

### 0.0.1 PDE-Constrained Optimization Problem

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

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

subject to:

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

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

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

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

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

Here, we have (+++ I am not sure how to write this in terms of  $\mathbf{K}(r, r')$ +++):

$$\mathcal{F}[\rho] = \int_{\Omega} \left( V_{ext} \rho + \rho(\log \rho - 1) + \frac{1}{2} \int_{\Omega} \rho(r) \rho(r') V_2(|r - r'|) dr' \right) dr.$$

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 (39) in Archer's paper.

### The Lagrangian

The Lagrangian for the above problem is:

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

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

### 0.0.2 Adjoint Equation 1

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

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

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

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

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

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:

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

swapping the order of integration. Then we have:

$$I_{2B} = \int_0^T \int_\Omega h(r') \left( \int_\Omega \rho(r) \mathbf{K}(r, r') \cdot \mathbf{p}(r) dr \right) dr' dt,$$

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

$$I_{2B} = \int_0^T \int_\Omega h(r) \left( \int_\Omega \rho(r') \mathbf{K}(r', r) \cdot \mathbf{p}(r') dr' \right) dr dt.$$

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

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

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

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

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:

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

Then the derivative becomes:

$$\begin{aligned}
&\int_0^T \int_{\Omega} \left( (\rho - \hat{\rho}) + m \frac{\partial \mathbf{v}}{\partial t} \cdot \mathbf{p} + m((\mathbf{v} \cdot \nabla)\mathbf{v}) \cdot \mathbf{p} + \nabla V_{ext} \cdot \mathbf{p} + \mathbf{f} \cdot \mathbf{p} - \mathbf{w} \cdot \mathbf{p} \right. \\
&- \eta \nabla^2 \mathbf{v} \cdot \mathbf{p} - \nabla \cdot \mathbf{p} - \nabla q \cdot \mathbf{v} - \frac{\partial q}{\partial t} + m\gamma \mathbf{v} \cdot \mathbf{p} \Big) h drdt \\
&+ \int_0^T \int_{\Omega} \left( \int_{\Omega} \rho(r')(\mathbf{p}(r) - \mathbf{p}(r')) \cdot \mathbf{K}(r, r') dr' \right) h drdt \\
&= 0.
\end{aligned}$$

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:

$$\begin{aligned}
\frac{\partial q}{\partial t} &= (\rho - \hat{\rho}) + m \frac{\partial \mathbf{v}}{\partial t} \cdot \mathbf{p} + m((\mathbf{v} \cdot \nabla)\mathbf{v}) \cdot \mathbf{p} + \nabla V_{ext} \cdot \mathbf{p} + \mathbf{f} \cdot \mathbf{p} - \mathbf{w} \cdot \mathbf{p} - \eta \nabla^2 \mathbf{v} \cdot \mathbf{p} \quad (1) \\
&- \nabla \cdot \mathbf{p} - \nabla q \cdot \mathbf{v} + m\gamma \mathbf{v} \cdot \mathbf{p} + \int_{\Omega} \rho(r')(\mathbf{p}(r) - \mathbf{p}(r')) \cdot \mathbf{K}(r, r') dr' \quad \text{in} \quad \Sigma
\end{aligned}$$

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

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

and again by a density argument:

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

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

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

Therefore, the first adjoint equation of this problem is:

$$\begin{aligned} \frac{\partial q}{\partial t} &= (\rho - \hat{\rho}) + m \frac{\partial \mathbf{v}}{\partial t} \cdot \mathbf{p} + m((\mathbf{v} \cdot \nabla)\mathbf{v}) \cdot \mathbf{p} + \nabla V_{ext} \cdot \mathbf{p} + \mathbf{f} \cdot \mathbf{p} - \mathbf{w} \cdot \mathbf{p} - \eta \nabla^2 \mathbf{v} \cdot \mathbf{p} \\ &\quad - \nabla \cdot \mathbf{p} - \nabla q \cdot \mathbf{v} + m\gamma \mathbf{v} \cdot \mathbf{p} + \int_{\Omega} \rho(r')(\mathbf{p}(r) - \mathbf{p}(r')) \cdot \mathbf{K}(r, r') dr' \quad \text{in } \Sigma \\ \mathbf{p} \cdot \mathbf{n} &= 0 \quad \text{on } \partial\Omega \\ q(T) &= 0. \end{aligned}$$

