PDE-Constrained Optimization Problem

The domain is $\Sigma = \Omega \times [0,T]$. There are two state variables, the particle density ρ and the velocity $\mathbf{v}$. The control is a force term $\mathbf{f}$.

$$\min_{\rho,\mathbf{v},\mathbf{f}} \quad \frac{1}{2}||\rho - \hat{\rho}||^2_{L_2(\Sigma)} + \frac{\alpha}{2}||\mathbf{v} - \hat{\mathbf{v}}||^2_{L_2(\Sigma)} + \frac{\beta}{2}||\mathbf{f}||^2_{L_2(\Sigma)}$$

subject to:

$$m\rho\frac{\partial \mathbf{v}}{\partial t} + m\rho(\mathbf{v}\cdot\nabla)\mathbf{v} + \rho\nabla V_{ext} + \nabla\rho + m\gamma\rho\mathbf{v} + \int_\Omega \rho(r)\rho(r')\nabla V_2(|r-r'|)dr' - \mathbf{f} = \mathbf{0} \qquad \text{in} \quad \Sigma$$

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{v}) = 0 \qquad \text{in} \quad \Sigma$$

$$\rho\mathbf{v}\cdot\mathbf{n} = 0 \qquad \text{on} \quad \partial\Sigma$$

$$\rho(r,0) = \rho_0$$

$$\mathbf{v}(r,0) = \mathbf{v}_0.$$

Here, we have:

$$\mathcal{F}[\rho] = \int_\Omega \left(V_{ext}\rho + \rho(\log\rho - 1) + \int_\Omega \rho(r)\rho(r')V_2(|r-r'|)dr' \right) dr.$$

Then:

$$\rho\nabla\frac{\delta\mathcal{F}[\rho]}{\delta\rho} = \rho\nabla V_{ext} + \nabla\rho + \int_\Omega \rho(r)\rho(r')\nabla V_2(|r-r'|)dr',$$

which matches Equation (29) in Archer's paper.

The Lagrangian

The Lagrangian for the above problem is:

$$\mathcal{L}(\rho,\mathbf{v},\mathbf{f},\mathbf{p}_\Sigma,q,p_{\partial\Sigma}) = \int_0^T\int_\Omega \frac{1}{2}(\rho-\hat{\rho})^2 drdt + \int_0^T\int_\Omega \frac{\alpha}{2}(\mathbf{v}-\hat{\mathbf{v}})^2 drdt + \int_0^T\int_\Omega \frac{\beta}{2}\mathbf{f}^2 drdt$$
$$+ \int_0^T\int_\Omega (m\rho\frac{\partial\mathbf{v}}{\partial t} + m\rho(\mathbf{v}\cdot\nabla)\mathbf{v} + \rho\nabla V_{ext} + \nabla\rho + m\gamma\rho\mathbf{v} + \int_\Omega \rho(r)\rho(r')\nabla V_2(|r-r'|)dr' - \mathbf{f})\cdot\mathbf{p}_\Sigma drdt$$
$$+ \int_0^T\int_\Omega (\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{v}))q drdt$$
$$+ \int_0^T\int_{\partial\Omega} \rho\mathbf{v}\cdot\mathbf{n}p_{\partial\Sigma} drdt,$$

where $\mathbf{p}_\Sigma$, q and $p_{\partial\Sigma}$ are Lagrange multipliers associated with the PDE for $\mathbf{v}$, the PDE for ρ and the boundary condition, respectively.

Adjoint Equation 1

The derivative of $\mathcal{L}$ with respect to ρ in some direction h is, where $h \in C_0^\infty(\Sigma)$:

$$\mathcal{L}_\rho(\rho, \mathbf{v}, \mathbf{f}, \mathbf{p}_\Sigma, q, p_{\partial\Sigma})h = \int_0^T \int_\Omega (\rho - \hat{\rho})h drdt$$
$$+ \int_0^T \int_\Omega (mh\frac{\partial \mathbf{v}}{\partial t} \cdot \mathbf{p}_\Sigma + mh((\mathbf{v} \cdot \nabla)\mathbf{v}) \cdot \mathbf{p}_\Sigma + h\nabla V_{ext} \cdot \mathbf{p}_\Sigma + \nabla h \cdot \mathbf{p}_\Sigma)drdt$$
$$+ \int_0^T \int_\Omega (m\gamma h\mathbf{v} + \int_\Omega h(r)\rho(r')\nabla V_2(|r - r'|)dr' + \int_\Omega \rho(r)h(r')\nabla V_2(|r - r'|)dr') \cdot \mathbf{p}_\Sigma drdt$$
$$+ \int_0^T \int_\Omega (q\frac{\partial h}{\partial t} + q\nabla \cdot (h\mathbf{v}))drdt + \int_0^T \int_{\partial\Omega} p_{\partial\Sigma} h\mathbf{v} \cdot \mathbf{n} drdt,$$

