial\left(\mathbf{b}^T\cdot\mathbf{v}\right)}{\partial b}\right)+\left(1+\frac{4}{3}D_6\,\frac{\rho_p}{\rho\cdot\Delta t}\right)\varepsilon=\mathrm{R}+\frac{4}{3}D_6\,\nabla\mathbf{v}\big|_{soll}$$

2. Slip boundaries

2.1. Simple Slip boundaries

Slip boundaries are mixed Neumann and Dirichlet boundaries. We introduce a slip coefficient α, such that we can formulate sliding along a solid wall boundary by

$$\begin{aligned}
&\alpha\cdot\mathbf{a}^T\cdot\mathbf{S}\cdot\mathbf{n}=\mathbf{a}^T\cdot\left(\mathbf{v}-\mathbf{v}_p\right)\\
&\alpha\cdot\mathbf{b}^T\cdot\mathbf{S}\cdot\mathbf{n}=\mathbf{b}^T\cdot\left(\mathbf{v}-\mathbf{v}_p\right)\\
&\mathbf{n}^T\cdot\left(\mathbf{v}-\mathbf{v}_p\right)=P
\end{aligned} \tag{2.1}$$

The last of the three equations describes a pure impermeable wall if $P=0$. If the wall shows permeable effects, then we have to formulate the flux term, for instance by a simple pressure law in the sense

$$P=\varepsilon\cdot\left(p-p_0\right) \tag{2.2}$$

Let us assume that P and α are given. Then system (2.1) can be reformulated as

$$\begin{aligned}
&\alpha\cdot\eta\cdot\left(\frac{\partial\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial a}\right)=\mathbf{a}^T\cdot\left(\mathbf{v}-\mathbf{v}_p\right)\\
&\alpha\cdot\eta\cdot\left(\frac{\partial\left(\mathbf{b}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial b}\right)=\mathbf{b}^T\cdot\left(\mathbf{v}-\mathbf{v}_p\right)\\
&\mathbf{n}^T\cdot\left(\mathbf{v}-\mathbf{v}_p\right)=P
\end{aligned} \tag{2.3}$$

And furthermore

$$
\begin{aligned}
&\alpha \cdot \eta \cdot \left(\mathbf{a}^T \cdot \frac{\partial \mathbf{v}}{\partial n} + \mathbf{n}^T \cdot \frac{\partial \mathbf{v}}{\partial a} \right) - \mathbf{a}^T \cdot \mathbf{v} = -\mathbf{a}^T \cdot \mathbf{v}_p \\
&\alpha \cdot \eta \cdot \left(\mathbf{b}^T \cdot \frac{\partial \mathbf{v}}{\partial n} + \mathbf{n}^T \cdot \frac{\partial \mathbf{v}}{\partial b} \right) - \mathbf{b}^T \cdot \mathbf{v} = -\mathbf{b}^T \cdot \mathbf{v}_p \\
&s \cdot \mathbf{n}^T \cdot \mathbf{v} = s \cdot P + s \cdot \mathbf{n}^T \cdot \mathbf{v}_p
\end{aligned}
\tag{2.4}
$$

The factor s can take the values 1 or -1 which enables us to toggle the sign of the last equation.

We now provide a normalization factor for the first two equations such that all the three equations are of the same order of magnitude. The normalization factor is simply

$$
X = \frac{1}{\alpha \cdot \eta \cdot c_{central} - 1} \tag{2.5}
$$

The term $c_{central}$ denotes the value of the central entry of the local $\frac{\partial}{\partial n}$, AND IT IS NEGATIVE!!!. Herewith, equation (2.4) finally looks like this:

$$
\begin{aligned}
&X \cdot \alpha \cdot \eta \cdot \left(\mathbf{a}^T \cdot \frac{\partial \mathbf{v}}{\partial n} + \mathbf{n}^T \cdot \frac{\partial \mathbf{v}}{\partial a} \right) - X \cdot \mathbf{a}^T \cdot \mathbf{v} = -X \cdot \mathbf{a}^T \cdot \mathbf{v}_p \\
&X \cdot \alpha \cdot \eta \cdot \left(\mathbf{b}^T \cdot \frac{\partial \mathbf{v}}{\partial n} + \mathbf{n}^T \cdot \frac{\partial \mathbf{v}}{\partial b} \right) - X \cdot \mathbf{b}^T \cdot \mathbf{v} = -X \cdot \mathbf{b}^T \cdot \mathbf{v}_p \\
&s \cdot \mathbf{n}^T \cdot \mathbf{v} + X \cdot \alpha \cdot \eta \cdot \mathbf{n}^T \cdot \frac{\partial \mathbf{v}}{\partial n} - X \cdot \alpha \cdot \eta \cdot \mathbf{n}^T \cdot \frac{\partial \mathbf{v}}{\partial n} = s \cdot P + s \cdot \mathbf{n}^T \cdot \mathbf{v}_p
\end{aligned}
\tag{2.6}
$$

Similarly to the considerations at the free surface, we now try to isolate $\frac{\partial \mathbf{v}}{\partial n}$ such that we are able to prescribe Neumann type boundary condition. In order to achieve this, let us write down equation (2.6) in matrix vector form, i.e.

$$
\begin{aligned}
&X \cdot \alpha \cdot \eta \cdot \begin{pmatrix} \mathbf{a}^T \\ \mathbf{b}^T \\ \mathbf{n}^T \end{pmatrix} \cdot \frac{\partial \mathbf{v}}{\partial n} + X \cdot \alpha \cdot \eta \cdot \begin{pmatrix} \mathbf{n}^T \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix} \cdot \frac{\partial \mathbf{v}}{\partial a} + X \cdot \alpha \cdot \eta \cdot \begin{pmatrix} \mathbf{0} \\ \mathbf{n}^T \\ \mathbf{0} \end{pmatrix} \cdot \frac{\partial \mathbf{v}}{\partial b} \\
&-X \cdot \alpha \cdot \eta \cdot \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{n}^T \end{pmatrix} \cdot \frac{\partial \mathbf{v}}{\partial n} + \begin{pmatrix} -X \cdot \mathbf{a}^T \\ -X \cdot \mathbf{b}^T \\ s \cdot \mathbf{n}^T \end{pmatrix} \cdot \mathbf{v} = \begin{pmatrix} -X \cdot \mathbf{a}^T \cdot \mathbf{v}_p \\ -X \cdot \mathbf{b}^T \cdot \mathbf{v}_p \\ s \cdot P + s \cdot \mathbf{n}^T \cdot \mathbf{v}_p \end{pmatrix}
\end{aligned}
\tag{2.7}
$$

As $\begin{pmatrix} \mathbf{a}^T \\ \mathbf{b}^T \\ \mathbf{n}^T \end{pmatrix}$ is a matrix of perpendicular unit vectors, its inverse is $\begin{pmatrix} \mathbf{a} & \mathbf{b} & \mathbf{n} \end{pmatrix}$ an thus we can transform (2.7) in order to isolate $\frac{\partial \mathbf{v}}{\partial n}$

$$\begin{aligned}
&X \cdot \alpha \cdot \eta \cdot \frac{\partial \mathbf{v}}{\partial n} + X \cdot \alpha \cdot \eta \cdot \left(\mathbf{a}\mathbf{n}^T\right) \cdot \frac{\partial \mathbf{v}}{\partial a} + X \cdot \alpha \cdot \eta \cdot \left(\mathbf{b}\mathbf{n}^T\right) \cdot \frac{\partial \mathbf{v}}{\partial b} \\
&-X \cdot \alpha \cdot \eta \cdot \left(\mathbf{n}\mathbf{n}^T\right) \cdot \frac{\partial \mathbf{v}}{\partial n} - X \cdot \left(\mathbf{a}\mathbf{a}^T + \mathbf{b}\mathbf{b}^T\right) \cdot \mathbf{v} + \left(s \cdot \mathbf{n}\mathbf{n}^T\right) \cdot \mathbf{v} = \\
&s \cdot P\mathbf{n} + s \cdot \left(\mathbf{n}\mathbf{n}^T\right) \cdot \mathbf{v}_p - X \cdot \left(\mathbf{a}\mathbf{a}^T + \mathbf{b}\mathbf{b}^T\right) \cdot \mathbf{v}_p
\end{aligned} \tag{2.8}$$

Even more easy, we find

$$\begin{aligned}
&X \cdot \alpha \cdot \eta \cdot \left(\mathbf{a}\mathbf{a}^T + \mathbf{b}\mathbf{b}^T\right) \cdot \frac{\partial \mathbf{v}}{\partial n} + X \cdot \alpha \cdot \eta \cdot \left(\mathbf{a}\mathbf{n}^T\right) \cdot \frac{\partial \mathbf{v}}{\partial a} + X \cdot \alpha \cdot \eta \cdot \left(\mathbf{b}\mathbf{n}^T\right) \cdot \frac{\partial \mathbf{v}}{\partial b} \\
&-X \cdot \left(\mathbf{a}\mathbf{a}^T + \mathbf{b}\mathbf{b}^T\right) \cdot \mathbf{v} + \left(s \cdot \mathbf{n}\mathbf{n}^T\right) \cdot \mathbf{v} = s \cdot P\mathbf{n} + \left(s \cdot \mathbf{n}\mathbf{n}^T\right) \cdot \mathbf{v}_p - X \cdot \left(\mathbf{a}\mathbf{a}^T + \mathbf{b}\mathbf{b}^T\right) \cdot \mathbf{v}_p
\end{aligned} \tag{2.9}$$

Let us sort the terms in (2.9) such that the contributions to the diagonal of some system matrix are in the beginning.

$$\begin{aligned}
&X \cdot \alpha \cdot \eta \cdot \left(\mathbf{a}\mathbf{a}^T + \mathbf{b}\mathbf{b}^T\right) \cdot \frac{\partial \mathbf{v}}{\partial n} - X \cdot \left(\mathbf{a}\mathbf{a}^T + \mathbf{b}\mathbf{b}^T\right) \cdot \mathbf{v} + \left(s \cdot \mathbf{n}\mathbf{n}^T\right) \cdot \mathbf{v} \\
&+X \cdot \alpha \cdot \eta \cdot \left(\mathbf{a}\mathbf{n}^T\right) \cdot \frac{\partial \mathbf{v}}{\partial a} + X \cdot \alpha \cdot \eta \cdot \left(\mathbf{b}\mathbf{n}^T\right) \cdot \frac{\partial \mathbf{v}}{\partial b} = s \cdot P\mathbf{n} + \left(s \cdot \mathbf{n}\mathbf{n}^T\right) \cdot \mathbf{v}_p - X \cdot \left(\mathbf{a}\mathbf{a}^T + \mathbf{b}\mathbf{b}^T\right) \cdot \mathbf{v}_p
\end{aligned} \tag{2.10}$$

For reasons of numerical stability, we have to choose $s = 1$.

2.2. Slip boundaries using momentum balance

The momentum balance along a tangential direction $\mathbf{a}$ for a slice with thickness δh and basis area A is given by

$$\begin{aligned}
&A\delta h \cdot \rho \cdot \left(\frac{d_p\left(\mathbf{a}^T \cdot \mathbf{v}\right)}{dt} + \left(\left(\mathbf{v} - \mathbf{v}_p\right)\nabla \mathbf{v}\right) \right) + A\delta h \cdot \left(\mathbf{a}^T \cdot \nabla \varepsilon\right) + A\delta h \cdot \left(\mathbf{a}^T \cdot \nabla \mathrm{p}\right) = \\
&\qquad A \cdot \eta \left(\frac{\partial\left(\mathbf{a}^T \cdot \mathbf{v}\right)}{\partial n} + \frac{\partial\left(\mathbf{n}^T \cdot \mathbf{v}\right)}{\partial a} \right) + A \cdot \mathbf{a}^T \cdot \mathbf{S} \cdot \mathbf{n} + A\delta h \cdot \rho \cdot \left(\mathbf{a}^T \cdot \mathbf{g}\right) + \\
&\qquad A\left(\mathbf{a}^T \cdot \mathbf{T}_W\right) - \frac{A}{\alpha}\left(\mathbf{a}^T \cdot \left(\mathbf{v} - \mathbf{v}_p\right)\right) - \delta \mathrm{h} \cdot \mathrm{A} \cdot \rho \cdot \beta \cdot \left(\mathbf{a}^T \cdot \bar{\mathbf{B}}\right) \cdot \mathbf{v}
\end{aligned} \tag{2.11}$$

The turbulent wall tension is

$$\mathbf{T}_W = -\tau_W \cdot \frac{\mathbf{v}-\mathbf{v}_p}{\left\|\mathbf{v}-\mathbf{v}_p\right\|} \tag{2.12}$$

The slip coefficient α determines sliding resistance along the wall by the viscous layer approach.

