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A
Residue vector and Jacobian matrix computation for fully implicit and coupled simulations of Newtonian incompressible flows

In this appendix, we write the entries of the residue vector and of the Jacobian matrix that we need to solve the non–linear system of equations 3-10 presented on Chapter 3 using Newton's method.

The residue vector entries for the first and second coordinate functions of the momentum equation on a node with index i are denoted by $\vec{r}[m_i^x]$ and $\vec{r}[m_i^y]$ and are written as follows:

$$\begin{aligned}
\vec{r}[m_i^x] = \; & \sum_{\tau\in\Lambda} \int_\tau \rho \frac{\partial \mathsf{u}^x}{\partial t}\phi_i + \; \rho \left[\mathsf{u}^x \frac{\partial \mathsf{u}^x}{\partial x} + \mathsf{u}^y \frac{\partial \mathsf{u}^x}{\partial y}\right] \phi_i - g^x \phi_i + \\
& \left[-\mathsf{p} + 2\mu \frac{\partial \mathsf{u}^x}{\partial x}\right] \frac{\partial \phi_i}{\partial x} + \; \mu \left[\frac{\partial \mathsf{u}^x}{\partial y} + \frac{\partial \mathsf{u}^y}{\partial x}\right] \frac{\partial \phi_i}{\partial y} \, \mathrm{d}\tau - \sum_{\epsilon\in\partial\Lambda} \int_\epsilon f^x \phi_i \, d\epsilon \\
\vec{r}[m_i^y] = \; & \sum_{\tau\in\Lambda} \int_\tau \rho \frac{\partial \mathsf{u}^y}{\partial t}\phi_i + \; \rho \left[\mathsf{u}^x \frac{\partial \mathsf{u}^y}{\partial x} + \mathsf{u}^y \frac{\partial \mathsf{u}^y}{\partial y}\right] \phi_i - g^y \phi_i + \\
& \left[-\mathsf{p} + 2\mu \frac{\partial \mathsf{u}^y}{\partial y}\right] \frac{\partial \phi_i}{\partial y} + \; \mu \left[\frac{\partial \mathsf{u}^x}{\partial y} + \frac{\partial \mathsf{u}^y}{\partial x}\right] \frac{\partial \phi_i}{\partial x} \, \mathrm{d}\tau - \sum_{\epsilon\in\partial\Lambda} \int_\epsilon f^y \phi_i \, d\epsilon
\end{aligned} \tag{A-1}$$

The residue entry for the continuity equation on a node with index i is denoted by $\vec{r}[c_i]$ and is computed using the following expression:

$$\vec{r}[c_i] = \sum_{\tau\in\Lambda} \int_\tau (\frac{\partial \mathsf{u}^x}{\partial x} + \frac{\partial \mathsf{u}^y}{\partial y}) \chi \, d\tau \tag{A-2}$$

To compute the entries of the Jacobian matrix, we must derivate the residue entries $\vec{r}[m_i^x]$ and $\vec{r}[m_i^y]$ in relation to the degrees of freedom u^x, u^y and p of a node with index j. The derivatives of the residue $\vec{r}[m_i^x]$ are denoted by $\mathbf{J}[m_i^x, \mathsf{u}_j^x]$, $\mathbf{J}[m_i^x, \mathsf{u}_j^y]$ and $\mathbf{J}[m_i^x, \mathsf{p}_j]$ and are written as:

$$\mathbf{J}[m_i^x, \mathsf{u}_j^x] = \sum_{\tau\in\Lambda} \int_\tau \left[\rho\frac{\phi_i\phi_j}{\delta \mathrm{t}}\right] + \rho\left[\phi_j\frac{\partial \mathsf{u}^x}{\partial x} + \mathsf{u}^x\frac{\partial \phi_j}{\partial x} + \mathsf{u}^y\frac{\partial \phi_j}{\partial y}\right]\phi_i + \left[2\mu\frac{\partial \phi_i}{\partial x}\frac{\partial \phi_j}{\partial x}\right] + \left[\mu\frac{\partial \phi_i}{\partial y}\frac{\partial \phi_j}{\partial y}\right]\mathrm{d}\tau$$