where the product rule is used to take the derivative of the interaction term. Looking at different integral terms individually:

$$I_1 = \int_0^T \int_\Omega \nabla h \cdot \mathbf{p}_\Sigma drdt = \int_0^T \int_{\partial\Omega} h\mathbf{p}_\Sigma \cdot \mathbf{n} drdt - \int_0^T \int_\Omega \nabla \cdot \mathbf{p}_\Sigma h drdt$$

$$I_2 = \int_0^T \int_\Omega q\frac{\partial h}{\partial t} drdt = \int_\Omega h(T)q(T)drdt - \int_0^T \int_\Omega \frac{\partial q}{\partial t} h drdt$$

Note that $h(r, 0) = 0$, (in order to satisfy the condition for all admissible h) and so the initial condition vanishes from the above expression.

$$I_3 = \int_0^T \int_\Omega q\nabla \cdot (h\mathbf{v})drdt = \int_0^T \int_{\partial\Omega} q\mathbf{v} \cdot \mathbf{n} h drdt - \int_0^T \int_\Omega \nabla q \cdot \mathbf{v} h drdt.$$

Furthermore, we have:

$$I_{2B} = \int_0^T \int_\Omega \left(\int_\Omega \rho(r)h(r')\nabla V_2(|r - r'|)dr' \right) \cdot \mathbf{p}_\Sigma(r)drdt$$
$$= \int_0^T \int_\Omega \int_\Omega \rho(r)h(r')\nabla V_2(|r - r'|) \cdot \mathbf{p}_\Sigma(r)drdr'dt,$$

swapping the order of integration. Then we have:

$$I_{2B} = \int_0^T \int_\Omega h(r') \left(\int_\Omega \rho(r)\nabla V_2(|r - r'|) \cdot \mathbf{p}_\Sigma(r)dr \right) dr'dt,$$

and relabelling $r \to r'$ and $r' \to r$ gives:

$$I_{2B} = \int_0^T \int_\Omega h(r) \left(\int_\Omega \rho(r')\nabla V_2(|r - r'|) \cdot \mathbf{p}_\Sigma(r')dr' \right) drdt,$$

Replacing I_1, I_2, I_{2B} and I_3 in the derivative gives:

$$
\begin{aligned}
&\mathcal{L}_\rho(\rho, \mathbf{v}, \mathbf{f}, \mathbf{p}_\Sigma, q, p_{\partial\Sigma})h = \int_\Omega h(T)q(T)drdt \\
&+ \int_0^T \int_\Omega ((\rho - \hat{\rho}) + m\frac{\partial \mathbf{v}}{\partial t} \cdot \mathbf{p}_\Sigma + m((\mathbf{v} \cdot \nabla)\mathbf{v}) \cdot \mathbf{p}_\Sigma + \nabla V_{ext} \cdot \mathbf{p}_\Sigma - \nabla \cdot \mathbf{p}_\Sigma - \ \nabla q \cdot \mathbf{v} - \frac{\partial q}{\partial t})hdrdt \\
&+ \int_0^T \int_\Omega \left(\int_\Omega \rho(r')(\mathbf{p}_\Sigma(r') + \mathbf{p}_\Sigma(r)) \cdot \nabla V_2(|r - r'|)dr' + m\gamma \mathbf{v} \cdot \mathbf{p}_\Sigma \right) hdrdt \\
&+ \int_0^T \int_{\partial\Omega} (\mathbf{p}_\Sigma \cdot \mathbf{n} + q\mathbf{v} \cdot \mathbf{n} + p_{\partial\Sigma}\mathbf{v} \cdot \mathbf{n})hdrdt
\end{aligned}
$$

Setting $\mathcal{L}_\rho(\rho, \mathbf{v}, \mathbf{f}, \mathbf{p}_\Sigma, q, p_{\partial\Sigma})h = 0$, and restricting the admissible set of choices of h to:

$$
\begin{aligned}
h = 0 \quad \text{on} \quad \partial\Sigma \\
h(T) = 0.
\end{aligned}
$$