Substituting  $\frac{\partial \mathbf{v}}{\partial t}$  from the forward equations gives:

$$\begin{aligned} \frac{\partial q}{\partial t} &= (\rho - \hat{\rho}) + \left( -m(\mathbf{v} \cdot \nabla)\mathbf{v} - \nabla V_{ext} - \mathbf{f} + \mathbf{w} - \frac{\nabla \rho}{\rho} - m\gamma \mathbf{v} + \eta \nabla^2 \mathbf{v} - \int_{\Omega} \rho(r') \mathbf{K}(r, r') dr' \right) \cdot \mathbf{p} \\ &\quad + m((\mathbf{v} \cdot \nabla)\mathbf{v}) \cdot \mathbf{p} + \nabla V_{ext} \cdot \mathbf{p} + \mathbf{f} \cdot \mathbf{p} - \mathbf{w} \cdot \mathbf{p} - \eta \nabla^2 \mathbf{v} \cdot \mathbf{p} \\ &\quad - \nabla \cdot \mathbf{p} - \nabla q \cdot \mathbf{v} + m\gamma \mathbf{v} \cdot \mathbf{p} + \int_{\Omega} \rho(r')(\mathbf{p}(r) - \mathbf{p}(r')) \cdot \mathbf{K}(r, r') dr' \quad \text{in } \Sigma \\ \mathbf{p} \cdot \mathbf{n} &= 0 \quad \text{on } \partial\Omega \\ q(T) &= 0. \end{aligned}$$

Cancelling terms and using that  $\nabla \rho = \rho \nabla \ln \rho$ :

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

### 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:

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

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

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

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

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

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

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

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

Replacing the rewritten integrals gives:

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

Then, setting  $\mathcal{L}_{\mathbf{v}}(\rho, \mathbf{v}, \mathbf{w}, \mathbf{p}, q, q_{\partial\Omega}) \mathbf{h} = \mathbf{0}$  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:

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

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:

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

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

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

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

$$\mathbf{p}(T) = \mathbf{0}. \quad (2)$$

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:

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

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

$$\begin{aligned} -\eta \rho \mathbf{p} \cdot \mathbf{n} &= 0 \\ \mathbf{p} \cdot \mathbf{n} &= 0 \quad \text{on } \partial\Omega. \end{aligned} \quad (3)$$

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

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

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:

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

Finally, substituting the expression for  $\frac{\partial \rho}{\partial t}$  from the forward equations gives:

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

And therefore, multiplying out the new term and cancelling, we get:

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

#### 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:

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

#### 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  $\rho$  remains positive, which is a natural condition for the particle density to satisfy. For now, neglect interaction term.

The forward equations become:

$$\frac{\partial \mathbf{v}}{\partial t} = -(\mathbf{v} \cdot \nabla)\mathbf{v} - \frac{1}{m} \nabla V_{ext} - \frac{1}{m} \mathbf{f} + \frac{1}{m} \mathbf{w} - \frac{1}{m} \nabla s - \gamma \mathbf{v} + \frac{\eta}{m} \nabla^2 \mathbf{v} \quad (4)$$

$$- \int_\Omega e^{s(r')} \mathbf{K}(r, r') dr' \quad (5)$$

$$\frac{\partial s}{\partial t} = -\mathbf{v} \cdot \nabla s - \nabla \cdot \mathbf{v}. \quad (6)$$

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:

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

and becomes:

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

The second adjoint equation was:

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

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:

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

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:

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

The second adjoint equation gives:

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