$$\mathbf{J}[m_i^x, \mathsf{u}_j^y] = \sum_{\tau\in\Lambda} \int_\tau \rho\left[\phi_i\phi_j\frac{\partial \mathsf{u}^x}{\partial y}\right] + \left[\mu\frac{\partial \phi_i}{\partial y}\frac{\partial \phi_j}{\partial x}\right]\mathrm{d}\tau \tag{A-3}$$

$$\mathbf{J}[m_i^x, \mathsf{p}_j] = \sum_{\tau\in\Lambda} \int_\tau -\left[\chi_j\frac{\partial \phi_i}{\partial x}\right]\mathrm{d}\tau$$

Analogously, we can compute the Jacobian entries related with the residue of the second coordinate function of the momentum equation $\vec{r}[m_i^y]$, that are denoted by $\mathbf{J}[m_i^y, \mathsf{u}_j^x]$, $\mathbf{J}[m_i^y, \mathsf{u}_j^y]$ and $\mathbf{J}[m_i^y, \mathsf{p}_j]$ and written as:

$$\mathbf{J}[m_i^y, \mathsf{u}_j^x] = \sum_{\tau\in\Lambda} \int_\tau \rho\left[\phi_i\phi_j\frac{\partial \mathsf{u}^y}{\partial x}\right] + \left[\mu\frac{\partial \phi_i}{\partial x}\frac{\partial \phi_j}{\partial y}\right]\mathrm{d}\tau$$

$$\mathbf{J}[m_i^y, \mathsf{u}_j^y] = \sum_{\tau\in\Lambda} \int_\tau \left[\rho\frac{\phi_i\phi_j}{\delta \mathrm{t}}\right] + \rho\left[\phi_j\frac{\partial \mathsf{u}^y}{\partial y} + \mathsf{u}^x\frac{\partial \phi_j}{\partial x} + \mathsf{u}^y\frac{\partial \phi_j}{\partial y}\right]\phi_i + \left[2\mu\frac{\partial \phi_i}{\partial y}\frac{\partial \phi_j}{\partial y}\right] + \left[\mu\frac{\partial \phi_i}{\partial x}\frac{\partial \phi_j}{\partial x}\right]\mathrm{d}\tau \tag{A-4}$$

$$\mathbf{J}[m_i^y, \mathsf{p}_j] = \sum_{\tau\in\Lambda} \int_\tau -\left[\chi_j\frac{\partial \phi_i}{\partial y}\right]\mathrm{d}\tau$$

Finally, the Jacobian entries that follows from the derivatives of the residue of the continuity equation $\vec{r}[c_i]$ are denoted by $\mathbf{J}[c_i, \mathsf{u}_j^x]$ and $\mathbf{J}[c_i, \mathsf{u}_j^y]$ and they are computed through the following expression:

$$\mathbf{J}[c_i, \mathsf{u}_j^x] = \sum_{\tau\in\Lambda} \int_\tau \left[\chi_i\frac{\partial \phi_j}{\partial x}\right]\mathrm{d}\tau$$

$$\mathbf{J}[c_i, \mathsf{u}_j^y] = \sum_{\tau\in\Lambda} \int_\tau \left[\chi_i\frac{\partial \phi_j}{\partial y}\right]\mathrm{d}\tau \tag{A-5}$$

In fact, as the basis functions ϕ_i have compact support, the summation in the residue vectors expression is computed only over the elements that are incident to the node i. Therefore, the boundary integral terms in $\vec{r}[m_i^x]$ and $\vec{r}[m_i^y]$ are computed only for the boundary nodes. This reduces and makes local the computational effort.

B
Residue vector and Jacobian matrix computation for fully implicit and coupled simulations of flows with suspended particles

In this appendix, we write the entries of the residue vector and of the Jacobian matrix that we need to solve the non–linear system of equations 4-25 and 4-26 derived on Chapter 4.