Equation (2.11) can be simplified by

$$\begin{aligned}
&\delta h \cdot \rho \cdot \left(\frac{d_p\left(\mathbf{a}^T \cdot \mathbf{v}\right)}{dt} + V_p \frac{\partial\left(\mathbf{a}^T \cdot \mathbf{v}\right)}{\partial m} \right) + \delta h \cdot \left(\mathbf{a}^T \cdot \nabla \varepsilon\right) + \delta h \cdot \left(\mathbf{a}^T \cdot \nabla \mathrm{p}\right) = \\
&\qquad \eta \left(\frac{\partial\left(\mathbf{a}^T \cdot \mathbf{v}\right)}{\partial n} + \frac{\partial\left(\mathbf{n}^T \cdot \mathbf{v}\right)}{\partial a} \right) + \mathbf{a}^T \cdot \mathbf{S} \cdot \mathbf{n} + \delta h \cdot \rho \cdot \left(\mathbf{a}^T \cdot \mathbf{g}\right) \\
&\qquad - \left(\frac{\tau_W}{\left\|\mathbf{v}-\mathbf{v}_p\right\|} + \frac{1}{\alpha} \right) \cdot \left(\mathbf{a}^T \cdot \left(\mathbf{v}-\mathbf{v}_p\right)\right) - \delta \mathrm{h} \cdot \rho \cdot \beta \cdot \left(\mathbf{a}^T \cdot \bar{\mathbf{B}}\right) \cdot \mathbf{v}
\end{aligned} \tag{2.13}$$

where the thickness parameter δh appears as regularization factor. If $\delta h = 0$, we find back the original slip boundary formulation

$$0 = \eta \left(\frac{\partial\left(\mathbf{a}^T \cdot \mathbf{v}\right)}{\partial n} + \frac{\partial\left(\mathbf{n}^T \cdot \mathbf{v}\right)}{\partial a} \right) + \mathbf{a}^T \cdot \mathbf{S} \cdot \mathbf{n} - \left(\frac{\tau_W}{\left\|\mathbf{v}-\mathbf{v}_p\right\|} + \frac{1}{\alpha} \right) \cdot \left(\mathbf{a}^T \cdot \left(\mathbf{v}-\mathbf{v}_p\right)\right) \tag{2.14}$$

Please compare (2.14) with equation (2.1). Let us rewrite equation (2.13)

$$\begin{aligned}
&\frac{\delta h \cdot \rho}{\Delta \mathrm{t}} \cdot \left(\mathbf{a}^T \cdot \mathbf{v}\right) + \left(\frac{\tau_W}{\left\|\mathbf{v}-\mathbf{v}_p\right\|} + \frac{1}{\alpha} \right) \cdot \left(\mathbf{a}^T \cdot \mathbf{v}\right) + \delta \mathrm{h} \cdot \rho \cdot \beta \cdot \left(\mathbf{a}^T \cdot \bar{\mathbf{B}}\right) \cdot \mathbf{v} \\
&+ \delta h \cdot \rho \cdot V_p \frac{\partial\left(\mathbf{a}^T \cdot \mathbf{v}\right)}{\partial m} - \eta \left(\frac{\partial\left(\mathbf{a}^T \cdot \mathbf{v}\right)}{\partial n} + \frac{\partial\left(\mathbf{n}^T \cdot \mathbf{v}\right)}{\partial a} \right) + \delta h \cdot \left(\mathbf{a}^T \cdot \nabla \varepsilon\right) = \\
&\frac{\delta h \cdot \rho}{\Delta \mathrm{t}} \cdot \left(\mathbf{a}^T \cdot \mathbf{v}_0\right) + \mathbf{a}^T \cdot \mathbf{S} \cdot \mathbf{n} + \left(\frac{\tau_W}{\left\|\mathbf{v}-\mathbf{v}_p\right\|} + \frac{1}{\alpha} \right) \cdot \left(\mathbf{a}^T \cdot \mathbf{v}_p\right) + \delta h \cdot \rho \cdot \left(\mathbf{a}^T \cdot \mathbf{g}\right) - \delta h \cdot \left(\mathbf{a}^T \cdot \nabla \mathrm{p}\right)
\end{aligned} \tag{2.15}$$

We define the term

$$\mathbf{R} = \frac{\delta h \cdot \rho}{\Delta \mathrm{t}} \cdot \mathbf{v}_0 + \mathbf{S} \cdot \mathbf{n} + \left(\frac{\tau_W}{\left\|\mathbf{v}-\mathbf{v}_p\right\|} + \frac{1}{\alpha} \right) \cdot \mathbf{v}_p + \delta h \cdot \rho \cdot \mathbf{g} - \delta h \cdot \nabla \mathrm{p} \tag{2.16}$$

And thus we are able to rewrite (2.15) in the sense

$$\left(\left(\frac{\delta h\cdot\rho}{\Delta t}+\frac{1}{\hat{\alpha}}\right)\cdot\mathbf{a}^T+\delta h\cdot\rho\cdot\beta\cdot\left(\mathbf{a}^T\cdot\bar{\mathbf{B}}\right)\right)\cdot\mathbf{v} + \delta h\cdot\rho\cdot V_p\frac{\partial\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\partial m} - \eta\left(\frac{\partial\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial a}\right)+\delta h\cdot\left(\mathbf{a}^T\cdot\nabla\varepsilon\right) = \mathbf{a}^T\cdot\mathbf{R} \quad (2.17)$$

We rewrite the first term by the definition

$$\left(\frac{\delta h\cdot\rho}{\Delta t}\cdot\mathbf{a}^T+\delta h\cdot\rho\cdot\beta\cdot\left(\mathbf{a}^T\cdot\bar{\mathbf{B}}\right)\right)=\frac{\delta h\cdot\rho}{\Delta t}(1+\Delta t\cdot\beta)\cdot\frac{\left(\frac{\delta h\cdot\rho}{\Delta t}\cdot\mathbf{a}^T+\delta h\cdot\rho\cdot\beta\cdot\left(\mathbf{a}^T\cdot\bar{\mathbf{B}}\right)\right)}{\frac{\delta h\cdot\rho}{\Delta t}(1+\Delta t\cdot\beta)}$$

$$=\frac{\delta h\cdot\rho}{\Delta t}(1+\Delta t\cdot\beta)\cdot\frac{\left(\mathbf{a}^T+\Delta t\cdot\beta\cdot\left(\mathbf{a}^T\cdot\bar{\mathbf{B}}\right)\right)}{(1+\Delta t\cdot\beta)}$$

$$=\frac{\delta h\cdot\rho}{\Delta t}(1+\Delta t\cdot\beta)\cdot\bar{\mathbf{a}}^T$$

We can nondimensionalize (2.17) by

$$\frac{\delta h\cdot\rho}{\Delta t}(1+\Delta t\cdot\beta)\frac{1}{N}\cdot\left(\bar{\mathbf{a}}^T\cdot\mathbf{v}\right)+\frac{1}{\hat{\alpha}}\frac{1}{N}\cdot\left(\mathbf{a}^T\cdot\mathbf{v}\right) + \frac{\delta h\cdot\rho\cdot V_p}{N}\frac{\partial\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\partial m} - \frac{\eta}{N}\left(\frac{\partial\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial a}\right)+\frac{\delta h}{N}\cdot\left(\mathbf{a}^T\cdot\nabla\varepsilon\right) = \frac{1}{N}\mathbf{a}^T\cdot\mathbf{R} \quad (2.18)$$

Determination of N is simply given by

$$N=\max\left(\left(\frac{\delta h\cdot\rho}{\Delta t}+\frac{1}{\hat{\alpha}}+\delta h\cdot\rho\cdot\beta\right),\ \eta\cdot c^{\mathrm{diff}}\right) \quad (2.19)$$

And thus we find

$$D_1\cdot\left(\bar{\mathbf{a}}^T\cdot\mathbf{v}\right)+\tilde{D}_1\cdot\left(\mathbf{a}^T\cdot\mathbf{v}\right)+D_6\frac{\partial\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\partial m} - D_2\left(\frac{\partial\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial a}\right)+D_3\cdot\left(\mathbf{a}^T\cdot\nabla\varepsilon\right) = \frac{1}{N}\mathbf{a}^T\cdot\mathbf{R} \quad (2.20)$$

Of course, the second tangential direction looks similar

$$D_1\cdot\left(\bar{\mathbf{b}}^T\cdot\mathbf{v}\right)+\tilde{D}_1\cdot\left(\mathbf{b}^T\cdot\mathbf{v}\right)+D_6\frac{\partial\left(\mathbf{b}^T\cdot\mathbf{v}\right)}{\partial m} - D_2\left(\frac{\partial\left(\mathbf{b}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial b}\right)+D_3\cdot\left(\mathbf{b}^T\cdot\nabla\varepsilon\right) = \frac{1}{N}\mathbf{b}^T\cdot\mathbf{R} \quad (2.21)$$

The third condition is a condition on the normal flux.

$$D_4\left(\mathbf{n}^T\cdot\mathbf{v}\right)-D_5\cdot\left(\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\partial a}+\frac{\partial\left(\mathbf{b}^T\cdot\mathbf{v}\right)}{\partial b}\right)=D_4\left(\mathbf{n}^T\cdot\mathbf{v}_p\right)-D_5\cdot D \quad (2.22)$$

We choose

$$\begin{aligned}
D_1 &= \frac{\delta h\cdot\rho}{\Delta t}\frac{\left(1+\Delta t\cdot\beta\right)}{N}\\
\tilde{D}_1 &= \frac{1}{\hat{\alpha}}\frac{1}{N}\\
D_2 &= \frac{\eta}{N}\\
D_3 &= \frac{\delta h}{N}\\
D_4 &= 1\\
D_5 &= D_4\cdot\beta\cdot\delta h\\
D_6 &= \frac{\delta h\cdot\rho\cdot V_p}{N}=\frac{\delta h\cdot\rho\cdot\left\|\mathbf{v}-\mathbf{v}_p\right\|}{N}
\end{aligned}$$

β is in the order of 1 and can be chosen by the user. This term forces the divergence of velocity towards a certain value D.

The three conditions (2.20), (2.21) and (2.22) can be written in matrix vector formulation

$$\begin{pmatrix} D_1\cdot\bar{\mathbf{a}}+\tilde{D}_1\cdot\mathbf{a}\\ CD_1\cdot\bar{\mathbf{b}}+C\tilde{D}_1\cdot\mathbf{b}\\ D_4\cdot\mathbf{n}\end{pmatrix}\cdot\mathbf{v}+\begin{pmatrix} D_6\cdot\mathbf{a}\\ D_6\cdot\mathbf{b}\\ 0\end{pmatrix}\frac{\partial\mathbf{v}}{\partial m}+\begin{pmatrix} -D_2\cdot\mathbf{a}\\ -CD_2\cdot\mathbf{b}\\ -D_5\cdot\mathbf{n}\end{pmatrix}\frac{\partial\mathbf{v}}{\partial n}+\begin{pmatrix} -D_2\cdot\mathbf{n}\\ 0\\ -D_5\cdot\mathbf{a}\end{pmatrix}\frac{\partial\mathbf{v}}{\partial a}+\begin{pmatrix} 0\\ -CD_2\cdot\mathbf{n}\\ -D_5\cdot\mathbf{b}\end{pmatrix}\frac{\partial\mathbf{v}}{\partial b}+$$

$$D_3\cdot\begin{pmatrix}\left(\mathbf{a}^T\cdot\nabla\varepsilon\right)\\ C\left(\mathbf{b}^T\cdot\nabla\varepsilon\right)\\ 0\end{pmatrix}=\begin{pmatrix}\frac{1}{N}\mathbf{a}^T\cdot\mathbf{R}\\ \frac{C}{N}\mathbf{b}^T\cdot\mathbf{R}\\ D_4\left(\mathbf{n}^T\cdot\mathbf{v}_p\right)-D_5\cdot D\end{pmatrix} \quad (2.23)$$

Where the extinction coefficient is $C=1-D_5$.*(No idea why I introduced this parameter, for the moment, set it to 1)*

Multiplication with a matrix yields

$$
\begin{aligned}
&(\mathbf{a}\quad \mathbf{b}\quad \mathbf{n})\begin{pmatrix} D_1\cdot\bar{\mathbf{a}}+\tilde{D}_1\cdot\mathbf{a}\\ D_1\cdot\bar{\mathbf{b}}+\tilde{D}_1\cdot\mathbf{b}\\ D_4\cdot\mathbf{n}\end{pmatrix}\cdot\mathbf{v}+(\mathbf{a}\quad \mathbf{b}\quad \mathbf{n})\begin{pmatrix} D_6\cdot\mathbf{a}\\ D_6\cdot\mathbf{b}\\ 0\end{pmatrix}\frac{\partial\mathbf{v}}{\partial m}+\\
&(\mathbf{a}\quad \mathbf{b}\quad \mathbf{n})\begin{pmatrix} -D_2\cdot\mathbf{a}\\ -D_2\cdot\mathbf{b}\\ -D_5\cdot\mathbf{n}\end{pmatrix}\frac{\partial\mathbf{v}}{\partial n}+(\mathbf{a}\quad \mathbf{b}\quad \mathbf{n})\begin{pmatrix} -D_2\cdot\mathbf{n}\\ 0\\ -D_5\cdot\mathbf{a}\end{pmatrix}\frac{\partial\mathbf{v}}{\partial a}+(\mathbf{a}\quad \mathbf{b}\quad \mathbf{n})\begin{pmatrix} 0\\ -D_2\cdot\mathbf{n}\\ -D_5\cdot\mathbf{b}\end{pmatrix}\frac{\partial\mathbf{v}}{\partial b}\\
&+D_3\cdot(\mathbf{a}\quad \mathbf{b}\quad \mathbf{n})\begin{pmatrix} (\mathbf{a}^T\cdot\nabla\varepsilon)\\ (\mathbf{b}^T\cdot\nabla\varepsilon)\\ 0\end{pmatrix}=(\mathbf{a}\quad \mathbf{b}\quad \mathbf{n})\begin{pmatrix} \frac{1}{N}\mathbf{a}^T\cdot\mathbf{R}\\ \frac{1}{N}\mathbf{b}^T\cdot\mathbf{R}\\ D_4\left(\mathbf{n}^T\cdot\mathbf{v}_p\right)-D_5\cdot D\end{pmatrix}
\end{aligned}
\tag{2.24}
$$