Then the derivative becomes:

$$
\begin{aligned}
&\int_0^T \int_\Omega ((\rho - \hat{\rho}) + m\frac{\partial \mathbf{v}}{\partial t} \cdot \mathbf{p}_\Sigma + m((\mathbf{v} \cdot \nabla)\mathbf{v}) \cdot \mathbf{p}_\Sigma + \nabla V_{ext} \cdot \mathbf{p}_\Sigma - \nabla \cdot \mathbf{p}_\Sigma - \ \nabla q \cdot \mathbf{v} - \frac{\partial q}{\partial t})hdrdt \\
&+ \int_0^T \int_\Omega \left(m\gamma \mathbf{v} \cdot \mathbf{p}_\Sigma + \int_\Omega \rho(r')(\mathbf{p}_\Sigma(r') + \mathbf{p}_\Sigma(r)) \cdot \nabla V_2(|r - r'|)dr' \right) hdrdt \\
&= 0.
\end{aligned}
$$

Since this has to hold for all $h \in C_0^\infty(\Sigma)$ and $C_0^\infty(\Sigma)$ is dense in $L_2(\Sigma)$, the first adjoint equation is derived as:

$$
\begin{aligned}
&(\rho - \hat{\rho}) + m\frac{\partial \mathbf{v}}{\partial t} \cdot \mathbf{p}_\Sigma + m((\mathbf{v} \cdot \nabla)\mathbf{v}) \cdot \mathbf{p}_\Sigma + \nabla V_{ext} \cdot \mathbf{p}_\Sigma - \nabla \cdot \mathbf{p}_\Sigma - \ \nabla q \cdot \mathbf{v} - \frac{\partial q}{\partial t} \qquad (1) \\
&+ m\gamma \mathbf{v} \cdot \mathbf{p}_\Sigma + \int_\Omega \rho(r')(\mathbf{p}_\Sigma(r') + \mathbf{p}_\Sigma(r)) \cdot \nabla V_2(|r - r'|)dr' = 0 \qquad \text{in} \quad \Sigma.
\end{aligned}
$$

Then, relaxing the conditions on h, such that $h(T) \neq 0$ is a permissible choice, gives:

$$
\int_\Omega h(T)q(T)drdt = 0,
$$

and by the same density argument as above, this gives the final time condition for q:

$$
q(T) = 0.
$$

Finally, allowing $h \neq 0 \quad \text{on} \quad \partial\Sigma$ result in:

$$
\int_0^T \int_{\partial\Omega} (\mathbf{p}_\Sigma \cdot \mathbf{n} + q\mathbf{v} \cdot \mathbf{n} + p_{\partial\Sigma}\mathbf{v} \cdot \mathbf{n})hdrdt = 0,
$$

and again by a density argument:

$$
\mathbf{p}_\Sigma \cdot \mathbf{n} + q\mathbf{v} \cdot \mathbf{n} + p_{\partial\Sigma}\mathbf{v} \cdot \mathbf{n} = 0 \qquad \text{on} \quad \partial\Sigma
$$

Since $\mathbf{v} \cdot \mathbf{n} = 0$ on $\partial\Sigma$, the boundary condition reduces to:

$$\mathbf{p}_\Sigma \cdot \mathbf{n} = 0 \qquad \text{on} \quad \partial\Sigma.$$

Therefore, the first adjoint equation of this problem is:

$$\begin{aligned}
&(\rho - \hat{\rho}) + m\frac{\partial \mathbf{v}}{\partial t} \cdot \mathbf{p}_\Sigma + m((\mathbf{v} \cdot \nabla)\mathbf{v}) \cdot \mathbf{p}_\Sigma + \nabla V_{ext} \cdot \mathbf{p}_\Sigma - \nabla \cdot \mathbf{p}_\Sigma - \ \nabla q \cdot \mathbf{v} - \frac{\partial q}{\partial t} \\
&+ m\gamma \mathbf{v} \cdot \mathbf{p}_\Sigma + \int_\Omega \rho(r')(\mathbf{p}_\Sigma(r') + \mathbf{p}_\Sigma(r)) \cdot \nabla V_2(|r - r'|)dr' = 0 \qquad\qquad \text{in} \quad \Sigma \\
&\mathbf{p}_\Sigma \cdot \mathbf{n} = 0 \qquad \text{on} \quad \partial\Sigma \\
&q(T) = 0.
\end{aligned}$$

