0.0.1 PDE-Constrained Optimization Problem

In the following we consider an optimal control problem constrained by (**??**). The domain is $\Sigma = \Omega \times [0, T]$. As described in the previous section, there are two state variables, the particle density ρ and the velocity $\mathbf{v}$. The control is applied through a background flow term $\mathbf{w}$ and the desired state is denoted by $\hat{\rho}$.

$$\min_{\rho,\mathbf{v},\mathbf{w}} \mathcal{J}(\rho, \mathbf{v}) := \quad \frac{1}{2}||\rho - \hat{\rho}||^2_{L_2(\Sigma)} + \frac{\beta}{2}||\mathbf{w}||^2_{L_2(\Sigma)}$$

subject to:

$$\frac{\partial \mathbf{v}}{\partial t} = -(\mathbf{v} \cdot \nabla)\mathbf{v} - \gamma \mathbf{v} + \frac{\eta}{m}\nabla^2 \mathbf{v} - \frac{1}{m}\mathbf{f} + \frac{1}{m}\mathbf{w} - \frac{1}{m}\nabla V_{ext} - \frac{1}{m}\nabla \ln \rho - \frac{1}{m}\int_\Omega \rho(r')\mathbf{K}(r, r')dr'$$

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

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

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

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

The Lagrangian

The Lagrangian for the above problem is:

$$\begin{aligned}
\mathcal{L}(\rho, \mathbf{v}, \mathbf{w}, \mathbf{p}, q, q_{\partial\Sigma}) = &\int_0^T \int_\Omega \frac{1}{2}(\rho - \hat{\rho})^2 drdt + \int_0^T \int_\Omega \frac{\beta}{2}\mathbf{w}^2 drdt \\
+ &\int_0^T \int_\Omega (\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} + \gamma \mathbf{v} - \frac{\eta}{m}\nabla^2 \mathbf{v} + \frac{1}{m}\mathbf{f} - \frac{1}{m}\mathbf{w} + \frac{1}{m}\nabla V_{ext} + \frac{1}{m}\nabla \ln \rho \\
&\quad + \frac{1}{m}\int_\Omega \rho(r')\mathbf{K}(r, r')dr') \cdot \mathbf{p} drdt \\
+ &\int_0^T \int_\Omega (\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}))q drdt \\
+ &\int_0^T \int_{\partial\Omega} \rho \mathbf{v} \cdot \mathbf{n} q_{\partial\Sigma} drdt,
\end{aligned}$$

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

0.0.2 Adjoint Equation 1

The derivative of $\mathcal{L}$ with respect to ρ in some direction h is taken where $h \in C_0^\infty(\Sigma)$. First, the derivative of $\nabla \ln \rho \cdot \mathbf{p}$ needs to be treated separately. +++ Add here after understanding++++

Then we get:

$$\mathcal{L}_\rho(\rho, \mathbf{v}, \mathbf{w}, \mathbf{p}, q, q_{\partial\Sigma})h = \int_0^T \int_\Omega (\rho - \hat{\rho}) h dr dt$$
$$+ \int_0^T \int_\Omega \left(\frac{1}{m} \nabla \left(\frac{h}{\rho} \right) \cdot \mathbf{p} \right) dr dt + \int_0^T \int_\Omega \left(\int_\Omega h(r') \mathbf{K}(r, r') dr' \right) \cdot \mathbf{p} dr dt$$
$$+ \int_0^T \int_\Omega (q \frac{\partial h}{\partial t} + q \nabla \cdot (h\mathbf{v})) dr dt + \int_0^T \int_{\partial\Omega} q_{\partial\Sigma} h \mathbf{v} \cdot \mathbf{n} dr dt,$$

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

$$I_1 = \int_0^T \int_\Omega \left(\frac{1}{m} \nabla \left(\frac{h}{\rho} \right) \cdot \mathbf{p} \right) dr dt = \int_0^T \int_{\partial\Omega} \frac{1}{\rho} \mathbf{p} \cdot \mathbf{n} h dr dt - \int_0^T \int_\Omega \frac{1}{\rho} \nabla \cdot \mathbf{p} h dr dt$$

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

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:

$$I_4 = \int_0^T \int_\Omega \left(\int_\Omega h(r') \mathbf{K}(r, r') dr' \right) \cdot \mathbf{p}(r) dr dt$$
$$= \int_0^T \int_\Omega \int_\Omega h(r') \mathbf{K}(r, r') \cdot \mathbf{p}(r) dr dr' dt,$$

swapping the order of integration. Then we have:

$$I_4 = \int_0^T \int_\Omega h(r') \left(\int_\Omega \mathbf{K}(r, r') \cdot \mathbf{p}(r) dr \right) dr' dt,$$