This is much simpler by writing

$$
\begin{aligned}
&\left(D_1\cdot\mathbf{a}\bar{\mathbf{a}}^T+D_1\cdot\mathbf{b}\bar{\mathbf{b}}^T+D_4\cdot\mathbf{n}\mathbf{n}^T\right)\cdot\mathbf{v}+\left(\tilde{D}_1\cdot\mathbf{a}\mathbf{a}^T+\tilde{D}_1\cdot\mathbf{b}\mathbf{b}^T\right)\cdot\mathbf{v}+\\
&\qquad+\left(D_6\cdot\mathbf{a}\mathbf{a}^T+D_6\cdot\mathbf{b}\mathbf{b}^T\right)\frac{\partial\mathbf{v}}{\partial m}\\
&\qquad\left(-D_2\cdot\mathbf{a}\mathbf{a}^T-D_2\cdot\mathbf{b}\mathbf{b}^T-D_5\cdot\mathbf{n}\mathbf{n}^T\right)\cdot\frac{\partial\mathbf{v}}{\partial n}+\\
&\qquad\left(-D_2\cdot\mathbf{a}\mathbf{n}^T-D_5\cdot\mathbf{n}\mathbf{a}^T\right)\cdot\frac{\partial\mathbf{v}}{\partial a}+\\
&\qquad\left(-D_2\cdot\mathbf{b}\mathbf{n}^T-D_5\cdot\mathbf{n}\mathbf{b}^T\right)\cdot\frac{\partial\mathbf{v}}{\partial b}+\\
&D_3\cdot\left(\mathbf{a}\frac{\partial\varepsilon}{\partial a}+\mathbf{b}\frac{\partial\varepsilon}{\partial b}\right)=\mathbf{a}\left(\mathbf{a}^T\cdot\frac{\mathbf{R}}{N}\right)+\mathbf{b}\left(\mathbf{b}^T\cdot\frac{\mathbf{R}}{N}\right)+\mathbf{n}\left(D_4\left(\mathbf{n}^T\cdot\mathbf{v}_p\right)-D_5\cdot D\right)
\end{aligned}
\tag{2.25}
$$

REMARK on the transport operator $\frac{\partial}{\partial m}$

In order to come up with numerically stable discretization, we do not evaluate $\frac{\partial}{\partial m}$ at the location of the boundary point, but upstream with the upwind distance of L_{uw}. In this way, the transport of a certain function u is given as

$$\frac{\partial u}{\partial m} \equiv \frac{\partial u}{\partial m}\left(\mathbf{x}-L_{uw}\mathbf{m}\right)=\frac{\partial u}{\partial m}(\mathbf{x})-L_{uw}\frac{\partial^2 u}{\partial m^2}(\mathbf{x})+HigerOrderTerms \tag{2.26}$$

The choice of the upwind length L_{uw} is naturally given by

$$L_{uw} = C \cdot V_p \cdot \Delta t \tag{2.27}$$

The value C can be defined by the user. $C=0.5$ means second order in space-time, $C=1$ still is first order (less precise, more stable).

Such, we represent the upwind term by a centralized gradient type and a centralized diffusion type (Gradient-Diffusion-formulation). For the central gradient, we can use the standard MESHFREE-operator, precalculated at every point and every time step:

$$\frac{\partial u}{\partial m}(\mathbf{x}_i) \approx \sum_j \left(\mathbf{m}_i^T \cdot \mathbf{c}_{ij}^{\nabla} \cdot u_j\right) \tag{2.28}$$

The diffusion operator

$$\frac{\partial^2 u}{\partial m^2}(\mathbf{x}_i) \approx \sum_j \left(c_{ij}^{mm} \cdot u_j\right) \tag{2.29}$$

does not exist explicitly precomputed in MESHFREE. A possibly cheap ansatz (analogously to classical finite differences) is

$$c_{ij}^{mm} = A\frac{W_{ij}}{r_{ij}^2} \tag{2.30}$$

We choose

$$\begin{aligned} r_{ij}^2 &= \left(\mathbf{x}_j - \mathbf{x}_i\right)^T \cdot \left(\mathbf{x}_j - \mathbf{x}_i\right) \\ W_{ij} &= \begin{cases} 1 & \text{if neighbor } j \text{ has the same boundary index than } i \\ \varepsilon & \text{otherwise} \end{cases} \end{aligned} \tag{2.31}$$

And determine A such that

$$\sum_j c_{ij}^{mm} \cdot \left(\mathbf{m}_i^T \cdot \mathbf{x}_j\right)^2 = 2 \tag{2.32}$$

In this way, it exactly reproduces quadratic functions in $\mathbf{m}$-direction. Moreover, c_{ii}^{mm} is adapted such that

$$\sum_j c_{ij}^{mm} = 0 \tag{2.33}$$

To come soon: The procedure (2.29) - (2.32) is the typical GFDM (least squares approximation LSQ) procedure, reduced to exactly two constraints (2.32) and (2.33) . Soon, we shall enrich the LSQ by the full set of constraints (second order in space).

$$\begin{aligned}
&\sum_j c_{ij}^{mm} = 0 \\
&\sum_j c_{ij}^{mm} \cdot \left(\mathbf{m}_i^T \cdot \mathbf{x}_j\right) = 0 \\
&\sum_j c_{ij}^{mm} \cdot \left(\mathbf{m}_i^T \cdot \mathbf{x}_j\right)^2 = 2 \\
&\sum_j c_{ij}^{mm} \cdot \left(\mathbf{a}_i^T \cdot \mathbf{x}_j\right)^n = 0, \qquad n = 1,2 \\
&\sum_j c_{ij}^{mm} \cdot \left(\mathbf{b}_i^T \cdot \mathbf{x}_j\right)^n = 0, \qquad n = 1,2
\end{aligned} \tag{2.34}$$

Where $\mathbf{a}_i$ and $\mathbf{b}_i$ are vectors perpendicular to $\mathbf{m}_i$.

2.3. Slip boundaries with no friction forces

Equation (2.11) becomes as simple as

$$\begin{aligned}
&A\delta h \cdot \rho \cdot \frac{d\left(\mathbf{a}^T \cdot \mathbf{v}\right)}{dt} + A\delta h \cdot \left(\mathbf{a}^T \cdot \nabla \varepsilon\right) + A\delta h \cdot \left(\mathbf{a}^T \cdot \nabla \mathrm{p}\right) = \\
&A \cdot \eta \left(\frac{\partial\left(\mathbf{a}^T \cdot \mathbf{v}\right)}{\partial n} + \frac{\partial\left(\mathbf{n}^T \cdot \mathbf{v}\right)}{\partial a} \right) + A\delta h \cdot \rho \cdot \left(\mathbf{a}^T \cdot \mathbf{g}\right)
\end{aligned} \tag{2.35}$$

and after division by the area term we obtain

$$\begin{aligned}
&\delta h \cdot \rho \cdot \frac{d\left(\mathbf{a}^T \cdot \mathbf{v}\right)}{dt} + \delta h \cdot \left(\mathbf{a}^T \cdot \nabla \varepsilon\right) + \delta h \cdot \left(\mathbf{a}^T \cdot \nabla \mathrm{p}\right) = \\
&\eta \left(\frac{\partial\left(\mathbf{a}^T \cdot \mathbf{v}\right)}{\partial n} + \frac{\partial\left(\mathbf{n}^T \cdot \mathbf{v}\right)}{\partial a} \right) + \delta h \cdot \rho \cdot \left(\mathbf{a}^T \cdot \mathbf{g}\right)
\end{aligned} \tag{2.36}$$

Finally,

$$\frac{\delta h\cdot\rho}{\Delta t}\cdot\left(\mathbf{a}^T\cdot\mathbf{v}\right)-\eta\left(\frac{\partial\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial a}\right)+\delta h\cdot\left(\mathbf{a}^T\cdot\nabla\varepsilon\right)=$$
$$\frac{\delta h\cdot\rho}{\Delta t}\cdot\left(\mathbf{a}^T\cdot\mathbf{v}_0\right)+\delta h\cdot\rho\cdot\left(\mathbf{a}^T\cdot\mathbf{g}\right)-\delta h\cdot\left(\mathbf{a}^T\cdot\nabla p\right) \tag{2.37}$$

Similarly to (2.16), we define the right hand side

$$\mathbf{R}=\frac{\delta h\cdot\rho}{\Delta t}\cdot\mathbf{v}_0+\delta h\cdot\rho\cdot\mathbf{g}-\delta h\cdot\nabla p \tag{2.38}$$

and hence, (2.37) appears as

$$\frac{\delta h\cdot\rho}{\Delta t}\cdot\left(\mathbf{a}^T\cdot\mathbf{v}\right)-\eta\left(\frac{\partial\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial a}\right)+\delta h\cdot\left(\mathbf{a}^T\cdot\nabla\varepsilon\right)=\mathbf{a}^T\cdot\mathbf{R} \tag{2.39}$$

Normalization yields

$$\frac{\delta h\cdot\rho}{\Delta t}\frac{1}{N}\cdot\left(\mathbf{a}^T\cdot\mathbf{v}\right)-\frac{\eta}{N}\left(\frac{\partial\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial a}\right)+\frac{\delta h}{N}\cdot\left(\mathbf{a}^T\cdot\nabla\varepsilon\right)=\mathbf{a}^T\cdot\frac{\mathbf{R}}{N} \tag{2.40}$$

and a similar definition of dummy constants leads to

$$D_1\cdot\left(\mathbf{a}^T\cdot\mathbf{v}\right)-D_2\left(\frac{\partial\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial a}\right)+D_3\cdot\left(\mathbf{a}^T\cdot\nabla\varepsilon\right)=\mathbf{a}^T\cdot\frac{\mathbf{R}}{N} \tag{2.41}$$

Equations (2.41) and (2.20) are exactly the same, such that the same algorithm works. The determination of the constants yields

$$N=\max\left(\frac{\delta h\cdot\rho}{\Delta t},\eta\cdot c^{\text{diff}}\right) \tag{2.42}$$

the value of c^{diff} is the biggest entry in the local differential operators for gradients.

2.4. Slip Boundaries Epsilon part

The equation to be solved throughout the domain is

$$\mathbf{v}^{n+1} - \tilde{\mathbf{v}}^{n+1} + \frac{\Delta t_{virt}}{\rho} \nabla \varepsilon = 0 \quad (2.43)$$

The term $\mathbf{v}^{n+1} - \tilde{\mathbf{v}}^{n+1}$ means how to correct the numerical solution. In fact, at the boundary we prescribe a normal flux, so $\frac{\Delta t_{virt}}{\rho} \mathbf{n} \cdot \nabla \varepsilon = 0$ would be sufficient, however we should better penalize the fact, that the flow does not assume the correct value of divergence of velocity. In fact we should set

$$\mathbf{n}^T \cdot \left(\mathbf{v}^{n+1} - \tilde{\mathbf{v}}^{n+1} \right) = -\alpha h \cdot \left(\nabla^T \mathbf{v} - \nabla^T \mathbf{v}_{required} \right) \quad (2.44)$$

an thus the boundary condition would be

$$\frac{\Delta t_{virt}}{\rho} \left(\mathbf{n}^T \cdot \nabla \varepsilon \right) = \frac{\Delta t_{virt}}{\rho} \frac{\partial \varepsilon}{\partial n} = \alpha h \cdot \left(\nabla^T \mathbf{v} - \nabla^T \mathbf{v}_{required} \right) \quad (2.45)$$

The value of $\nabla^T \mathbf{v}_{required}$ is

$$\nabla^T \mathbf{v}_{required} = -\frac{\rho_p}{\rho} \frac{\varepsilon}{\Delta t} + \overline{\nabla^T \mathbf{v}} \quad (2.46)$$

Thus, the boundary condition is

$$\frac{\Delta t_{virt}}{\rho} \frac{\partial \varepsilon}{\partial n} = \alpha h \cdot \left(\nabla^T \mathbf{v} + \frac{\rho_p}{\rho} \frac{\varepsilon}{\Delta t} - \overline{\nabla^T \mathbf{v}} \right) \quad (2.47)$$

Bringing everything on the right side of the equation, we obtain

$$\frac{\partial \varepsilon}{\partial n} - \alpha h \cdot \frac{\rho_p}{\Delta t_{virt} \Delta t} \varepsilon - \alpha h \cdot \frac{\rho}{\Delta t_{virt}} \nabla^T \mathbf{v} = -\alpha h \cdot \frac{\rho}{\Delta t_{virt}} \cdot \overline{\nabla^T \mathbf{v}} \quad (2.48)$$

or a bit different

$$\frac{\partial \varepsilon}{\partial n} - \left(\alpha h \cdot \frac{\rho}{\Delta t_{virt}} \right) \cdot \left(\frac{\rho_p}{\rho \cdot \Delta t} \right) \varepsilon - \left(\alpha h \cdot \frac{\rho}{\Delta t_{virt}} \right) \nabla^T \mathbf{v} = - \left(\alpha h \cdot \frac{\rho}{\Delta t_{virt}} \right) \cdot \overline{\nabla^T \mathbf{v}} \qquad (2.49)$$

With dedicated constants

$$\frac{\partial \varepsilon}{\partial n} - D_7 \cdot D_6 \cdot \varepsilon - D_7 \cdot \nabla^T \mathbf{v} = -D_7 \cdot \overline{\nabla^T \mathbf{v}} \qquad (2.50)$$

3. Contact boundary

We can consider a phase boundary (i.e. a boundary being in contact with some other, different material) either as a free surface boundary with additional terms (compared to chapter 1) or as slip boundary with additional terms (similarly to chapter 2).

The first of these two cases will be applied, if the local dynamic viscosity is bigger than the one of the opposite material. The second of these cases will be applied in the other way, namely if the viscosity is smaller than the opposite one. An example would be the two phase flow of air and water. Seen from the water side, the air does not have much impact on the heavy water, so the surface of the water is like a free surface with slight modifications concerning pressure. Seen from the air, the surface of the water is almost like an impermeable wall that moves. That means, that for phase boundaries, from one side we have to provide a free surface type condition, from the other side, be will have to provide a slip wall condition.