Adjoint Equation 2

Taking the derivative of the above Lagrangian with respect to $\mathbf{v}$ in the direction $\mathbf{h} \in C_0^\infty(\Sigma)$, gives:

$$\begin{aligned}
\mathcal{L}_\mathbf{v}(\rho, \mathbf{v}, \mathbf{f}, \mathbf{p}_\Sigma, q, p_{\partial\Sigma})\mathbf{h} = &\int_0^T \int_\Omega \alpha(\mathbf{v} - \hat{\mathbf{v}}) \cdot \mathbf{h} dr dt \\
&+ \int_0^T \int_\Omega (m\rho \frac{\partial \mathbf{h}}{\partial t} + m\rho(\mathbf{h} \cdot \nabla)\mathbf{v} + m\rho(\mathbf{v} \cdot \nabla)\mathbf{h} + m\gamma\rho\mathbf{h}) \cdot \mathbf{p}_\Sigma dr dt \\
&+ \int_0^T \int_\Omega (\nabla \cdot (\rho\mathbf{h}))q dr dt \\
&+ \int_0^T \int_{\partial\Omega} \rho\mathbf{h} \cdot \mathbf{n} p_{\partial\Sigma} dr dt.
\end{aligned}$$

Some of the terms are considered separately, as in the previous calculations:

$$\begin{aligned}
I_4 &= \int_0^T \int_\Omega m\rho \frac{\partial \mathbf{h}}{\partial t} \cdot \mathbf{p}_\Sigma dr dt \\
&= \int_\Omega m\rho(T)\mathbf{p}_\Sigma(T) \cdot \mathbf{h}(T) dr dt - \int_0^T \int_\Omega m \frac{\partial \rho}{\partial t} \mathbf{p}_\Sigma \cdot \mathbf{h} dr dt - \int_0^T \int_\Omega m\rho \frac{\partial \mathbf{p}_\Sigma}{\partial t} \cdot \mathbf{h} dr dt.
\end{aligned}$$

Note that $\mathbf{h}(0) = \mathbf{0}$, in order to satisfy the conditions on $\mathbf{h}$, as before.

$$I_5 = \int_0^T \int_\Omega q\nabla \cdot (\rho\mathbf{h}) dr dr = \int_0^T \int_{\partial\Omega} q\rho\mathbf{n} \cdot \mathbf{h} dr dt - \int_0^T \int_\Omega \rho\nabla q \cdot \mathbf{h} dr dt$$

$$I_6 = \int_0^T \int_\Omega m\rho((\mathbf{h} \cdot \nabla)\mathbf{v}) \cdot \mathbf{p}_\Sigma dr dt = \int_0^T \int_\Omega m\rho((\nabla\mathbf{v})^\top \mathbf{p}_\Sigma) \cdot \mathbf{h} dr dt$$

$$
\begin{aligned}
I_7 = \int_0^T \int_\Omega m\rho((\mathbf{v}\cdot\nabla)\mathbf{h})\cdot\mathbf{p}_\Sigma drdt &= \int_0^T \int_{\partial\Omega} m\rho(\mathbf{v}\cdot\mathbf{p}_\Sigma)(\mathbf{n}\cdot\mathbf{h})drdt \\
&- \int_0^T \int_\Omega (m\rho((\mathbf{v}\cdot\nabla)\mathbf{p}_\Sigma)\cdot\mathbf{h} + m\rho(\nabla\cdot\mathbf{v})(\mathbf{p}_\Sigma\cdot\mathbf{h}) + m(\mathbf{v}\cdot\nabla\rho)(\mathbf{p}_\Sigma\cdot\mathbf{h}))drdt
\end{aligned}
$$

Replacing the rewritten integrals gives:

$$
\begin{aligned}
&\mathcal{L}_\mathbf{v}(\rho,\mathbf{v},\mathbf{f},\mathbf{p}_\Sigma,q,p_{\partial\Sigma})\mathbf{h} = \int_\Omega m\rho(T)\mathbf{p}_\Sigma(T)\cdot\mathbf{h}(T)drdt \\
&+ \int_0^T \int_\Omega \bigg(\alpha(\mathbf{v}-\hat{\mathbf{v}}) - m\frac{\partial\rho}{\partial t}\mathbf{p}_\Sigma - m\rho\frac{\partial\mathbf{p}_\Sigma}{\partial t} + m\gamma\rho\mathbf{p}_\Sigma \\
&- \rho\nabla q + m\rho(\nabla\mathbf{v})^\top\mathbf{p}_\Sigma - m\rho(\mathbf{v}\cdot\nabla)\mathbf{p}_\Sigma - m\rho(\nabla\cdot\mathbf{v})\mathbf{p}_\Sigma - m(\mathbf{v}\cdot\nabla\rho)\mathbf{p}_\Sigma\bigg)\cdot\mathbf{h}drdt \\
&+ \int_0^T \int_{\partial\Omega} (m\rho(\mathbf{v}\cdot\mathbf{p}_\Sigma) + \rho p_{\partial\Sigma} + q\rho)\mathbf{n}\cdot\mathbf{h}drdt
\end{aligned}
$$