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

$$I_4 = \int_0^T \int_\Omega h(r) \left(\int_\Omega \mathbf{K}(r', r) \cdot \mathbf{p}(r') dr' \right) dr dt.$$

If we assume that $\mathbf{K}(r', r) = -\mathbf{K}(r, r')$, we get:

$$I_4 = -\int_0^T \int_\Omega h(r) \left(\int_\Omega \mathbf{K}(r, r') \cdot \mathbf{p}(r') dr' \right) dr dt.$$

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

$$\mathcal{L}_\rho(\rho, \mathbf{v}, \mathbf{w}, \mathbf{p}, q, q_{\partial\Sigma})h = \int_\Omega h(T)q(T)drdt$$
$$+ \int_0^T \int_\Omega \left((\rho - \hat{\rho}) - \frac{\partial q}{\partial t} - \nabla q \cdot \mathbf{v} - \frac{1}{\rho} \nabla \cdot \mathbf{p} - \int_\Omega \mathbf{p}(r') \cdot \mathbf{K}(r, r')dr' \right) hdrdt$$
$$+ \int_0^T \int_{\partial\Omega} \left(\frac{1}{\rho} \mathbf{p} \cdot \mathbf{n} + q\mathbf{v} \cdot \mathbf{n} + q_{\partial\Sigma} \mathbf{v} \cdot \mathbf{n} \right) hdrdt$$

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

$$h = 0 \quad \text{on} \quad \partial\Omega$$
$$h(T) = 0.$$

Then the derivative becomes:

$$\int_0^T \int_\Omega \left((\rho - \hat{\rho}) - \frac{\partial q}{\partial t} - \nabla q \cdot \mathbf{v} - \frac{1}{\rho} \nabla \cdot \mathbf{p} - \int_\Omega \mathbf{p}(r') \cdot \mathbf{K}(r, r')dr' \right) hdrdt = 0.$$

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:

$$(\rho - \hat{\rho}) - \frac{\partial q}{\partial t} - \nabla q \cdot \mathbf{v} - \frac{1}{\rho} \nabla \cdot \mathbf{p} - \int_\Omega \mathbf{p}(r') \cdot \mathbf{K}(r, r')dr' \qquad \text{in} \quad \Sigma$$

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 $\partial\Omega$ result in:

$$\int_0^T \int_{\partial\Omega} \left(\frac{1}{\rho} \mathbf{p} \cdot \mathbf{n} + q\mathbf{v} \cdot \mathbf{n} + q_{\partial\Sigma} \mathbf{v} \cdot \mathbf{n} \right) hdrdt = 0,$$

and again by a density argument:

$$\frac{1}{\rho} \mathbf{p} \cdot \mathbf{n} + q\mathbf{v} \cdot \mathbf{n} + q_{\partial\Sigma} \mathbf{v} \cdot \mathbf{n} = 0 \qquad \text{on} \quad \partial\Omega$$

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

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

Therefore, the first adjoint equation of this problem is:

$$
\begin{aligned}
&\frac{\partial q}{\partial t} = (\rho - \hat{\rho}) - \nabla q \cdot \mathbf{v} - \frac{1}{\rho}\nabla \cdot \mathbf{p} - \int_{\Omega} \mathbf{p}(r') \cdot \mathbf{K}(r,r')dr' \qquad \text{in} \quad \Sigma \\
&\mathbf{p} \cdot \mathbf{n} = 0 \qquad \text{on} \quad \partial\Omega \\
&q(T) = 0.
\end{aligned}
$$

If instead we substitute $\frac{\partial \mathbf{v}}{\partial t}$ from the forward equations, cancel terms and use that $\nabla\rho = \rho\nabla \ln \rho$ we get:

$$
\begin{aligned}
&\frac{\partial q}{\partial t} = (\rho - \hat{\rho}) - \nabla(\ln \rho) \cdot \mathbf{p} - \nabla \cdot \mathbf{p} - \nabla q \cdot \mathbf{v} - \int_{\Omega} \rho(r')\mathbf{p}(r') \cdot \mathbf{K}(r,r')dr' \qquad \text{in} \quad \Sigma \\
&\mathbf{p} \cdot \mathbf{n} = 0 \qquad \text{on} \quad \partial\Omega \\
&q(T) = 0.
\end{aligned}
$$