3.1. Phase boundary, free surface type

Similarly to equation (1.1), we state the equilibrium equation for such a boundary

$$\begin{aligned} \mathbf{a}^T \cdot \mathbf{S} \cdot \mathbf{n} &= \mathbf{a}^T \cdot \mathbf{S}_o \cdot \mathbf{n} \\ \mathbf{b}^T \cdot \mathbf{S} \cdot \mathbf{n} &= \mathbf{b}^T \cdot \mathbf{S}_o \cdot \mathbf{n} \\ \mathbf{n}^T \cdot \mathbf{S} \cdot \mathbf{n} - \mathrm{p} &= \mathbf{n}^T \cdot \mathbf{S}_o \cdot \mathbf{n} - \mathrm{p}_0 \end{aligned} \qquad (3.1)$$

Again, as the last equation will be fulfilled by implementing boundary conditions for the pressure Poisson equation, we are able replace tha last line.

$$\begin{aligned}&\mathbf{a}^T \cdot \mathbf{S} \cdot \mathbf{n} = \mathbf{a}^T \cdot \mathbf{S}_o \cdot \mathbf{n}\\&\mathbf{b}^T \cdot \mathbf{S} \cdot \mathbf{n} = \mathbf{b}^T \cdot \mathbf{S}_o \cdot \mathbf{n}\\&div(\mathbf{v}) = D\end{aligned} \tag{3.2}$$

If there is no viscous tension along the free surface at the opposite side (i.e. $\mathbf{a}^T \cdot \mathbf{S}_o \cdot \mathbf{n} = 0,\ \mathbf{b}^T \cdot \mathbf{S}_o \cdot \mathbf{n} = 0$), then equation (3.2) reduces to equation (1.2) and therefore to a simple free surface condition. We rewrite (3.2) by

$$\begin{aligned}&\eta \cdot \left(\frac{\partial\left(\mathbf{a}^T \cdot \left(\mathbf{v} - \phi \mathbf{v}_o\right)\right)}{\partial n} + \frac{\partial\left(\mathbf{n}^T \cdot \left(\mathbf{v} - \phi \mathbf{v}_o\right)\right)}{\partial a} \right) = 0\\&\eta \cdot \left(\frac{\partial\left(\mathbf{b}^T \cdot \left(\mathbf{v} - \phi \mathbf{v}_o\right)\right)}{\partial n} + \frac{\partial\left(\mathbf{n}^T \cdot \left(\mathbf{v} - \phi \mathbf{v}_o\right)\right)}{\partial b} \right) = 0\\&\frac{\partial\left(\mathbf{n}^T \cdot \mathbf{v}\right)}{\partial n} + \frac{\partial\left(\mathbf{a}^T \cdot \mathbf{v}\right)}{\partial a} + \frac{\partial\left(\mathbf{b}^T \cdot \mathbf{v}\right)}{\partial b} = D\end{aligned} \tag{3.3}$$

We have the definition

$$\phi = \frac{\eta_o}{\eta} \tag{3.4}$$

In matrix vector notation, we find

$$\begin{pmatrix} \mathbf{a}^T \\ \mathbf{b}^T \\ \mathbf{n}^T \end{pmatrix} \cdot \frac{\partial\left(\mathbf{v} - \phi \mathbf{v}_o\right)}{\partial n} + \begin{pmatrix} \mathbf{n}^T \\ \mathbf{0} \\ \mathbf{a}^T \end{pmatrix} \cdot \frac{\partial\left(\mathbf{v} - \phi \mathbf{v}_o\right)}{\partial a} + \begin{pmatrix} \mathbf{0} \\ \mathbf{n}^T \\ \mathbf{b}^T \end{pmatrix} \cdot \frac{\partial\left(\mathbf{v} - \phi \mathbf{v}_o\right)}{\partial b} = \begin{pmatrix} 0 \\ 0 \\ D - \phi D_o \end{pmatrix} \tag{3.5}$$

Isolation of the term

$$\frac{\partial\left(\mathbf{v} - \phi \mathbf{v}_o\right)}{\partial n} + \left(\mathbf{a}\mathbf{n}^T + \mathbf{n}\mathbf{a}^T\right) \cdot \frac{\partial\left(\mathbf{v} - \phi \mathbf{v}_o\right)}{\partial a} + \left(\mathbf{b}\mathbf{n}^T + \mathbf{n}\mathbf{b}^T\right) \cdot \frac{\partial\left(\mathbf{v} - \phi \mathbf{v}_o\right)}{\partial b} = \mathbf{n} \cdot \left(D - \phi D_o\right) \tag{3.6}$$

3.2. Phase boundary, free surface type including momentum balance, tangential direction

A more sophisticated ansatz for the free surfaces includes the momentum balance. Suppose we have a slice of material of thickness δh normal to the surface. The mometum balance taken in the tangential direction of $\mathbf{a}$ is

$$\delta h \cdot A \cdot \rho \frac{d\mathbf{v}}{dt} + \delta h \cdot A \cdot \left(\mathbf{a}^T \cdot \nabla \varepsilon\right) = A \cdot \left(\mathbf{a}^T \cdot \mathbf{S} \cdot \mathbf{n} - \mathbf{a}^T \cdot \mathbf{S}_{Opp} \cdot \mathbf{n}\right) + \delta h \cdot A \cdot \left(\mathbf{a}^T \cdot \mathbf{g}\right) - \delta h \cdot A \cdot \left(\mathbf{a}^T \cdot \nabla p\right) \quad (3.7)$$

Division by A yields

$$\delta h \cdot \rho \frac{d\mathbf{v}}{dt} + \delta h \cdot \left(\mathbf{a}^T \cdot \nabla \varepsilon\right) = \left(\mathbf{a}^T \cdot \mathbf{S} \cdot \mathbf{n} - \mathbf{a}^T \cdot \mathbf{S}_{Opp} \cdot \mathbf{n}\right) + \delta h \cdot \rho \cdot \left(\mathbf{a}^T \cdot \mathbf{g}\right) - \delta h \cdot \left(\mathbf{a}^T \cdot \nabla p\right) \quad (3.8)$$

which is equally

$$\delta h \cdot \rho \frac{d\left(\mathbf{a}^T \cdot \mathbf{v}\right)}{dt} + \delta h \cdot \left(\mathbf{a}^T \cdot \nabla \varepsilon\right) = \eta \cdot \left(\frac{\partial\left(\mathbf{a}^T \cdot \mathbf{v}\right)}{\partial n} + \frac{\partial\left(\mathbf{n}^T \cdot \mathbf{v}\right)}{\partial a}\right) - \eta_{Opp} \cdot \left(\frac{\partial\left(\mathbf{a}^T \cdot \mathbf{v}_{Opp}\right)}{\partial n} + \frac{\partial\left(\mathbf{n}^T \cdot \mathbf{v}_{Opp}\right)}{\partial a}\right) \quad (3.9)$$
$$+ \delta h \cdot \rho \cdot \left(\mathbf{a}^T \cdot \mathbf{g}\right) - \delta h \cdot \left(\mathbf{a}^T \cdot \nabla p\right)$$

As a numerical scheme, it looks like

$$\begin{aligned} &\delta h \cdot \rho \cdot \mathbf{a}^T \cdot \frac{\mathbf{v} - \mathbf{v}_0}{\Delta t} + \delta h \cdot \left(\mathbf{a}^T \cdot \tilde{\nabla} \varepsilon\right) = \\ &\eta \cdot \left(\frac{\tilde{\partial}\left(\mathbf{a}^T \cdot \mathbf{v}\right)}{\tilde{\partial} n} + \frac{\tilde{\partial}\left(\mathbf{n}^T \cdot \mathbf{v}\right)}{\tilde{\partial} a}\right) - \eta_{Opp} \cdot \left(\frac{\tilde{\partial}\left(\mathbf{a}^T \cdot \mathbf{v}_{Opp}\right)}{\tilde{\partial} n} + \frac{\tilde{\partial}\left(\mathbf{n}^T \cdot \mathbf{v}_{Opp}\right)}{\tilde{\partial} a}\right) \\ &+ \delta h \cdot \rho \cdot \left(\mathbf{a}^T \cdot \mathbf{g}\right) - \delta h \cdot \left(\mathbf{a}^T \cdot \nabla p\right) \end{aligned} \quad (3.10)$$

and we can put the unknow values on the left hand side and all the other ones on the right hand side.

$$\begin{aligned} &\frac{\delta h \cdot \rho}{\Delta t} \cdot \left(\mathbf{a}^T \cdot \mathbf{v}\right) - \eta \cdot \left(\frac{\tilde{\partial}\left(\mathbf{a}^T \cdot \mathbf{v}\right)}{\tilde{\partial} n} - \phi \frac{\tilde{\partial}\left(\mathbf{a}^T \cdot \mathbf{v}_{Opp}\right)}{\tilde{\partial} n} + \frac{\tilde{\partial}\left(\mathbf{n}^T \cdot \mathbf{v}\right)}{\tilde{\partial} a} - \phi \frac{\tilde{\partial}\left(\mathbf{n}^T \cdot \mathbf{v}_{Opp}\right)}{\tilde{\partial} a}\right) + \delta h \cdot \left(\mathbf{a}^T \cdot \tilde{\nabla} \varepsilon\right) = \\ &\frac{\delta h \cdot \rho}{\Delta t} \cdot \left(\mathbf{a}^T \cdot \mathbf{v}_0\right) + \delta h \cdot \rho \cdot \left(\mathbf{a}^T \cdot \mathbf{g}\right) - \delta h \cdot \left(\mathbf{a}^T \cdot \nabla p\right) \end{aligned} \quad (3.11)$$

Let us also divide by a nondimsionalizing term N

$$\frac{\delta h\cdot\rho}{\Delta t\cdot N}\cdot\left(\mathbf{a}^T\cdot\mathbf{v}\right)-\frac{\eta}{N}\cdot\left(\frac{\tilde{\partial}\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\tilde{\partial}n}-\phi\frac{\tilde{\partial}\left(\mathbf{a}^T\cdot\mathbf{v}_{Opp}\right)}{\tilde{\partial}n}+\frac{\tilde{\partial}\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\tilde{\partial}a}-\phi\frac{\tilde{\partial}\left(\mathbf{n}^T\cdot\mathbf{v}_{Opp}\right)}{\tilde{\partial}a}\right)+\frac{\delta h}{N}\cdot\left(\mathbf{a}^T\cdot\tilde{\nabla}\varepsilon\right)= \frac{\delta h\cdot\rho}{\Delta t\cdot N}\cdot\left(\mathbf{a}^T\cdot\mathbf{v}_0\right)+\frac{\delta h\cdot\rho}{N}\cdot\left(\mathbf{a}^T\cdot\mathbf{g}\right)-\frac{\delta h}{N}\cdot\left(\mathbf{a}^T\cdot\nabla p\right) \tag{3.12}$$

The choice of N is

$$N=\frac{\delta h\cdot\rho}{\Delta t}+\eta\cdot c^{diff} \tag{3.13}$$

N is chooses such that one of the terms on the right hand side has possibly order 1, the others less. In a simpler way, we can write

$$D_1\cdot\left(\mathbf{a}^T\cdot\mathbf{v}\right)-D_2\cdot\left(\frac{\tilde{\partial}\left(\mathbf{a}^T\cdot\left(\mathbf{v}-\phi\mathbf{v}_{Opp}\right)\right)}{\tilde{\partial}n}+\frac{\tilde{\partial}\left(\mathbf{n}^T\cdot\left(\mathbf{v}-\phi\mathbf{v}_{Opp}\right)\right)}{\tilde{\partial}a}\right)+D_3\cdot\left(\mathbf{a}^T\cdot\tilde{\nabla}\varepsilon\right)=\mathbf{a}^T\cdot\mathbf{R} \tag{3.14}$$

Similarly, for the second tangential vector, we have

$$D_1\cdot\left(\mathbf{b}^T\cdot\mathbf{v}\right)-D_2\cdot\left(\frac{\tilde{\partial}\left(\mathbf{b}^T\cdot\left(\mathbf{v}-\phi\mathbf{v}_{Opp}\right)\right)}{\tilde{\partial}n}+\frac{\tilde{\partial}\left(\mathbf{n}^T\cdot\left(\mathbf{v}-\phi\mathbf{v}_{Opp}\right)\right)}{\tilde{\partial}b}\right)+D_3\cdot\left(\mathbf{b}^T\cdot\tilde{\nabla}\varepsilon\right)=\mathbf{b}^T\cdot\mathbf{R} \tag{3.15}$$

Written in matrix vector formulation we obtain

$$D_1\begin{pmatrix}\mathbf{a}^T\\ \mathbf{b}^T\\ \mathbf{0}\end{pmatrix}\cdot\mathbf{v}-\begin{pmatrix}D_2\mathbf{a}^T\\ D_2\mathbf{b}^T\\ D_4\mathbf{n}^T\end{pmatrix}\cdot\frac{\partial\mathbf{v}}{\partial n}+\begin{pmatrix}D_2\phi\mathbf{a}^T\\ D_2\phi\mathbf{b}^T\\ 0\end{pmatrix}\cdot\frac{\partial\mathbf{v}_{Opp}}{\partial n}-\begin{pmatrix}D_2\mathbf{n}^T\\ \mathbf{0}\\ D_4\mathbf{a}^T\end{pmatrix}\cdot\frac{\partial\mathbf{v}}{\partial a}+\begin{pmatrix}D_2\phi\mathbf{n}^T\\ \mathbf{0}\\ 0\end{pmatrix}\cdot\frac{\partial\mathbf{v}_{Opp}}{\partial a} -\begin{pmatrix}\mathbf{0}\\ D_2\mathbf{n}^T\\ D_4\mathbf{b}^T\end{pmatrix}\cdot\frac{\partial\mathbf{v}}{\partial b}+\begin{pmatrix}\mathbf{0}\\ D_2\phi\mathbf{n}^T\\ 0\end{pmatrix}\cdot\frac{\partial\mathbf{v}_{Opp}}{\partial b}+\begin{pmatrix}D_3\cdot\frac{\partial\varepsilon}{\partial a}\\ D_3\cdot\frac{\partial\varepsilon}{\partial b}\\ -D_4\cdot D_5\cdot\varepsilon\end{pmatrix}=\begin{pmatrix}\mathbf{a}^T\cdot\mathbf{R}\\ \mathbf{b}^T\cdot\mathbf{R}\\ -D_4\cdot D\end{pmatrix} \tag{3.16}$$