The residue vector entries for the first and second coordinate functions of the momentum equation on a node with index i are analogous with the ones shown in Appendix A, but now we need to add to the residue the Lagrange multipliers term. The momentum residues for simulations of flows with suspended particles are denoted by $\vec{r}[m_i^x]$ and $\vec{r}[m_i^y]$ and are written as follows:

$$
\begin{aligned}
\vec{r}[m_i^x] \; &= \sum_{\tau\in\Lambda} \int_{\tau} \rho \frac{\partial \mathsf{u}^x}{\partial t}\phi_i + \; \rho \left[\mathsf{u}^x \frac{\partial \mathsf{u}^x}{\partial x} + \mathsf{u}^y \frac{\partial \mathsf{u}^x}{\partial y} - g^x \right] \phi_i + \left[-\mathsf{p} + 2\mu \frac{\partial \mathsf{u}^x}{\partial x} \right] \frac{\partial \phi_i}{\partial x} + \\
&+ \mu \left[\frac{\partial \mathsf{u}^x}{\partial y} + \frac{\partial \mathsf{u}^y}{\partial x} \right] \frac{\partial \phi_i}{\partial y} - \mu \left[\frac{\partial \mathsf{l}^x}{\partial x}\frac{\partial \phi_i}{\partial x} + \frac{\partial \mathsf{l}^y}{\partial x}\frac{\partial \phi_i}{\partial y} \right] - [\alpha \mathsf{l}^x]\, \phi_i d\tau + \\
&+ \sum_{\epsilon\in\partial\Lambda} \int_{\epsilon} (\mu t^x - f^x)\phi_i \, d\epsilon \\
\\
\vec{r}[m_i^y] \; &= \sum_{\tau\in\Lambda} \int_{\tau} \rho \frac{\partial \mathsf{u}^y}{\partial t}\phi_i + \; \rho \left[\mathsf{u}^x \frac{\partial \mathsf{u}^y}{\partial x} + \mathsf{u}^y \frac{\partial \mathsf{u}^y}{\partial y} - g^y \right] \phi_i + \left[-\mathsf{p} + 2\mu \frac{\partial \mathsf{u}^y}{\partial y} \right] \frac{\partial \phi_i}{\partial y} + \\
&+ \mu \left[\frac{\partial \mathsf{u}^x}{\partial y} + \frac{\partial \mathsf{u}^y}{\partial x} \right] \frac{\partial \phi_i}{\partial x} - \mu \left[\frac{\partial \mathsf{l}^x}{\partial y}\frac{\partial \phi_i}{\partial x} + \frac{\partial \mathsf{l}^y}{\partial y}\frac{\partial \phi_i}{\partial y} \right] - [\alpha \mathsf{l}^y]\, \phi_i d\tau \; + \\
&+ \sum_{\epsilon\in\partial\Lambda} \int_{\epsilon} (\mu t^y - f^y)\phi_i \, d\epsilon
\end{aligned}
\tag{B-1}
$$

The residue entry for the continuity equation on a node with index i is exactly the same as in the case of Newtonian incompressible fluids. It is denoted by $\vec{r}[c_i]$ and computed using the expression:

$$
\vec{r}[c_i] = \sum_{\tau\in\Lambda} \int_{\tau} \left(\frac{\partial \mathsf{u}^x}{\partial x} + \frac{\partial \mathsf{u}^y}{\partial y}\right) \chi \, d\tau \tag{B-2}
$$

The residue entries for the first and second coordinates of the linear velocity and the entry related with the angular velocity of a particle with index p_i are denoted by $\vec{r}[U^x_{p_i}]$, $\vec{r}[U^y_{p_i}]$ and $\vec{r}[w_{p_i}]$ and their expressions are:

$$\begin{aligned}
\vec{r}[U^x_{p_i}] &= \sum_{\tau\in\Lambda_{p_i}} \int_\tau (\rho_{p_i} - \rho_f)\frac{\partial U^y_{p_i}}{\partial t} - \rho_{p_i} g^x + \frac{\partial \mathsf{p}}{\partial x} + \alpha \mathsf{l}^x \, d\tau \\
\vec{r}[U^y_{p_i}] &= \sum_{\tau\in\Lambda_{p_i}} \int_\tau (\rho_{p_i} - \rho_f)\frac{\partial U^y_{p_i}}{\partial t} - \rho_{p_i} g^y + \frac{\partial \mathsf{p}}{\partial y} + \alpha \mathsf{l}^y \, d\tau \\
\vec{r}[w_{p_i}] &= \sum_{\tau\in\Lambda_{p_i}} \int_\tau \omega_{p_i} + \frac{1}{2}(\frac{\partial \mathsf{u}^x}{\partial y} - \frac{\partial \mathsf{u}^y}{\partial x}) \, d\tau
\end{aligned} \tag{B-3}$$