Then, setting $\mathcal{L}_\mathbf{v}(\rho,\mathbf{v},\mathbf{f},\mathbf{p}_\Sigma,q,p_{\partial\Sigma})\mathbf{h} = \mathbf{0}$ and placing the restrictions on $\mathbf{h}$, as before:

$$
\begin{aligned}
\mathbf{h} = 0 \quad &\text{on} \quad \partial\Sigma \\
\mathbf{h}(T) = 0&,
\end{aligned}
$$

gives:

$$
\begin{aligned}
&\int_0^T \int_\Omega \bigg(\alpha(\mathbf{v}-\hat{\mathbf{v}}) - m\frac{\partial\rho}{\partial t}\mathbf{p}_\Sigma - m\rho\frac{\partial\mathbf{p}_\Sigma}{\partial t} + m\gamma\rho\mathbf{p}_\Sigma \\
&- \rho\nabla q + m\rho(\nabla\mathbf{v})^\top\mathbf{p}_\Sigma - m\rho(\mathbf{v}\cdot\nabla)\mathbf{p}_\Sigma - m\rho(\nabla\cdot\mathbf{v})\mathbf{p}_\Sigma - m(\mathbf{v}\cdot\nabla\rho)\mathbf{p}_\Sigma\bigg)\cdot\mathbf{h}drdt = 0.
\end{aligned}
$$

Employing the density argument that $C_0^\infty(\Sigma)$ is dense in $L_2(\Sigma)$, which has to hold for all $\mathbf{h}\in C_0^\infty(\Sigma)$, results in:

$$
\begin{aligned}
&\alpha(\mathbf{v}-\hat{\mathbf{v}}) - m\frac{\partial\rho}{\partial t}\mathbf{p}_\Sigma - m\rho\frac{\partial\mathbf{p}_\Sigma}{\partial t} - \rho\nabla q + m\rho(\nabla\mathbf{v})^\top\mathbf{p}_\Sigma + m\gamma\rho\mathbf{p}_\Sigma \\
&- m\rho(\mathbf{v}\cdot\nabla)\mathbf{p}_\Sigma - m\rho(\nabla\cdot\mathbf{v})\mathbf{p}_\Sigma - m(\mathbf{v}\cdot\nabla\rho)\mathbf{p}_\Sigma = \mathbf{0} \qquad \text{in} \quad \Sigma.
\end{aligned}
$$

Then, relaxing the conditions on $\mathbf{h}$, so that $\mathbf{h}(T)\neq 0$ is permissible, gives

$$
\int_\Omega m\rho(T)\mathbf{p}_\Sigma(T)\cdot\mathbf{h}(T)drdt = 0,
$$

and so, since $\rho\neq 0$, this results in the final time condition for $\mathbf{p}_\Sigma$:

$$
\mathbf{p}_\Sigma(T) = \mathbf{0}. \tag{2}
$$

Finally, relaxing the condition $\mathbf{h} = 0 \quad \text{on} \quad \partial\Sigma$ gives:

$$\int_0^T \int_{\partial\Omega} (m\rho(\mathbf{v} \cdot \mathbf{p}_\Sigma) + \rho p_{\partial\Sigma} + q\rho)\mathbf{n} \cdot \mathbf{h} dr dt = 0,$$

and by the same density argument as above, this results in:

$$(m\rho(\mathbf{v} \cdot \mathbf{p}_\Sigma) + \rho p_{\partial\Sigma} + q\rho)\mathbf{n} = \mathbf{0} \qquad \text{on} \quad \partial\Sigma.$$

This condition can be rewritten, since $\rho \neq 0$:

$$(m(\mathbf{v} \cdot \mathbf{p}_\Sigma) + p_{\partial\Sigma} + q)\mathbf{n} = \mathbf{0}$$