0.0.3 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:

$$
\begin{aligned}
\mathcal{L}_{\mathbf{v}}(\rho, \mathbf{v}, \mathbf{w}, \mathbf{p}, q, q_{\partial\Sigma})\mathbf{h} = &\int_0^T \int_\Omega (m\rho\frac{\partial \mathbf{h}}{\partial t} + m\rho(\mathbf{h}\cdot\nabla)\mathbf{v} + m\rho(\mathbf{v}\cdot\nabla)\mathbf{h} + m\gamma\rho\mathbf{h} - \eta\rho\nabla^2\mathbf{h}) \cdot \mathbf{p}drdt \\
&+ \int_0^T \int_\Omega (\nabla \cdot (\rho\mathbf{h}))qdrdt \\
&+ \int_0^T \int_{\partial\Omega} \rho\mathbf{h} \cdot \mathbf{n}q_{\partial\Sigma}drdt.
\end{aligned}
$$

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

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

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

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

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

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

$$
\begin{aligned}
I_8 &= \int_0^T \int_\Omega \eta\rho\nabla^2\mathbf{h}\cdot\mathbf{p}drdt = \int_0^T \int_{\partial\Omega} \eta(\nabla\cdot\mathbf{h})(\rho\mathbf{p}\cdot\mathbf{n})drdt - \int_0^T \int_\Omega \Big(\nabla\cdot(\rho\mathbf{p})\Big)\Big(\nabla\cdot\mathbf{h}\Big)drdt \\
&= \int_0^T \int_{\partial\Omega} \eta(\nabla\cdot\mathbf{h})(\rho\mathbf{p}\cdot\mathbf{n})drdt - \int_0^T \int_{\partial\Omega} \eta\Big(\nabla\cdot(\rho\mathbf{p})\Big)(\mathbf{h}\cdot\mathbf{n})drdt + \int_0^T \int_\Omega \eta\nabla^2(\rho\mathbf{p})\cdot\mathbf{h}drdt.
\end{aligned}
$$

Replacing the rewritten integrals gives:

$$
\begin{aligned}
&\mathcal{L}_\mathbf{v}(\rho,\mathbf{v},\mathbf{w},\mathbf{p},q,q_{\partial\Sigma})\mathbf{h} = \int_\Omega m\rho(T)\mathbf{p}(T)\cdot\mathbf{h}(T)drdt \\
&+ \int_0^T \int_\Omega \Big(-\eta\nabla^2(\rho\mathbf{p}) - m\frac{\partial\rho}{\partial t}\mathbf{p} - m\rho\frac{\partial\mathbf{p}}{\partial t} + m\gamma\rho\mathbf{p} \\
&- \rho\nabla q + m\rho(\nabla\mathbf{v})^\top\mathbf{p} - m\rho(\mathbf{v}\cdot\nabla)\mathbf{p} - m\rho(\nabla\cdot\mathbf{v})\mathbf{p} - m(\mathbf{v}\cdot\nabla\rho)\mathbf{p}\Big)\cdot\mathbf{h}drdt \\
&+ \int_0^T \int_{\partial\Omega} (m\rho(\mathbf{v}\cdot\mathbf{p}) + \rho q_{\partial\Sigma} + q\rho)\mathbf{n}\cdot\mathbf{h}drdt + \int_0^T \int_{\partial\Omega} \Big(\eta\Big(\nabla\cdot(\rho\mathbf{p})\Big)(\mathbf{h}\cdot\mathbf{n}) - \eta(\nabla\cdot\mathbf{h})(\rho\mathbf{p}\cdot\mathbf{n})\Big)drdt
\end{aligned}
$$

We can substitute the definition of $\frac{\partial\rho}{\partial t}$ from the forward equations and cancel terms to get:

$$
\begin{aligned}
&\mathcal{L}_\mathbf{v}(\rho,\mathbf{v},\mathbf{w},\mathbf{p},q,q_{\partial\Sigma})\mathbf{h} = \int_\Omega m\rho(T)\mathbf{p}(T)\cdot\mathbf{h}(T)drdt \\
&+ \int_0^T \int_\Omega \Big(-\eta\nabla^2(\rho\mathbf{p}) - m\rho\frac{\partial\mathbf{p}}{\partial t} + m\gamma\rho\mathbf{p} - \rho\nabla q + m\rho(\nabla\mathbf{v})^\top\mathbf{p} - m\rho(\mathbf{v}\cdot\nabla)\mathbf{p}\Big)\cdot\mathbf{h}drdt \\
&+ \int_0^T \int_{\partial\Omega} (m\rho(\mathbf{v}\cdot\mathbf{p}) + \rho q_{\partial\Sigma} + q\rho)\mathbf{n}\cdot\mathbf{h}drdt + \int_0^T \int_{\partial\Omega} \Big(\eta\Big(\nabla\cdot(\rho\mathbf{p})\Big)(\mathbf{h}\cdot\mathbf{n}) - \eta(\nabla\cdot\mathbf{h})(\rho\mathbf{p}\cdot\mathbf{n})\Big)drdt
\end{aligned}
$$