The last entries needed to compute the residue vector are the ones of the Lagrange multipliers equations inside and outside the particle's region and the equation of the position of the particle p_i. Those entries are denoted by $\vec{r}[l^x_i]$, $\vec{r}[l^y_i]$, $\vec{r}[X^x_{p_i}]$ and $\vec{r}[X^y_{p_i}]$. Their expressions are:

$$\begin{aligned}
\vec{r}[l^x_i] &= \sum_{\tau\in\Lambda_f} \int_\tau \mathsf{l}^x \phi_i \, d\tau && \text{in } \Lambda_f \\
\vec{r}[l^x_i] &= \sum_{\tau\in\Lambda_{p_i}} \int_\tau \left[\left(\mathsf{u}^x - U^x_{p_i}\right) - \omega_{p_i}\left(x^y - X^y_{p_i}\right)\right] \phi_i \, d\tau && \text{in } \Lambda_{p_i} \\
\vec{r}[l^y_i] &= \sum_{\tau\in\Lambda_f} \int_\tau \mathsf{l}^y \phi_i \, d\tau && \text{in } \Lambda_f \\
\vec{r}[l^y_i] &= \sum_{\tau\in\Lambda_{p_i}} \int_\tau \left[\left(\mathsf{u}^y - U^y_{p_i}\right) - \omega_{p_i}\left(x^x - X^x_{p_i}\right)\right] \phi_i \, d\tau && \text{in } \Lambda_{p_i} \\
\vec{r}[X^x_{p_i}] &= \frac{\partial X^x_{p_i}}{\partial t} - U^x_{p_i} && \text{for } p_i \in (1 \ldots n_p) \\
\vec{r}[X^y_{p_i}] &= \frac{\partial X^y_{p_i}}{\partial t} - U^y_{p_i} && \text{for } p_i \in (1 \ldots n_p)
\end{aligned} \tag{B-4}$$

The Jacobian matrix entries are computed deriving the residues in relation to the degrees of freedom of the problem. The derivatives of the momentum residue in relation to the extended fluid's velocity and pressure is analogous to the ones shown in the previous appendix and will be omitted here. The derivatives of the momentum residue in a node of index i in relation to the Lagrange multipliers unknowns l^x_j and l^y_j of a node with index j are denoted by $\mathbf{J}[m^x_i, \mathsf{l}^x_j]$, $\mathbf{J}[m^x_i, \mathsf{l}^y_j]$, $\mathbf{J}[m^y_i, \mathsf{l}^x_j]$ and $\mathbf{J}[m^y_i, \mathsf{l}^y_j]$ and computed using the expressions:

$$
\begin{aligned}
\mathbf{J}[m_i^x, \mathsf{l}_j^x] &= \sum_{\tau\in\Lambda} \int_\tau -\left[\mu \frac{\partial\phi_i}{\partial x}\frac{\partial\phi_j}{\partial x} + \alpha\phi_i\phi_j\right] d\tau \\
\mathbf{J}[m_i^x, \mathsf{l}_j^y] &= \sum_{\tau\in\Lambda} \int_\tau -\left[\mu \frac{\partial\phi_i}{\partial y}\frac{\partial\phi_j}{\partial x}\right] d\tau \\
\mathbf{J}[m_i^y, \mathsf{l}_j^x] &= \sum_{\tau\in\Lambda} \int_\tau -\left[\mu \frac{\partial\phi_i}{\partial x}\frac{\partial\phi_j}{\partial y}\right] d\tau \\
\mathbf{J}[m_i^y, \mathsf{l}_j^y] &= \sum_{\tau\in\Lambda} \int_\tau -\left[\mu \frac{\partial\phi_i}{\partial y}\frac{\partial\phi_j}{\partial y} + \alpha\phi_i\phi_j\right] d\tau
\end{aligned}
\tag{B-5}
$$