Multiplication with the inverse matrix yields

$$D_1\begin{pmatrix}\mathbf{a} & \mathbf{b} & \mathbf{n}\end{pmatrix}\begin{pmatrix}\mathbf{a}^T\\ \mathbf{b}^T\\ \mathbf{0}\end{pmatrix}\cdot\mathbf{v}-\begin{pmatrix}\mathbf{a} & \mathbf{b} & \mathbf{n}\end{pmatrix}\begin{pmatrix}0\\ 0\\ D_4\mathbf{n}^T\end{pmatrix}\cdot\frac{\partial\mathbf{v}}{\partial n}-\begin{pmatrix}\mathbf{a} & \mathbf{b} & \mathbf{n}\end{pmatrix}\begin{pmatrix}D_2\mathbf{a}^T\\ D_2\mathbf{b}^T\\ 0\end{pmatrix}\cdot\frac{\partial\left(\mathbf{v}-\phi\mathbf{v}_{Opp}\right)}{\partial n}$$
$$-\begin{pmatrix}\mathbf{a} & \mathbf{b} & \mathbf{n}\end{pmatrix}\begin{pmatrix}0\\ \mathbf{0}\\ D_4\mathbf{a}^T\end{pmatrix}\cdot\frac{\partial\mathbf{v}}{\partial a}-\begin{pmatrix}\mathbf{a} & \mathbf{b} & \mathbf{n}\end{pmatrix}\begin{pmatrix}D_2\mathbf{n}^T\\ \mathbf{0}\\ 0\end{pmatrix}\cdot\frac{\partial\left(\mathbf{v}-\phi\mathbf{v}_{Opp}\right)}{\partial a}$$
$$-\begin{pmatrix}\mathbf{a} & \mathbf{b} & \mathbf{n}\end{pmatrix}\begin{pmatrix}\mathbf{0}\\ 0\\ D_4\mathbf{b}^T\end{pmatrix}\cdot\frac{\partial\mathbf{v}}{\partial b}-\begin{pmatrix}\mathbf{a} & \mathbf{b} & \mathbf{n}\end{pmatrix}\begin{pmatrix}\mathbf{0}\\ D_2\mathbf{n}^T\\ 0\end{pmatrix}\cdot\frac{\partial\left(\mathbf{v}-\phi\mathbf{v}_{Opp}\right)}{\partial b}$$
$$+\begin{pmatrix}\mathbf{a} & \mathbf{b} & \mathbf{n}\end{pmatrix}\begin{pmatrix}D_3\cdot\frac{\partial\varepsilon}{\partial a}\\ D_3\cdot\frac{\partial\varepsilon}{\partial b}\\ -D_4\cdot D_5\cdot\varepsilon\end{pmatrix}=\begin{pmatrix}\mathbf{a} & \mathbf{b} & \mathbf{n}\end{pmatrix}\begin{pmatrix}\mathbf{a}^T\cdot\mathbf{R}\\ \mathbf{b}^T\cdot\mathbf{R}\\ -D_4\cdot D\end{pmatrix} \tag{3.17}$$

And more easy

$$D_1\left(\mathbf{a}\mathbf{a}^T+\mathbf{b}\mathbf{b}^T\right)\cdot\mathbf{v}-\left(D_4\mathbf{n}\mathbf{n}^T\right)\cdot\frac{\partial\mathbf{v}}{\partial n}-\left(D_2\mathbf{a}\mathbf{a}^T+D_2\mathbf{b}\mathbf{b}^T\right)\cdot\frac{\partial\left(\mathbf{v}-\phi\mathbf{v}_{Opp}\right)}{\partial n}$$
$$-\left(D_4\mathbf{n}\mathbf{a}^T\right)\cdot\frac{\partial\mathbf{v}}{\partial a}-\left(D_2\mathbf{a}\mathbf{n}^T\right)\cdot\frac{\partial\left(\mathbf{v}-\phi\mathbf{v}_{Opp}\right)}{\partial a}-\left(D_4\mathbf{n}\mathbf{b}^T\right)\cdot\frac{\partial\mathbf{v}}{\partial b}-\left(D_2\mathbf{b}\mathbf{n}^T\right)\cdot\frac{\partial\left(\mathbf{v}-\phi\mathbf{v}_{Opp}\right)}{\partial b} \tag{3.18}$$
$$+D_3\cdot\left(\mathbf{a}\frac{\partial\varepsilon}{\partial a}+\mathbf{b}\frac{\partial\varepsilon}{\partial b}\right)-\mathbf{n}\cdot D_4\cdot D_5\cdot\varepsilon=\mathbf{a}\left(\mathbf{a}^T\cdot\mathbf{R}\right)+\mathbf{b}\left(\mathbf{b}^T\cdot\mathbf{R}\right)+\mathbf{n}\left(-D_4\cdot D\right)$$

3.3. Phase boundary, free surface type, including momentum balance, normal direction

$$\delta\mathrm{h}\cdot\mathrm{A}\cdot\rho\frac{d\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{dt}+\mathrm{A}\cdot\left(\mathrm{p}+\varepsilon-\mathrm{p}_{Opp}-\varepsilon_{Opp}\right)=\mathrm{A}\cdot\left(\mathbf{n}^T\cdot\left(\mathbf{S}-\mathbf{S}_{Opp}\right)\cdot\mathbf{n}\right)+\delta\mathrm{h}\cdot\mathrm{A}\cdot\rho\cdot\left(\mathbf{n}^T\cdot\mathbf{g}\right) \tag{3.19}$$

Equaly written as

$$\delta\mathrm{h}\cdot\rho\frac{d\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{dt}+\left(\mathrm{p}+\varepsilon-\mathrm{p}_{Opp}-\varepsilon_{Opp}\right)=2\eta\left(\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial n}-\frac{\eta_{\mathrm{Opp}}}{\eta}\left.\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial n}\right|_{Opp}\right)+\delta\mathrm{h}\cdot\rho\cdot\left(\mathbf{n}^T\cdot\mathbf{g}\right) \tag{3.20}$$

As numerical scheme, with $\phi=\frac{\eta_{\mathrm{Opp}}}{\eta}$ it appears as

$$\frac{\delta h \cdot \rho}{\Delta t}\left(\mathbf{n}^T \cdot \mathbf{v} - \mathbf{n}^T \cdot \mathbf{v}_0\right) + \left(p + \varepsilon - p_0 - \varepsilon_{Opp}\right) = 2\eta\left(\frac{\partial\left(\mathbf{n}^T \cdot \mathbf{v}\right)}{\partial n} - \frac{1}{3}D - \phi \left.\frac{\partial\left(\mathbf{n}^T \cdot \mathbf{v}\right)}{\partial n}\right|_{Opp} + \frac{1}{3}\phi D_{Opp}\right) + \delta h \cdot \rho \cdot \left(\mathbf{n}^T \cdot \mathbf{g}\right) \tag{3.21}$$

After reordering of terms, we obtain

$$\frac{\delta h \cdot \rho}{\Delta t}\left(\mathbf{n}^T \cdot \mathbf{v}\right) - 2\eta\left(\frac{\partial\left(\mathbf{n}^T \cdot \mathbf{v}\right)}{\partial n} - \frac{1}{3}D - \phi \left.\frac{\partial\left(\mathbf{n}^T \cdot \mathbf{v}\right)}{\partial n}\right|_{Opp} + \frac{1}{3}\phi D_{Opp}\right) + \varepsilon - \varepsilon_{Opp} = \frac{\delta h \cdot \rho}{\Delta t}\left(\mathbf{n}^T \cdot \mathbf{v}_0\right) + \delta h \cdot \rho \cdot \left(\mathbf{n}^T \cdot \mathbf{g}\right) - \left(p - p_{Opp}\right) \tag{3.22}$$

Simplification yields

$$D_5\left(\mathbf{n}^T \cdot \mathbf{v}\right) - D_6\left(\frac{\partial\left(\mathbf{n}^T \cdot \mathbf{v}\right)}{\partial n} - \phi \left.\frac{\partial\left(\mathbf{n}^T \cdot \mathbf{v}\right)}{\partial n}\right|_{Opp} - \frac{1}{3}\left(D - \phi D_{Opp}\right)\right) + \varepsilon - \varepsilon_{Opp} = R \tag{3.23}$$

With the already prepared operators $\frac{\partial_\phi^{Opp}}{\partial n} = \frac{\partial}{\partial n} - \phi \left.\frac{\partial}{\partial n}\right|_{Opp}$ we finally reach

$$D_5\left(\mathbf{n}^T \cdot \mathbf{v}\right) - D_6\left(\frac{\partial_\phi^{Opp}\left(\mathbf{n}^T \cdot \mathbf{v}\right)}{\partial n} - \frac{1}{3}\left(\nabla_\phi^{OppT} \cdot \mathbf{v}\right)\right) + \varepsilon - \varepsilon_{Opp} = R \tag{3.24}$$

3.4. Phase boundary, slip wall type

The formulation of the slip interphase condition is similar to the formulation in equation (2.1), with the same meaning of the slip coefficient α as above.

$$\begin{aligned} &\alpha \cdot \mathbf{a}^T \cdot \mathbf{S} \cdot \mathbf{n} = \mathbf{a}^T \cdot \left(\mathbf{v} - \mathbf{v}_o\right) \\ &\alpha \cdot \mathbf{b}^T \cdot \mathbf{S} \cdot \mathbf{n} = \mathbf{b}^T \cdot \left(\mathbf{v} - \mathbf{v}_o\right) \\ &\mathbf{n}^T \cdot \left(\mathbf{v} - \mathbf{v}_o\right) = 0 \end{aligned} \tag{3.25}$$

The index „o“ means the values of the opposite material. Let us rewrite this system in terms of derivatives of velocities.

$$\alpha \cdot \eta \cdot \left(\frac{\partial\left(\mathbf{a}^T \cdot \mathbf{v}\right)}{\partial n} + \frac{\partial\left(\mathbf{n}^T \cdot \mathbf{v}\right)}{\partial a} \right) = \mathbf{a}^T \cdot \left(\mathbf{v} - \mathbf{v}_o\right)$$
$$\alpha \cdot \eta \cdot \left(\frac{\partial\left(\mathbf{b}^T \cdot \mathbf{v}\right)}{\partial n} + \frac{\partial\left(\mathbf{n}^T \cdot \mathbf{v}\right)}{\partial b} \right) = \mathbf{b}^T \cdot \left(\mathbf{v} - \mathbf{v}_o\right) \qquad (3.26)$$
$$s \cdot \mathbf{n}^T \cdot \left(\mathbf{v} - \mathbf{v}_o\right) = 0$$

Again, we have to normalize the first two equations such that they are in the same order of magnitude.

$$X \cdot \alpha \cdot \eta \cdot \left(\mathbf{a}^T \cdot \frac{\partial \mathbf{v}}{\partial n} + \mathbf{n}^T \cdot \frac{\partial \mathbf{v}}{\partial a} \right) - X \cdot \mathbf{a}^T \cdot \left(\mathbf{v} - \mathbf{v}_o\right) = 0$$
$$X \cdot \alpha \cdot \eta \cdot \left(\mathbf{b}^T \cdot \frac{\partial \mathbf{v}}{\partial n} + \mathbf{n}^T \cdot \frac{\partial \mathbf{v}}{\partial b} \right) - X \cdot \mathbf{b}^T \cdot \left(\mathbf{v} - \mathbf{v}_o\right) = 0 \qquad (3.27)$$
$$s \cdot \mathbf{n}^T \cdot \left(\mathbf{v} - \mathbf{v}_o\right) + X \cdot \alpha \cdot \eta \cdot \mathbf{n}^T \cdot \frac{\partial \mathbf{v}}{\partial n} - X \cdot \alpha \cdot \eta \cdot \mathbf{n}^T \cdot \frac{\partial \mathbf{v}}{\partial n} = 0$$

That leads to the matrix vector formulation

$$X \cdot \alpha \cdot \eta \cdot \begin{pmatrix} \mathbf{a}^T \\ \mathbf{b}^T \\ \mathbf{n}^T \end{pmatrix} \cdot \frac{\partial \mathbf{v}}{\partial n} + X \cdot \alpha \cdot \eta \cdot \begin{pmatrix} \mathbf{n}^T \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix} \cdot \frac{\partial \mathbf{v}}{\partial a} + X \cdot \alpha \cdot \eta \cdot \begin{pmatrix} \mathbf{0} \\ \mathbf{n}^T \\ \mathbf{0} \end{pmatrix} \cdot \frac{\partial \mathbf{v}}{\partial b}$$
$$-X \cdot \alpha \cdot \eta \cdot \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{n}^T \end{pmatrix} \cdot \frac{\partial \mathbf{v}}{\partial n} + \begin{pmatrix} -X \cdot \mathbf{a}^T \\ -X \cdot \mathbf{b}^T \\ s \cdot \mathbf{n}^T \end{pmatrix} \cdot \left(\mathbf{v} - \mathbf{v}_o\right) = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \qquad (3.28)$$