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

$$
\begin{aligned}
\mathbf{h} = \mathbf{0}, \quad \nabla\cdot\mathbf{h} = 0 \quad \text{on} \quad \partial\Omega \\
\mathbf{h}(T) = \mathbf{0},
\end{aligned}
$$

gives:

$$
\int_0^T \int_\Omega \Big(-\eta\nabla^2(\rho\mathbf{p}) - m\rho\frac{\partial\mathbf{p}}{\partial t} + m\gamma\rho\mathbf{p} - \rho\nabla q + m\rho(\nabla\mathbf{v})^\top\mathbf{p} - m\rho(\mathbf{v}\cdot\nabla)\mathbf{p}\Big)\cdot\mathbf{h}drdt = 0
$$

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:

$$m\rho\frac{\partial \mathbf{p}}{\partial t} = -\eta\nabla^2(\rho\mathbf{p}) + m\gamma\rho\mathbf{p} - \rho\nabla q + m\rho(\nabla\mathbf{v})^\top\mathbf{p} - m\rho(\mathbf{v}\cdot\nabla)\mathbf{p} \qquad \text{in} \quad \Sigma.$$

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

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

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

$$\mathbf{p}(T) = \mathbf{0}. \tag{1}$$

Finally, relaxing the conditions on the boundary terms to choose $\mathbf{h} = \mathbf{0}$ and $\nabla\cdot\mathbf{h} \neq 0$ on $\partial\Omega$ gives:

$$\int_0^T \int_{\partial\Omega} -\eta(\nabla\cdot\mathbf{h})(\rho\mathbf{p}\cdot\mathbf{n})drdt = 0,$$

which, by the same density argument as above, gives, since $\rho \neq 0$ by assumption:

$$\begin{aligned} -\eta\rho\mathbf{p}\cdot\mathbf{n} &= 0 \\ \mathbf{p}\cdot\mathbf{n} &= 0 \quad \text{on} \quad \partial\Omega. \end{aligned} \tag{2}$$

Then relaxing the final condition, such that $\mathbf{h} \neq 0$ on $\partial\Omega$, we get:

$$\int_0^T \int_{\partial\Omega} \Big(m\rho(\mathbf{v}\cdot\mathbf{p}) + \rho q_{\partial\Sigma} + q\rho + \eta\nabla\cdot(\rho\mathbf{p})\Big)(\mathbf{n}\cdot\mathbf{h})drdt = 0.$$

By the same density argument as above, this results in:

$$(m\rho(\mathbf{v}\cdot\mathbf{p}) + \rho q_{\partial\Sigma} + q\rho + \eta\nabla\cdot(\rho\mathbf{p}))\mathbf{n} = \mathbf{0}$$

+++ Now not sure if any more simplification possible...+++ The second adjoint equation of the above problem is:

$$\begin{aligned} &m\rho\frac{\partial \mathbf{p}}{\partial t} = -\eta\nabla^2(\rho\mathbf{p}) + m\gamma\rho\mathbf{p} - \rho\nabla q + m\rho(\nabla\mathbf{v})^\top\mathbf{p} - m\rho(\mathbf{v}\cdot\nabla)\mathbf{p} && \text{in} \quad \Sigma \\ &\mathbf{p}\cdot\mathbf{n} = 0 && \text{on} \quad \partial\Omega \\ &\mathbf{p}(T) = \mathbf{0} \end{aligned}$$

+++ Same as before +++

0.0.4 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:

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

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

$$\mathbf{w} = \frac{1}{\beta} \rho \mathbf{p} \quad \text{in} \quad \Sigma \quad \text{and on} \quad \partial\Omega.$$

0.0.5 Rewriting the equations for implementation

We employ the transformation $\rho = e^s$, so that $s = \ln \rho$. This is in order to ensure that ρ remains positive, which is a natural condition for the particle density to satisfy. For now, neglect interaction term.