The Jacobian entries related with the continuity equation of the extended fluid velocity also remain unchanged in relation to the ones presented in the previous appendix. The Jacobian entries for the residue of the linear and angular velocities of a particle with index p_i are given by:

$$
\begin{aligned}
\mathbf{J}[U_{p_i}^x, \mathsf{l}_j^x] = \mathbf{J}(U_{p_i}^y, \mathsf{l}_j^y) &= \sum_{\tau\in\Lambda_{p_i}} \int_\tau \alpha\phi_j \, d\tau \\
\mathbf{J}[U_{p_i}^x, U_{p_i}^x] = \mathbf{J}(U_{p_i}^y, U_{p_i}^y) &= \sum_{\tau\in\Lambda_{p_i}} \int_\tau \frac{(\rho_{p_i} - \rho_f)}{\delta t} \, d\tau \\
\mathbf{J}[w_{p_i}, \mathsf{u}_j^x] &= \sum_{\tau\in\Lambda_{p_i}} \int_\tau \frac{\partial\phi_j}{\partial y} \, d\tau \\
\mathbf{J}[w_{p_i}, \mathsf{u}_j^y] &= \sum_{\tau\in\Lambda_{p_i}} \int_\tau -\frac{\partial\phi_j}{\partial x} \, d\tau \\
\mathbf{J}[w_{p_i}, \omega_{p_i}] &= \sum_{\tau\in\Lambda_{p_i}} \int_\tau 2 \, d\tau
\end{aligned}
\tag{B-6}
$$

The non–zero Jacobian entries of the Lagrange multiplier equations in a node i are:

$$
\begin{aligned}
\mathbf{J}[l_i^x, \mathsf{l}_j^x] = \mathbf{J}[l_i^y, \mathsf{l}_j^y] &= \sum_{\tau \in \Lambda_f} \int_\tau \phi_i \phi_j \, d\tau \\
\mathbf{J}[l_i^x, \mathsf{l}_j^x] = \mathbf{J}[l_i^y, \mathsf{l}_j^y] &= \sum_{\tau \in \Lambda_{p_i}} \int_\tau \phi_i \phi_j \, d\tau \\
\mathbf{J}[l_i^x, U_{p_j}^x] = \mathbf{J}[l_i^y, U_{p_j}^y] &= \sum_{\tau \in \Lambda_{p_i}} \int_\tau -\phi_i \, d\tau \\
\mathbf{J}[l_i^x, \omega_{p_j}] &= \sum_{\tau \in \Lambda_{p_i}} \int_\tau \left(x_i^y - X_{p_j}^y \right) \, d\tau \\
\mathbf{J}[l_i^y, \omega_{p_j}] &= \sum_{\tau \in \Lambda_{p_i}} \int_\tau \left(X_{p_j}^x - x_i^x \right) \, d\tau \\
\mathbf{J}[l_i^x, X_{p_j}^x] = -\mathbf{J}[l_i^y, X_{p_j}^y] &= \sum_{\tau \in \Lambda_{p_i}} \int_\tau \omega_{p_j} \phi_i \, d\tau
\end{aligned}
\tag{B-7}
$$

Finally, the Jacobian entries for the particle's position are computed using the following expression:

$$
\begin{aligned}
\mathbf{J}[X_{p_i}^x, U_{p_i}^x] = \mathbf{J}[X_{p_i}^y, U_{p_i}^y] &= -1 \\
\mathbf{J}[X_{p_i}^x, X_{p_i}^x] = \mathbf{J}[X_{p_i}^y, X_{p_i}^y] &= \frac{1}{\delta t}
\end{aligned}
\tag{B-8}
$$

Again, the basis functions ϕ_i have compact support, which implies that the summation in the residue vectors and Jacobian matrix entries expression are computed only over the elements that are incident to the node i, which again reduces and makes local the computational effort.