And the solution for $\frac{\partial \mathbf{v}}{\partial n}$ is given directly by

$$X \cdot \alpha \cdot \eta \cdot \frac{\partial \mathbf{v}}{\partial n} + X \cdot \alpha \cdot \eta \cdot \left(\mathbf{a}\mathbf{n}^T\right) \cdot \frac{\partial \mathbf{v}}{\partial a} + X \cdot \alpha \cdot \eta \cdot \left(\mathbf{b}\mathbf{n}^T\right) \cdot \frac{\partial \mathbf{v}}{\partial b} - X \cdot \alpha \cdot \eta \cdot \left(\mathbf{n}\mathbf{n}^T\right) \cdot \frac{\partial \mathbf{v}}{\partial n}$$
$$+\left(-X \cdot \mathbf{a}\mathbf{a}^T - X \cdot \mathbf{b}\mathbf{b}^T + s \cdot \mathbf{n}\mathbf{n}^T\right) \cdot \left(\mathbf{v} - \mathbf{v}_o\right) = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \qquad (3.29)$$

This is equivalent to

$$X\cdot\alpha\cdot\eta\cdot\left(\mathbf{aa}^T+\cdot\mathbf{bb}^T\right)\cdot\frac{\partial\mathbf{v}}{\partial n}+X\cdot\alpha\cdot\eta\cdot\left(\mathbf{an}^T\right)\cdot\frac{\partial\mathbf{v}}{\partial a}+X\cdot\alpha\cdot\eta\cdot\left(\mathbf{bn}^T\right)\cdot\frac{\partial\mathbf{v}}{\partial b}$$
$$+\left(-X\cdot\mathbf{aa}^T-X\cdot\mathbf{bb}^T+s\cdot\mathbf{nn}^T\right)\cdot\left(\mathbf{v}-\mathbf{v}_o\right)=\begin{pmatrix}0\\0\\0\end{pmatrix} \qquad (3.30)$$

We choose $s=1$ in order to provide well conditioned lines in the operator matrix.

3.5. Phase boundary, Slip type using momentum balance

The momentum balance along a tangential direction $\mathbf{a}$ for a slice with thickness δh and basis area A is given by

$$A\delta h\cdot\rho\cdot\frac{d\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{dt}+A\delta h\cdot\left(\mathbf{a}^T\cdot\nabla\varepsilon\right)+A\delta h\cdot\left(\mathbf{a}^T\cdot\nabla \mathrm{p}\right)\ =$$
$$A\cdot\eta\left(\frac{\partial\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial a}\right)+A\left(\mathbf{a}^T\cdot\mathbf{T}_W\right)-\frac{A}{\alpha}\left(\mathbf{a}^T\cdot\left(\mathbf{v}-\mathbf{v}_{Opp}\right)\right)+A\delta h\cdot\rho\cdot\left(\mathbf{a}^T\cdot\mathbf{g}\right) \qquad (3.31)$$

The turbulent wall tension is

$$\mathbf{T}_W=-\tau_W\cdot\frac{\mathbf{v}-\mathbf{v}_{Opp}}{\left\|\mathbf{v}-\mathbf{v}_{Opp}\right\|} \qquad (3.32)$$

The slip coefficient α determines sliding resistance along the wall by the viscous layer approach.

Equation (3.31) can be simplified by

$$\delta h\cdot\rho\cdot\frac{d\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{dt}+\delta h\cdot\left(\mathbf{a}^T\cdot\nabla\varepsilon\right)+\delta h\cdot\left(\mathbf{a}^T\cdot\nabla \mathrm{p}\right)\ =$$
$$\eta\left(\frac{\partial\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial a}\right)-\left(\frac{\tau_W}{\left\|\mathbf{v}-\mathbf{v}_{Opp}\right\|}+\frac{1}{\alpha}\right)\left(\mathbf{a}^T\cdot\left(\mathbf{v}-\mathbf{v}_{Opp}\right)\right)+\delta h\cdot\rho\cdot\left(\mathbf{a}^T\cdot\mathbf{g}\right) \qquad (3.33)$$

where the thickness parameter δh appears as regularization factor. If $\delta h=0$, we find back the original slip boundary formulation

$$0\ =\eta\left(\frac{\partial\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial a}\right)-\left(\frac{\tau_W}{\left\|\mathbf{v}-\mathbf{v}_{Opp}\right\|}+\frac{1}{\alpha}\right)\left(\mathbf{a}^T\cdot\left(\mathbf{v}-\mathbf{v}_{Opp}\right)\right) \qquad (3.34)$$

Please compare (3.34) with equation (2.1). Let us rewrite equation (3.33)

$$\frac{\delta h\cdot\rho}{\Delta t}\cdot\left(\mathbf{a}^T\cdot\mathbf{v}\right)-\eta\left(\frac{\partial\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial a}\right)+\frac{1}{\alpha}\left(\mathbf{a}^T\cdot\mathbf{v}\right)+\delta h\cdot\left(\mathbf{a}^T\cdot\nabla\varepsilon\right) = \frac{\delta h\cdot\rho}{\Delta t}\cdot\left(\mathbf{a}^T\cdot\mathbf{v}_0\right)+\frac{1}{\hat{\alpha}}\left(\mathbf{a}^T\cdot\mathbf{v}_{Opp}\right)+\delta h\cdot\rho\cdot\left(\mathbf{a}^T\cdot\mathbf{g}\right)-\delta h\cdot\left(\mathbf{a}^T\cdot\nabla\mathrm{p}\right) \tag{3.35}$$

We define the term

$$\mathbf{R}=\frac{\delta h\cdot\rho}{\Delta t}\cdot\mathbf{v}_0+\delta h\cdot\rho\cdot\mathbf{g}-\delta h\cdot\nabla\mathrm{p} \tag{3.36}$$

And thus we are able to rewrite (3.35) in the sense

$$\left(\frac{\delta h\cdot\rho}{\Delta t}\right)\cdot\left(\mathbf{a}^T\cdot\mathbf{v}\right)+\left(\frac{1}{\hat{\alpha}}\right)\cdot\left(\mathbf{a}^T\cdot\left(\mathbf{v}-\mathbf{v}_{Opp}\right)\right)-\eta\left(\frac{\partial\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial a}\right)+\delta h\cdot\left(\mathbf{a}^T\cdot\nabla\varepsilon\right) =\mathbf{a}^T\cdot\mathbf{R} \tag{3.37}$$

We can nondimensionalize (3.37) by

$$\left(\frac{\delta h\cdot\rho}{\Delta t\cdot N}\right)\cdot\left(\mathbf{a}^T\cdot\mathbf{v}\right)+\left(\frac{1}{\hat{\alpha}\cdot N}\right)\cdot\left(\mathbf{a}^T\cdot\left(\mathbf{v}-\mathbf{v}_{Opp}\right)\right)-\frac{\eta}{N}\left(\frac{\partial\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial a}\right)+\frac{\delta h}{N}\cdot\left(\mathbf{a}^T\cdot\nabla\varepsilon\right) =\mathbf{a}^T\cdot\frac{\mathbf{R}}{N} \tag{3.38}$$

Determination of N is simply given by

$$N=\max\left(\left(\frac{\delta h\cdot\rho}{\Delta t}+\frac{1}{\hat{\alpha}}\right),\ \eta\cdot\mathbf{c}^{\mathrm{diff}}\right) \tag{3.39}$$

And thus, we find

$$D_1\cdot\left(\mathbf{a}^T\cdot\mathbf{v}\right)+\tilde{D}_1\cdot\left(\mathbf{a}^T\cdot\left(\mathbf{v}-\mathbf{v}_{Opp}\right)\right)-D_2\left(\frac{\partial\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial a}\right)+D_3\cdot\left(\mathbf{a}^T\cdot\nabla\varepsilon\right) =\mathbf{a}^T\cdot\frac{\mathbf{R}}{N} \tag{3.40}$$

Of course, the second tangential direction looks similar

$$D_1\cdot\left(\mathbf{b}^T\cdot\mathbf{v}\right)+\tilde{D}_1\cdot\left(\mathbf{b}^T\cdot\left(\mathbf{v}-\mathbf{v}_{Opp}\right)\right)-D_2\left(\frac{\partial\left(\mathbf{b}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial b}\right)+D_3\cdot\left(\mathbf{b}^T\cdot\nabla\varepsilon\right) =\mathbf{b}^T\cdot\frac{\mathbf{R}}{N} \tag{3.41}$$

The third condition is a condition on the normal flux.

$$D_4\left(\mathbf{n}^T\cdot\mathbf{v}\right)+D_5\cdot\left(\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{a}^T\cdot\mathbf{v}\right)}{\partial a}+\frac{\partial\left(\mathbf{b}^T\cdot\mathbf{v}\right)}{\partial b}\right)=D_4\left(\mathbf{n}^T\cdot\mathbf{v}_{Opp}\right)+D_4\cdot R_{Opp}+D_5\cdot D \quad (3.42)$$

where we require that $D_4\left(\mathbf{n}^T\cdot\left(\mathbf{v}-\mathbf{v}_{Opp}\right)\right)=D_4\cdot R_{Opp}$ and R_{Opp} is determined by the fact that we want to move adjacent particles into an optimal distance to each other.

We choose

$$D_4=1$$
$$D_5=D_4\cdot\beta\cdot\delta h$$

β is in the order of 1 and can be chosen by the user. This term forces the divergence of velocity towards a certain value D.

The three conditions (2.20), (2.21) and (2.22) can be written in matrix vector formulation

$$\begin{pmatrix} D_1\cdot\mathbf{a} \\ D_1\cdot\mathbf{b} \\ 0 \end{pmatrix}\cdot\mathbf{v}+\begin{pmatrix} \tilde{D}_1\cdot\mathbf{a} \\ \tilde{D}_1\cdot\mathbf{b} \\ D_4\cdot\mathbf{n} \end{pmatrix}\cdot\left(\mathbf{v}-\mathbf{v}_{Opp}\right)+$$

$$\begin{pmatrix} -D_2\cdot\mathbf{a} \\ -D_2\cdot\mathbf{b} \\ D_5\cdot\mathbf{n} \end{pmatrix}\frac{\partial\mathbf{v}}{\partial n}+\begin{pmatrix} -D_2\cdot\mathbf{n} \\ 0 \\ D_5\cdot\mathbf{a} \end{pmatrix}\frac{\partial\mathbf{v}}{\partial a}+\begin{pmatrix} 0 \\ -D_2\cdot\mathbf{n} \\ D_5\cdot\mathbf{b} \end{pmatrix}\frac{\partial\mathbf{v}}{\partial b}+D_3\cdot\begin{pmatrix} \left(\mathbf{a}^T\cdot\nabla\varepsilon\right) \\ \left(\mathbf{b}^T\cdot\nabla\varepsilon\right) \\ 0 \end{pmatrix}=\begin{pmatrix} \frac{1}{N}\mathbf{a}^T\cdot\mathbf{R} \\ \frac{1}{N}\mathbf{b}^T\cdot\mathbf{R} \\ D_5\cdot D+D_4\cdot R_{Opp} \end{pmatrix} \quad (3.43)$$

Multiplication with a matrix yields

$$\begin{aligned}
&(\mathbf{a} \quad \mathbf{b} \quad \mathbf{n})\begin{pmatrix} D_1 \cdot \mathbf{a} \\ D_1 \cdot \mathbf{b} \\ 0 \end{pmatrix}\cdot \mathbf{v} + (\mathbf{a} \quad \mathbf{b} \quad \mathbf{n})\begin{pmatrix} \tilde{D}_1 \cdot \mathbf{a} \\ \tilde{D}_1 \cdot \mathbf{b} \\ D_4 \cdot \mathbf{n} \end{pmatrix}\cdot\left(\mathbf{v} - \mathbf{v}_{Opp}\right) + \\
&(\mathbf{a} \quad \mathbf{b} \quad \mathbf{n})\begin{pmatrix} -D_2 \cdot \mathbf{a} \\ -D_2 \cdot \mathbf{b} \\ D_5 \cdot \mathbf{n} \end{pmatrix}\frac{\partial \mathbf{v}}{\partial n} + (\mathbf{a} \quad \mathbf{b} \quad \mathbf{n})\begin{pmatrix} -D_2 \cdot \mathbf{n} \\ 0 \\ D_5 \cdot \mathbf{a} \end{pmatrix}\frac{\partial \mathbf{v}}{\partial a} + \\
&(\mathbf{a} \quad \mathbf{b} \quad \mathbf{n})\begin{pmatrix} 0 \\ -D_2 \cdot \mathbf{n} \\ D_5 \cdot \mathbf{b} \end{pmatrix}\frac{\partial \mathbf{v}}{\partial b} + D_3 \cdot (\mathbf{a} \quad \mathbf{b} \quad \mathbf{n})\begin{pmatrix} \left(\mathbf{a}^T \cdot \nabla\varepsilon\right) \\ \left(\mathbf{b}^T \cdot \nabla\varepsilon\right) \\ 0 \end{pmatrix} = (\mathbf{a} \quad \mathbf{b} \quad \mathbf{n})\begin{pmatrix} \frac{1}{N}\mathbf{a}^T \cdot \mathbf{R} \\ \frac{1}{N}\mathbf{b}^T \cdot \mathbf{R} \\ D_5 \cdot D + D_4 \cdot R_{Opp} \end{pmatrix}
\end{aligned} \tag{3.44}$$