The forward equations become:

$$\begin{aligned}\frac{\partial \mathbf{v}}{\partial t} = &-(\mathbf{v} \cdot \nabla)\mathbf{v} - \frac{1}{m}\nabla V_{ext} - \frac{1}{m}\mathbf{f} + \frac{1}{m}\mathbf{w} - \frac{1}{m}\nabla s - \gamma \mathbf{v} + \frac{\eta}{m}\nabla^2 \mathbf{v} \qquad (3) \\ &- \int_\Omega e^{s(r')} \mathbf{K}(r, r') dr' \qquad (4) \\ \frac{\partial s}{\partial t} = &-\mathbf{v} \cdot \nabla s - \nabla \cdot \mathbf{v}. \qquad (5)\end{aligned}$$

Here, we only divided the first equation by $m\rho$ and used the fact that $\nabla \rho = \rho \nabla \ln \rho$.

The first adjoint equation does not change much. It was: +++ depends now on what happens!!+++

$$\frac{\partial q}{\partial t} = (\rho - \hat{\rho}) - \nabla(\ln \rho) \cdot \mathbf{p} - \nabla \cdot \mathbf{p} - \nabla q \cdot \mathbf{v} - \int_\Omega \rho(r')\mathbf{p}(r') \cdot \mathbf{K}(r, r') dr' \qquad \text{in} \quad \Sigma$$

and becomes:

$$\frac{\partial q}{\partial t} = (e^s - \hat{\rho}) - \nabla s \cdot \mathbf{p} - \nabla \cdot \mathbf{p} - \nabla q \cdot \mathbf{v} - \int_\Omega e^{s(r')}\mathbf{p}(r') \cdot \mathbf{K}(r, r') dr' \qquad \text{in} \quad \Sigma.$$

The second adjoint equation was:

$$m\rho \frac{\partial \mathbf{p}}{\partial t} = -\eta \nabla^2(\rho \mathbf{p}) + m\gamma\rho\mathbf{p} - \rho \nabla q + m\rho(\nabla \mathbf{v})^\top \mathbf{p} - m\rho(\mathbf{v} \cdot \nabla)\mathbf{p} \qquad \text{in} \quad \Sigma$$

Rewriting the first term in the new variable s gives:

$$-\eta\nabla^2(\rho\mathbf{p}) = -e^s\left(2\eta\nabla\mathbf{p}\cdot\nabla s + \eta\mathbf{p}\cdot(\nabla s)^2 + \eta\mathbf{p}\cdot\nabla^2 s + \eta\nabla^2\mathbf{p}\right)$$

And therefore the new adjoint equation is:

$$\begin{aligned}\frac{\partial\mathbf{p}}{\partial t} =& -\frac{2\eta}{m}\nabla\mathbf{p}\cdot\nabla s - \frac{\eta}{m}\mathbf{p}\cdot(\nabla s)^2 - \frac{\eta}{m}\mathbf{p}\cdot\nabla^2 s - \frac{\eta}{m}\nabla^2\mathbf{p}\\ &+ \gamma\mathbf{p} - \rho\nabla q + (\nabla\mathbf{v})^\top\mathbf{p} - (\mathbf{v}\cdot\nabla)\mathbf{p} \qquad\qquad \text{in} \quad \Sigma\end{aligned}$$

Finally, in both adjoints, time is reversed due to the negative Laplacian term and the final time conditions, using $\tau = T - t$. The first adjoint equation becomes:

$$\frac{\partial q}{\partial\tau} = -(e^s - \hat{\rho}) + \nabla s\cdot\mathbf{p} + \nabla\cdot\mathbf{p} + \nabla q\cdot\mathbf{v} + \int_\Omega e^{s(r')}\mathbf{p}(r')\cdot\mathbf{K}(r,r')dr' \qquad \text{in} \quad \Sigma.$$

The second adjoint equation gives:

$$\begin{aligned}\frac{\partial\mathbf{p}}{\partial\tau} =& \frac{2\eta}{m}\nabla\mathbf{p}\cdot\nabla s + \frac{\eta}{m}\mathbf{p}\cdot(\nabla s)^2 + \frac{\eta}{m}\mathbf{p}\cdot\nabla^2 s + \frac{\eta}{m}\nabla^2\mathbf{p}\\ &- \gamma\mathbf{p} + \rho\nabla q - (\nabla\mathbf{v})^\top\mathbf{p} + (\mathbf{v}\cdot\nabla)\mathbf{p} \qquad\qquad \text{in} \quad \Sigma\end{aligned}$$