

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} .

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

subject to:

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

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

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

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

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

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:

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

where \mathbf{p}_{Σ} , 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 $h \in C_0^\infty(\Sigma)$:

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

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

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

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

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.

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

Furthermore, we have:

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

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 $r \rightarrow r'$ and $r' \rightarrow r$ gives:

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

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

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

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:

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

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:

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

in Σ .

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 $h \neq 0$ on $\partial\Sigma$ result in:

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

and again by a density argument:

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

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

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

Therefore, the first adjoint equation of this problem is:

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

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:

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

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

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

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

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

Replacing the rewritten integrals gives:

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

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:

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

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:

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

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}_{Σ} :

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

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

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

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}_Σ 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:

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

Then:

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

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

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

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:

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

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:

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

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.