This is much more simple by finally writing

$$\begin{aligned}
&\left(D_1 \cdot \mathbf{a}\mathbf{a}^T + D_1 \cdot \mathbf{b}\mathbf{b}^T\right)\cdot \mathbf{v} + \left(\tilde{D}_1 \cdot \mathbf{a}\mathbf{a}^T + \tilde{D}_1 \cdot \mathbf{b}\mathbf{b}^T + D_4 \cdot \mathbf{n}\mathbf{n}^T\right)\cdot\left(\mathbf{v} - \mathbf{v}_{Opp}\right) + \\
&\left(-D_2 \cdot \mathbf{a}\mathbf{a}^T - D_2 \cdot \mathbf{b}\mathbf{b}^T + D_5 \cdot \mathbf{n}\mathbf{n}^T\right)\cdot\frac{\partial \mathbf{v}}{\partial n} + \\
&\left(-D_2 \cdot \mathbf{a}\mathbf{n}^T + D_5 \cdot \mathbf{n}\mathbf{a}^T\right)\cdot\frac{\partial \mathbf{v}}{\partial a} + \\
&\left(-D_2 \cdot \mathbf{b}\mathbf{n}^T + D_5 \cdot \mathbf{n}\mathbf{b}^T\right)\cdot\frac{\partial \mathbf{v}}{\partial b} + \\
&D_3 \cdot \left(\mathbf{a}\frac{\partial \varepsilon}{\partial \mathrm{a}} + \mathbf{b}\frac{\partial \varepsilon}{\partial b}\right) = \mathbf{a}\left(\mathbf{a}^T \cdot \frac{\mathbf{R}}{N}\right) + \mathbf{b}\left(\mathbf{b}^T \cdot \frac{\mathbf{R}}{N}\right) + \mathbf{n}\left(D_5 \cdot D + D_4 \cdot R_{Opp}\right)
\end{aligned} \tag{3.45}$$

The direct implementation of this is kept similar to a simple slip boundary (2.25) by

$$\begin{aligned}
&\left(D_1 \cdot \mathbf{a}\mathbf{a}^T + D_1 \cdot \mathbf{b}\mathbf{b}^T\right)\cdot \mathbf{v} + \left(\tilde{D}_1 \cdot \mathbf{a}\mathbf{a}^T + \tilde{D}_1 \cdot \mathbf{b}\mathbf{b}^T + D_4 \cdot \mathbf{n}\mathbf{n}^T\right)\cdot \mathbf{v} + \\
&+\left(\tilde{D}_1 \cdot \mathbf{a}\mathbf{a}^T + \tilde{D}_1 \cdot \mathbf{b}\mathbf{b}^T + D_4 \cdot \mathbf{n}\mathbf{n}^T\right)\cdot\left(\left(\mathbf{v} - \mathbf{v}_{Opp}\right) - \mathbf{v}\right) \\
&\left(-D_2 \cdot \mathbf{a}\mathbf{a}^T - D_2 \cdot \mathbf{b}\mathbf{b}^T + D_5 \cdot \mathbf{n}\mathbf{n}^T\right)\cdot\frac{\partial \mathbf{v}}{\partial n} + \\
&\left(-D_2 \cdot \mathbf{a}\mathbf{n}^T + D_5 \cdot \mathbf{n}\mathbf{a}^T\right)\cdot\frac{\partial \mathbf{v}}{\partial a} + \\
&\left(-D_2 \cdot \mathbf{b}\mathbf{n}^T + D_5 \cdot \mathbf{n}\mathbf{b}^T\right)\cdot\frac{\partial \mathbf{v}}{\partial b} + \\
&D_3 \cdot \left(\mathbf{a}\frac{\partial \varepsilon}{\partial \mathrm{a}} + \mathbf{b}\frac{\partial \varepsilon}{\partial b}\right) = \mathbf{a}\left(\mathbf{a}^T \cdot \frac{\mathbf{R}}{N}\right) + \mathbf{b}\left(\mathbf{b}^T \cdot \frac{\mathbf{R}}{N}\right) + \mathbf{n}\left(D_5 \cdot D + D_4 \cdot R_{Opp}\right)
\end{aligned} \tag{3.46}$$

3.6. Phase boundary, free surface pressure type

$$0=-\left(\varepsilon+p_d\right)\cdot\mathbf{n}+\mathbf{S}\cdot\mathbf{n}-\left(\varepsilon^o+p_d^o\right)\cdot(-\mathbf{n})+\mathbf{S}^o\cdot(-\mathbf{n}) \tag{3.47}$$

$$0=-\left(\varepsilon+p_d\right)+\eta\left(2\frac{\partial v_n}{\partial n}-\frac{2}{3}\nabla^T\mathbf{v}\right)+\left(\varepsilon^o+p_d^o\right)-\eta^o\left(2\frac{\partial v_n^o}{\partial n}-\frac{2}{3}\nabla^T\mathbf{v}^o\right) \tag{3.48}$$

$$0=\left(\varepsilon+p_d\right)-\left(\varepsilon^o+p_d^o\right)-\left(\eta\left(2\frac{\partial v_n}{\partial n}-\frac{2}{3}\nabla^T\mathbf{v}\right)-\eta^o\left(2\frac{\partial v_n^o}{\partial n}-\frac{2}{3}\nabla^T\mathbf{v}^o\right)\right) \tag{3.49}$$

$$-\left(p_d-p_d^o\right)=\left(\varepsilon-\varepsilon^o\right)-2\eta\left(\left(\frac{\partial v_n}{\partial n}-\phi\frac{\partial v_n^o}{\partial n}\right)-\frac{1}{3}\left(\nabla^T\mathbf{v}-\phi\nabla^T\mathbf{v}^o\right)\right) \tag{3.50}$$

Alternatively:

$$-\left(p_d-p_d^o\right)=\left(\varepsilon-\varepsilon^o\right)-2\eta\left(\left(\nabla^T\mathbf{v}-\frac{\partial v_a}{\partial a}-\frac{\partial v_b}{\partial b}-\phi\left(\nabla^T\mathbf{v}^o-\frac{\partial v_a^o}{\partial a}-\frac{\partial v_b^o}{\partial b}\right)\right)-\frac{1}{3}\left(\nabla^T\mathbf{v}-\phi\nabla^T\mathbf{v}^o\right)\right) \tag{3.51}$$

$$-\left(p_d-p_d^o\right)=\left(\varepsilon-\varepsilon^o\right)-2\eta\left(\left(-\frac{\partial v_a}{\partial a}-\frac{\partial v_b}{\partial b}-\phi\left(-\frac{\partial v_a^o}{\partial a}-\frac{\partial v_b^o}{\partial b}\right)\right)+\frac{2}{3}\left(\nabla^T\mathbf{v}-\phi\nabla^T\mathbf{v}^o\right)\right) \tag{3.52}$$

$$-\left(p_d-p_d^o\right)=\left(\varepsilon-\varepsilon^o\right)+2\eta\left(\left(+\frac{\partial v_a}{\partial a}+\frac{\partial v_b}{\partial b}+\phi\left(-\frac{\partial v_a^o}{\partial a}-\frac{\partial v_b^o}{\partial b}\right)\right)-\frac{2}{3}\left(\nabla^T\mathbf{v}-\phi\nabla^T\mathbf{v}^o\right)\right) \tag{3.53}$$

$$-\left(p_d-p_d^o\right)=\left(\varepsilon-\varepsilon^o\right)+2\eta\left(\left(\frac{\partial v_a}{\partial a}-\phi\frac{\partial v_a^o}{\partial a}\right)+\left(\frac{\partial v_b}{\partial b}-\phi\frac{\partial v_b^o}{\partial b}\right)-\frac{2}{3}\left(\nabla^T\mathbf{v}-\phi\nabla^T\mathbf{v}^o\right)\right) \tag{3.54}$$

4. Coulomb-Friction, using momentum balance

In the direction of the velocity, q, we have the following equilibrium of forces:

$$
\begin{aligned}
&A\delta h\cdot \rho\cdot \frac{d\left(\mathbf{q}^T\cdot\mathbf{v}\right)}{dt}+A\delta h\cdot\left(\mathbf{q}^T\cdot\nabla\varepsilon\right)+A\delta h\cdot\left(\mathbf{q}^T\cdot\nabla \mathrm{p}\right) \ = \\
&A\cdot\mathbf{q}^T\cdot\mathbf{S}_S\cdot\mathbf{n}-A\cdot\mu\left(p-\mathbf{n}^T\cdot\mathbf{S}_S\cdot\mathbf{n}\right)+ \\
&A\cdot\eta\left(\frac{\partial\left(\mathbf{q}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial q}\right)-A\cdot\mu\left(\varepsilon-\eta\left(2\frac{\partial\left(\mathbf{q}^T\cdot\mathbf{v}\right)}{\partial n}-\frac{2}{3}D\right)\right) \\
&+A\delta h\cdot\rho\cdot\left(\mathbf{q}^T\cdot\mathbf{g}\right)
\end{aligned}
\tag{4.1}
$$

Simplification (division by A) yields

$$
\begin{aligned}
&\frac{\delta h\cdot\rho}{dt}\cdot\left(\mathbf{q}^T\cdot\left(\mathbf{v}-\mathbf{v}_0\right)\right)+\delta h\cdot\left(\mathbf{q}^T\cdot\nabla\varepsilon\right)+\delta h\cdot\left(\mathbf{q}^T\cdot\nabla \mathrm{p}\right) \ = \\
&\mathbf{q}^T\cdot\mathbf{S}_S\cdot\mathbf{n}-\mu\left(p-\mathbf{n}^T\cdot\mathbf{S}_S\cdot\mathbf{n}\right)+ \\
&\eta\left(\frac{\partial\left(\mathbf{q}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial q}\right)-\mu\left(\varepsilon-\eta\left(2\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial n}-\frac{2}{3}D\right)\right) \\
&+\delta h\cdot\rho\cdot\left(\mathbf{q}^T\cdot\mathbf{g}\right)
\end{aligned}
\tag{4.2}
$$

Bring all the variable terms to the left hand side and order them a little bit:

$$
\begin{aligned}
&\frac{\delta h\cdot\rho}{dt}\cdot\left(\mathbf{q}^T\cdot\mathbf{v}\right)-\eta\left(\frac{\partial\left(\mathbf{q}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial q}\right)+\delta h\cdot\left(\mathbf{q}^T\cdot\nabla\varepsilon\right) \\
&+\mu\varepsilon-\mu\cdot\eta\left(2\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial n}-\frac{2}{\nu}D\right) \ = \\
&\frac{\delta h\cdot\rho}{dt}\cdot\left(\mathbf{q}^T\cdot\mathbf{v}_0\right)-\delta h\cdot\left(\mathbf{q}^T\cdot\nabla \mathrm{p}\right) \\
&\mathbf{q}^T\cdot\mathbf{S}_S\cdot\mathbf{n}-\mu\left(p-\mathbf{n}^T\cdot\mathbf{S}_S\cdot\mathbf{n}\right)+\delta h\cdot\rho\cdot\left(\mathbf{q}^T\cdot\mathbf{g}\right)
\end{aligned}
\tag{4.3}
$$

And more simple, it becomes

$$
\begin{aligned}
&\frac{\delta h\cdot\rho}{dt}\cdot\left(\mathbf{q}^T\cdot\mathbf{v}\right)-\eta\left(\frac{\partial\left(\mathbf{q}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial q}\right)+\delta h\cdot\left(\mathbf{q}^T\cdot\nabla\varepsilon\right) \\
&+\mu\varepsilon-\mu\cdot\eta\left(2\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial n}-\frac{2}{\nu}D\right) \ = R_q
\end{aligned}
\tag{4.4}
$$

Aftern normalization, we have

$$\frac{\delta h\cdot\rho}{dt\cdot N}\cdot\left(\mathbf{q}^T\cdot\mathbf{v}\right)-\frac{\eta}{\mathrm{N}}\left(\frac{\partial\left(\mathbf{q}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial q}\right)+\frac{\delta h}{N}\cdot\left(\mathbf{q}^T\cdot\nabla\varepsilon\right)$$
$$+\frac{\mu}{N}\varepsilon-\frac{\mu\cdot\eta}{N}\left(2\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial n}-\frac{2}{\nu}D\right)=\frac{R_q}{N} \quad (4.5)$$

and finally we abbreviate with the D constants

$$D_1\cdot\left(\mathbf{q}^T\cdot\mathbf{v}\right)-D_2\left(\frac{\partial\left(\mathbf{q}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial q}\right)+D_3\cdot\left(\mathbf{q}^T\cdot\nabla\varepsilon\right)$$
$$+D_8\varepsilon-D_9\left(2\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial n}-\frac{2}{\nu}D\right)=\frac{R_q}{N} \quad (4.6)$$

In the perpendicular direction s, no friction is acting

$$A\delta h\cdot\rho\cdot\frac{d\left(\mathbf{s}^T\cdot\mathbf{v}\right)}{dt}+A\delta h\cdot\left(\mathbf{s}^T\cdot\nabla\varepsilon\right)+A\delta h\cdot\left(\mathbf{s}^T\cdot\nabla\mathrm{p}\right)=$$
$$A\cdot\eta\left(\frac{\partial\left(\mathbf{s}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial s}\right)+A\delta h\cdot\rho\cdot\left(\mathbf{s}^T\cdot\mathbf{g}\right)+A\cdot\mathbf{s}^T\mathbf{S}_s\mathbf{n} \quad (4.7)$$