The vectors $\mathbf{v}$ and $\mathbf{p}_\Sigma$ can be decomposed in terms of the normal direction $\mathbf{n}$ and all perpendicular directions $\mathbf{n}^\perp$:

$$\begin{aligned}\mathbf{v} &= |\mathbf{v}^n|\mathbf{n} + |\mathbf{v}^\perp|\mathbf{n}^\perp \\ \mathbf{p}_\Sigma &= |\mathbf{p}_\Sigma^n|\mathbf{n} + |\mathbf{p}_\Sigma^\perp|\mathbf{n}^\perp.\end{aligned}$$

Therefore:

$$m\Big((|\mathbf{v}^n|\mathbf{n} + |\mathbf{v}^\perp|\mathbf{n}^\perp) \cdot (|\mathbf{p}_\Sigma^n|\mathbf{n} + |\mathbf{p}_\Sigma^\perp|\mathbf{n}^\perp) \Big)\mathbf{n} + p_{\partial\Sigma}\mathbf{n} + q\mathbf{n} = \mathbf{0}.$$

Then:

$$m\Big((|\mathbf{v}^n||\mathbf{p}_\Sigma^n|\mathbf{n} \cdot \mathbf{n} + |\mathbf{v}^\perp||\mathbf{p}_\Sigma^n|\mathbf{n}^\perp \cdot \mathbf{n} + |\mathbf{v}^n||\mathbf{p}_\Sigma^\perp|\mathbf{n} \cdot \mathbf{n}^\perp + |\mathbf{v}^\perp||\mathbf{p}_\Sigma^\perp|\mathbf{n}^\perp \cdot \mathbf{n}^\perp) \Big)\mathbf{n} + p_{\partial\Sigma}\mathbf{n} + q\mathbf{n} = \mathbf{0}.$$

This reduces, since $\mathbf{v} \cdot \mathbf{n} = 0$ on $\partial\Sigma$ and $\mathbf{n}^\perp \cdot \mathbf{n} = 0$ by orthogonality. Therefore:

$$m\Big(|\mathbf{v}|^\perp |\mathbf{p}_\Sigma|^\perp \Big)\mathbf{n} + p_{\partial\Sigma}\mathbf{n} + q\mathbf{n} = \mathbf{0}.$$

Then there is the following relationship between the three Lagrange multipliers:

$$m|\mathbf{v}|^\perp |\mathbf{p}_\Sigma|^\perp + p_{\partial\Sigma} + q = 0.$$

The second adjoint equation of the above problem is:

$$\begin{aligned}&\alpha(\mathbf{v} - \hat{\mathbf{v}}) - m\frac{\partial\rho}{\partial t}\mathbf{p}_\Sigma - m\rho\frac{\partial \mathbf{p}_\Sigma}{\partial t} - \rho\nabla q + m\rho(\nabla\mathbf{v})^\top\mathbf{p}_\Sigma + m\gamma\rho\mathbf{p}_\Sigma \\ &- m\rho(\mathbf{v} \cdot \nabla)\mathbf{p}_\Sigma - m\rho(\nabla \cdot \mathbf{v})\mathbf{p}_\Sigma - m(\mathbf{v} \cdot \nabla\rho)\mathbf{p}_\Sigma = \mathbf{0} \qquad \text{in} \quad \Sigma \\ &\mathbf{p}_\Sigma(T) = \mathbf{0}.\end{aligned}$$

The Gradient Equation

Taking the derivative of the Lagrangian with respect to $\mathbf{f}$, in the direction $\mathbf{h} \in C_0^\infty(\Sigma)$, gives:

$$\begin{aligned}\mathcal{L}_{\mathbf{f}}(\rho, \mathbf{v}, \mathbf{f}, \mathbf{p}_\Sigma, q, p_{\partial\Sigma})\mathbf{h} &= \int_0^T \int_\Omega \beta \mathbf{f} \cdot \mathbf{h} dr dt - \int_0^T \int_\Omega \mathbf{p}_\Sigma \cdot \mathbf{h} dr dt \\ &= \int_0^T \int_\Omega (\beta \mathbf{f} - \mathbf{p}_\Sigma) \cdot \mathbf{h} dr dt.\end{aligned}$$

Employing the same density argument for the permissible $\mathbf{h}$ gives the gradient equation of the problem:

$$\beta \mathbf{f} - \mathbf{p}_\Sigma = 0 \quad \text{in} \quad \Sigma \quad \text{and on} \quad \partial\Sigma.$$

1 Reference

The paper that the forward equation is taken from is:

A. J. Archer, Dynamical Density Functional Theory for Molecular and Colloidal Fluids: A Microscopic Approach to Fluid Mechanics. *The Journal of Chemical Physics*. 130, 2009.