Division by A yields

$$\frac{\delta h\cdot\rho}{dt}\cdot\left(\mathbf{s}^T\cdot\mathbf{v}-\mathbf{s}^T\cdot\mathbf{v}_0\right)+\delta h\cdot\left(\mathbf{s}^T\cdot\nabla\varepsilon\right)+\delta h\cdot\left(\mathbf{s}^T\cdot\nabla\mathrm{p}\right)=$$
$$\eta\left(\frac{\partial\left(\mathbf{s}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial s}\right)+\delta h\cdot\rho\cdot\left(\mathbf{s}^T\cdot\mathbf{g}\right)+\mathbf{s}^T\mathbf{S}_s\mathbf{n} \quad (4.8)$$

Reordering of terms gives

$$\frac{\delta h\cdot\rho}{dt}\cdot\left(\mathbf{s}^T\cdot\mathbf{v}\right)-\eta\left(\frac{\partial\left(\mathbf{s}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial s}\right)+\delta h\cdot\left(\mathbf{s}^T\cdot\nabla\varepsilon\right)=$$
$$\frac{\delta h\cdot\rho}{dt}\cdot\left(\mathbf{s}^T\cdot\mathbf{v}_0\right)-\delta h\cdot\left(\mathbf{s}^T\cdot\nabla\mathrm{p}\right)+\delta h\cdot\rho\cdot\left(\mathbf{s}^T\cdot\mathbf{g}\right)+\mathbf{s}^T\mathbf{S}_s\mathbf{n} \quad (4.9)$$

With the same normalization as in equation (4.5), we obtain

$$\frac{\delta h\cdot\rho}{dt\cdot N}\cdot\left(\mathbf{s}^T\cdot\mathbf{v}\right)-\frac{\eta}{N}\left(\frac{\partial\left(\mathbf{s}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial s}\right)+\frac{\delta h}{N}\cdot\left(\mathbf{s}^T\cdot\nabla\varepsilon\right)=\frac{R_s}{N} \tag{4.10}$$

and henceforth

$$D_1\cdot\left(\mathbf{s}^T\cdot\mathbf{v}\right)-D_2\left(\frac{\partial\left(\mathbf{s}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial s}\right)+D_3\cdot\left(\mathbf{s}^T\cdot\nabla\varepsilon\right)=\frac{R_s}{N} \tag{4.11}$$

The third equation is the non-penetration clause given by

$$D_4\left(\mathbf{n}^T\cdot\mathbf{v}\right)+D_5\cdot\left(\frac{\partial\left(\mathbf{n}^T\cdot\mathbf{v}\right)}{\partial n}+\frac{\partial\left(\mathbf{q}^T\cdot\mathbf{v}\right)}{\partial q}+\frac{\partial\left(\mathbf{s}^T\cdot\mathbf{v}\right)}{\partial s}\right)=D_4\left(\mathbf{n}^T\cdot\mathbf{v}_{Opp}\right)+D_5\cdot D \tag{4.12}$$

where we choose (so far) $D_4=1,\ D_5=0$.

We define

$$\mathbf{R}=\frac{R_q}{N}\cdot\mathbf{q}+\frac{R_s}{N}\cdot\mathbf{s}+D_5\cdot D\cdot\mathbf{n} \tag{4.13}$$

All equations together give

$$\begin{pmatrix}D_1\cdot\mathbf{q}\\D_1\cdot\mathbf{s}\\0\end{pmatrix}\cdot\mathbf{v}+\begin{pmatrix}0\\0\\D_4\cdot\mathbf{n}\end{pmatrix}\cdot\left(\mathbf{v}-\mathbf{v}_{Opp}\right)+$$

$$\begin{pmatrix}-D_2\cdot\mathbf{q}\\-D_2\cdot\mathbf{s}\\+D_5\cdot\mathbf{n}\end{pmatrix}\frac{\partial\mathbf{v}}{\partial n}+\begin{pmatrix}-D_2\cdot\mathbf{n}\\0\\+D_5\cdot\mathbf{q}\end{pmatrix}\frac{\partial\mathbf{v}}{\partial q}+\begin{pmatrix}0\\-D_2\cdot\mathbf{n}\\+D_5\cdot\mathbf{s}\end{pmatrix}\frac{\partial\mathbf{v}}{\partial s}+D_3\cdot\begin{pmatrix}\left(\mathbf{q}^T\cdot\nabla\varepsilon\right)\\\left(\mathbf{s}^T\cdot\nabla\varepsilon\right)\\0\end{pmatrix} \tag{4.14}$$

$$+\begin{pmatrix}-D_9\left(2-\frac{2}{\nu}\right)\cdot\mathbf{n}\\0\\0\end{pmatrix}\frac{\partial\mathbf{v}}{\partial n}+\begin{pmatrix}D_9\cdot\frac{2}{\nu}\cdot\mathbf{q}\\0\\0\end{pmatrix}\frac{\partial\mathbf{v}}{\partial q}+\begin{pmatrix}D_9\cdot\frac{2}{\nu}\cdot\mathbf{s}\\0\\0\end{pmatrix}\frac{\partial\mathbf{v}}{\partial s}+\begin{pmatrix}D_8\cdot\varepsilon\\0\\0\end{pmatrix}=\begin{pmatrix}\mathbf{q}^T\cdot\mathbf{R}\\\mathbf{s}^T\cdot\mathbf{R}\\\mathbf{n}^T\cdot\mathbf{R}\end{pmatrix}$$

We multiply with the inverse

$$\left(D_1 \cdot \mathbf{qq}^T + D_1 \cdot \mathbf{ss}^T\right) \cdot \mathbf{v} + \left(D_4 \cdot \mathbf{nn}^T\right) \cdot \left(\mathbf{v} - \mathbf{v}_{Opp}\right) +$$

$$\left(-D_2 \cdot \mathbf{qq}^T - D_2 \cdot \mathbf{ss}^T - D_5 \cdot \mathbf{nn}^T\right) \frac{\partial \mathbf{v}}{\partial n} + \left(-D_2 \cdot \mathbf{qn}^T - D_5 \cdot \mathbf{nq}^T\right) \frac{\partial \mathbf{v}}{\partial q} + \left(-D_2 \cdot \mathbf{sn}^T - D_5 \cdot \mathbf{ns}^T\right) \frac{\partial \mathbf{v}}{\partial s} +$$

$$D_3 \cdot \left(\left(\mathbf{qq}^T \cdot \nabla \varepsilon\right) + \left(\mathbf{ss}^T \cdot \nabla \varepsilon\right)\right)$$

$$-\left(D_9 \left(2 - \tfrac{2}{\nu}\right) \cdot \mathbf{qn}^T\right) \frac{\partial \mathbf{v}}{\partial n} + \left(D_9 \cdot \tfrac{2}{\nu} \cdot \mathbf{qq}^T\right) \frac{\partial \mathbf{v}}{\partial q} + \left(D_9 \cdot \tfrac{2}{\nu} \cdot \mathbf{qs}^T\right) \frac{\partial \mathbf{v}}{\partial s} + \left(D_8 \cdot \mathbf{q} \varepsilon\right) =$$

$$\mathbf{qq}^T \cdot \mathbf{R} + \mathbf{ss}^T \cdot \mathbf{R} + \mathbf{nn}^T \cdot \mathbf{R} = \mathbf{R}$$

5. Temperature conditions

5.1. Contact boundaries: Equilibrium of fluxes

$$h \cdot A \cdot \rho \cdot c_v \cdot \frac{T^{n+1} - T^n}{\Delta t} + h_{opp} \cdot A \cdot \rho_{opp} \cdot c_{v,opp} \cdot \frac{T_{opp}^{n+1} - T_{opp}^n}{\Delta t} = -A \cdot \lambda_{opp} \cdot \frac{\partial T_{opp}^{n+1}}{\partial n} + A \cdot \lambda \cdot \frac{\partial T^{n+1}}{\partial n} \quad (4.15)$$

Simplificaation:

$$\frac{\partial T^{n+1}}{\partial n} - \frac{\lambda_{opp}}{\lambda} \cdot \frac{\partial T_{opp}^{n+1}}{\partial n} - \frac{h \cdot \rho \cdot c_v}{\Delta t \cdot \lambda} \cdot \left(T^{n+1} - T^n\right) - \frac{h_{opp} \cdot \rho_{opp} \cdot c_{v,opp}}{\Delta t \cdot \lambda} \cdot \left(T_{opp}^{n+1} - T_{opp}^n\right) = 0 \quad (4.16)$$

Bringing terms of previous time step to the other side:

$$\frac{\partial T^{n+1}}{\partial n} - \frac{\lambda_{opp}}{\lambda} \cdot \frac{\partial T_{opp}^{n+1}}{\partial n} - \frac{h \cdot \rho \cdot c_v}{\Delta t \cdot \lambda} \cdot T^{n+1} - \frac{h_{opp} \cdot \rho_{opp} \cdot c_{v,opp}}{\Delta t \cdot \lambda} \cdot T_{opp}^{n+1} = -\frac{h \cdot \rho \cdot c_v}{\Delta t \cdot \lambda} \cdot T^n - \frac{h_{opp} \cdot \rho_{opp} \cdot c_{v,opp}}{\Delta t \cdot \lambda} \cdot T_{opp}^n \quad (4.17)$$

Addition of zero yields

$$\frac{\partial T^{n+1}}{\partial n} - \frac{\lambda_{opp}}{\lambda} \cdot \frac{\partial T_{opp}^{n+1}}{\partial n} - \frac{h \cdot \rho \cdot c_v}{\Delta t \cdot \lambda} \cdot T^{n+1} - \frac{h_{opp} \cdot \rho_{opp} \cdot c_{v,opp}}{\Delta t \cdot \lambda} \cdot T^{n+1} + \frac{h_{opp} \cdot \rho_{opp} \cdot c_{v,opp}}{\Delta t \cdot \lambda} \cdot T^{n+1} - \frac{h_{opp} \cdot \rho_{opp} \cdot c_{v,opp}}{\Delta t \cdot \lambda} \cdot T_{opp}^{n+1} = -\frac{h \cdot \rho \cdot c_v}{\Delta t \cdot \lambda} \cdot T^n - \frac{h_{opp} \cdot \rho_{opp} \cdot c_{v,opp}}{\Delta t \cdot \lambda} \cdot T_{opp}^n \quad (4.18)$$

Collecting terms leads to

$$\frac{\partial T^{n+1}}{\partial n} - \frac{\lambda_{opp}}{\lambda} \cdot \frac{\partial T_{opp}^{n+1}}{\partial n} - \left(\frac{h \cdot \rho \cdot c_v}{\Delta t \cdot \lambda} + \frac{h_{opp} \cdot \rho_{opp} \cdot c_{v,opp}}{\Delta t \cdot \lambda}\right) \cdot T^{n+1} + \frac{h_{opp} \cdot \rho_{opp} \cdot c_{v,opp}}{\Delta t \cdot \lambda} \cdot \left(T^{n+1} - T_{opp}^{n+1}\right) = -\frac{h \cdot \rho \cdot c_v}{\Delta t \cdot \lambda} \cdot T^n - \frac{h_{opp} \cdot \rho_{opp} \cdot c_{v,opp}}{\Delta t \cdot \lambda} \cdot T_{opp}^n \quad (4.19)$$

Final simplification

$$\frac{\partial T^{n+1}}{\partial n} - D_1 \cdot \frac{\partial T_{opp}^{n+1}}{\partial n} - D_2 \cdot T^{n+1} + D_3 \cdot \left(T^{n+1} - T_{opp}^{n+1}\right) = R \tag{4.20}$$

With the values

$$R = -\frac{h \cdot \rho \cdot c_v}{\Delta t \cdot \lambda} \cdot T^n - \frac{h_{opp} \cdot \rho_{opp} \cdot c_{v,opp}}{\Delta t \cdot \lambda} \cdot T_{opp}^n$$

$$D_1 = \frac{\lambda_{opp}}{\lambda}$$

$$D_2 = -\left(\frac{h \cdot \rho \cdot c_v}{\Delta t \cdot \lambda} + \frac{h_{opp} \cdot \rho_{opp} \cdot c_{v,opp}}{\Delta t \cdot \lambda}\right)$$

$$D_3 = \frac{h_{opp} \cdot \rho_{opp} \cdot c_{v,opp}}{\Delta t \cdot \lambda}$$

5.2. Formulation for the temperature difference

The heat balance around a boundary point is settled in a control volume of a boundary point, representing a boundary area A and a thickness H (which form a control volume for the energy balance):

$$\begin{aligned}
&H \cdot A \cdot \rho \cdot c_v \cdot \frac{T^{n+1} - T^n}{\Delta t} = -\alpha \cdot A \cdot \left(T^{n+1} - T_{opp}^{n+1}\right) + \lambda \cdot A \cdot \frac{\partial T^{n+1}}{\partial n} \\
&H \cdot \rho \cdot c_v \cdot \frac{T^{n+1} - T^n}{\Delta t} = -\alpha \cdot \left(T^{n+1} - T_{opp}^{n+1}\right) + \lambda \cdot \frac{\partial T^{n+1}}{\partial n} \\
&\frac{H \cdot \rho \cdot c_v}{\Delta t} \cdot \left(T^{n+1} - T^n\right) = -\alpha \cdot \left(T^{n+1} - T_{opp}^{n+1}\right) + \lambda \cdot \frac{\partial T^{n+1}}{\partial n} \\
&\left(\frac{H \cdot \rho \cdot c_v}{\Delta t} + \alpha\right) \cdot T^{n+1} - \lambda \cdot \frac{\partial T^{n+1}}{\partial n} = \alpha T_{opp}^{n+1} + \frac{H \cdot \rho \cdot c_v}{\Delta t} \cdot T^n
\end{aligned} \tag{4.21}$$

The thickness is a partition of the local smoothing length

$$H = const \cdot h \tag{4.22}$$

The balance is taken in normal direction, assuming that H is always small enough such that the tangential fluxes are minor to the normal one.