### 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 $\mathbf{w}$. The additional variable $\mathbf{f}$ is an imposed flow and a fixed variable.

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

subject to:

$$m\rho\frac{\partial \mathbf{v}}{\partial t} = -m\rho(\mathbf{v}\cdot\nabla)\mathbf{v} - \rho\nabla V_{ext} - \rho\mathbf{f} - \rho\mathbf{w} - \nabla\rho - m\gamma\rho\mathbf{v} + \eta\rho\nabla^2\mathbf{v}$$
$$- \int_\Omega \rho(r)\rho(r')\nabla V_2(|r - r'|)dr'$$
$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{v}) = 0 \qquad \text{in} \quad \Sigma$$

$$\rho\mathbf{v}\cdot\mathbf{n} = 0 \qquad \text{on} \quad \partial\Sigma$$
$$\rho(r, 0) = \rho_0$$
$$\mathbf{v}(r, 0) = \mathbf{v}_0.$$

Here, we have:

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

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:

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

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 $h \in C_0^\infty(\Sigma)$:

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

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

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

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

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.

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

Furthermore, we have:

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

swapping the order of integration. Then we have:

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

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

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

The introduction of the minus sign is due to the relationship $\nabla_r V_2(|r-r'|) = \nabla_{r'} V_2(|r'-r|)$. (++ Check correct location of comment)+++ Replacing $I_1, I_2, I_{2B}$ and $I_3$ in the derivative gives:

$$
\begin{aligned}
&\mathcal{L}_\rho(\rho, \mathbf{v}, \mathbf{w}, \mathbf{p}, q, q_{\partial\Sigma})h = \int_\Omega h(T)q(T)drdt \\
&+ \int_0^T \int_\Omega \Big( (\rho - \hat{\rho}) + m\frac{\partial \mathbf{v}}{\partial t} \cdot \mathbf{p} + m((\mathbf{v}\cdot\nabla)\mathbf{v})\cdot\mathbf{p} + \nabla V_{ext}\cdot\mathbf{p} + \mathbf{f}\cdot\mathbf{p} + \mathbf{w}\cdot\mathbf{p} \\
&- \eta\nabla^2\mathbf{v}\cdot\mathbf{p} - \nabla\cdot\mathbf{p} - \ \nabla q\cdot\mathbf{v} - \frac{\partial q}{\partial t} + m\gamma\mathbf{v}\cdot\mathbf{p}\Big) hdrdt \\
&+ \int_0^T \int_\Omega \Big( \int_\Omega \rho(r')(\mathbf{p}(r) - \mathbf{p}(r'))\cdot\nabla V_2(|r-r'|)dr' \Big) hdrdt \\
&+ \int_0^T \int_{\partial\Omega} (\mathbf{p}\cdot\mathbf{n} + q\mathbf{v}\cdot\mathbf{n} + q_{\partial\Sigma}\mathbf{v}\cdot\mathbf{n})hdrdt
\end{aligned}
$$

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:

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

Then the derivative becomes:

$$
\begin{aligned}
&\int_0^T \int_\Omega \Big( (\rho - \hat{\rho}) + m\frac{\partial \mathbf{v}}{\partial t} \cdot \mathbf{p} + m((\mathbf{v}\cdot\nabla)\mathbf{v})\cdot\mathbf{p} + \nabla V_{ext}\cdot\mathbf{p} + \mathbf{f}\cdot\mathbf{p} + \mathbf{w}\cdot\mathbf{p} \\
&- \eta\nabla^2\mathbf{v}\cdot\mathbf{p} - \nabla\cdot\mathbf{p} - \ \nabla q\cdot\mathbf{v} - \frac{\partial q}{\partial t} + m\gamma\mathbf{v}\cdot\mathbf{p}\Big) hdrdt \\
&+ \int_0^T \int_\Omega \Big( \int_\Omega \rho(r')(\mathbf{p}(r) - \mathbf{p}(r'))\cdot\nabla V_2(|r-r'|)dr' \Big) hdrdt \\
&= 0.
\end{aligned}
$$

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:

$$
\begin{aligned}
\frac{\partial q}{\partial t} &= (\rho - \hat{\rho}) + m\frac{\partial \mathbf{v}}{\partial t} \cdot \mathbf{p} + m((\mathbf{v}\cdot\nabla)\mathbf{v})\cdot\mathbf{p} + \nabla V_{ext}\cdot\mathbf{p} + \mathbf{f}\cdot\mathbf{p} + \mathbf{w}\cdot\mathbf{p} - \eta\nabla^2\mathbf{v}\cdot\mathbf{p} \\
&- \nabla\cdot\mathbf{p} - \nabla q\cdot\mathbf{v} + m\gamma\mathbf{v}\cdot\mathbf{p} + \int_\Omega \rho(r')(\mathbf{p}(r) - \mathbf{p}(r'))\cdot\nabla V_2(|r-r'|)dr' \qquad \text{in} \quad \Sigma
\end{aligned}
$$

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:

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

and again by a density argument:

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

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

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

Therefore, the first adjoint equation of this problem is:

$$\begin{aligned}
&\frac{\partial q}{\partial t} = (\rho - \hat{\rho}) + m\frac{\partial \mathbf{v}}{\partial t}\cdot\mathbf{p} + m((\mathbf{v}\cdot\nabla)\mathbf{v})\cdot\mathbf{p} + \nabla V_{ext}\cdot\mathbf{p} + \mathbf{f}\cdot\mathbf{p} + \mathbf{w}\cdot\mathbf{p} - \eta\nabla^2\mathbf{v}\cdot\mathbf{p} \\
&- \nabla\cdot\mathbf{p} - \nabla q\cdot\mathbf{v} + m\gamma\mathbf{v}\cdot\mathbf{p} + \int_\Omega \rho(r')(\mathbf{p}(r) - \mathbf{p}(r'))\cdot\nabla V_2(|r - r'|)dr' \qquad \text{in} \quad \Sigma \\
&\mathbf{p}\cdot\mathbf{n} = 0 \qquad \text{on} \quad \partial\Sigma \\
&q(T) = 0.
\end{aligned} \tag{1}$$

### 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:

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

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

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

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

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

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

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

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

Replacing the rewritten integrals gives:

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

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:

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

gives:

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

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:

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

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

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

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

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

Finally, relaxing the conditions on the boundary terms to choose $\mathbf{h} = 0$ and $\frac{\partial \mathbf{h}}{\partial n} \neq 0$ on $\partial\Sigma$ gives:

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

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

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

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

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

Applying 3, this reduces to:

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

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

$$(\rho q_{\partial\Sigma} + q\rho)\mathbf{n} = \mathbf{0} \qquad \text{on} \quad \partial\Sigma.$$

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

$$(q_{\partial\Sigma} + q)\mathbf{n} = \mathbf{0}$$

And the relationship between the adjoints becomes:

$$q_{\partial\Sigma} = -q.$$

The second adjoint equation of the above problem is:

$$\begin{aligned} m\rho \frac{\partial \mathbf{p}}{\partial t} =& -\eta \nabla^2(\rho\mathbf{p}) - m\frac{\partial \rho}{\partial t}\mathbf{p} + m\gamma\rho\mathbf{p} - \rho\nabla q + m\rho(\nabla\mathbf{v})^\top \mathbf{p} \\ & - m\rho(\mathbf{v}\cdot\nabla)\mathbf{p} - m\rho(\nabla\cdot\mathbf{v})\mathbf{p} - m(\mathbf{v}\cdot\nabla\rho)\mathbf{p} \qquad \text{in} \quad \Sigma \\ & \mathbf{p}(T) = \mathbf{0}. \end{aligned} \tag{4}$$

### 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:

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

### 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.
The forward equations become:

$$\begin{aligned}\frac{\partial \mathbf{v}}{\partial t} &= -(\mathbf{v} \cdot \nabla)\mathbf{v} - \frac{1}{m}\nabla V_{ext} - \frac{1}{m}\mathbf{f} - \frac{1}{m}\mathbf{w} - \frac{1}{m}\nabla s - \gamma \mathbf{v} + \frac{\eta}{m}\nabla^2 \mathbf{v} \\ &\quad - \int_\Omega e^{s(r')} \nabla V_2(|r - r'|) dr' \end{aligned} \tag{5}$$

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

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 1 doesn't change much. Although it should be noted that the integral term would enter the adjoints here, so we would get an integral involving $e^s$.

$$\begin{aligned}\frac{\partial q}{\partial t} &= (e^s - \hat{\rho}) + m\frac{\partial \mathbf{v}}{\partial t} \cdot \mathbf{p} + m((\mathbf{v} \cdot \nabla)\mathbf{v}) \cdot \mathbf{p} + \nabla V_{ext} \cdot \mathbf{p} + \mathbf{f} \cdot \mathbf{p} + \mathbf{w} \cdot \mathbf{p} - \eta \nabla^2 \mathbf{v} \cdot \mathbf{p} \\ &\quad - \nabla \cdot \mathbf{p} - \nabla q \cdot \mathbf{v} + m\gamma \mathbf{v} \cdot \mathbf{p} + \int_\Omega e^{s(r')}(\mathbf{p}(r) - \mathbf{p}(r')) \cdot \nabla V_2(|r - r'|) dr'\end{aligned}$$

Substituting the definition of $\frac{\partial \mathbf{v}}{\partial t}$ from the forward Equation 5 gives:

$$\begin{aligned}\frac{\partial q}{\partial t} &= (e^s - \hat{\rho}) + m\Big( - (\mathbf{v} \cdot \nabla)\mathbf{v} - \frac{1}{m}\nabla V_{ext} - \frac{1}{m}\mathbf{f} - \frac{1}{m}\mathbf{w} - \frac{1}{m}\nabla s - \gamma \mathbf{v} + \frac{\eta}{m}\nabla^2 \mathbf{v}\Big) \cdot \mathbf{p} \\ &\quad + m((\mathbf{v} \cdot \nabla)\mathbf{v}) \cdot \mathbf{p} + \nabla V_{ext} \cdot \mathbf{p} + \mathbf{f} \cdot \mathbf{p} + \mathbf{w} \cdot \mathbf{p} - \eta \nabla^2 \mathbf{v} \cdot \mathbf{p} \\ &\quad - \nabla \cdot \mathbf{p} - \nabla q \cdot \mathbf{v} + m\gamma \mathbf{v} \cdot \mathbf{p} + \int_\Omega e^{s(r')}(\mathbf{p}(r) - \mathbf{p}(r')) \cdot \nabla V_2(|r - r'|) dr'\end{aligned}$$

Which cancels to give:

$$\frac{\partial q}{\partial t} = (e^s - \hat{\rho}) - \nabla s \cdot \mathbf{p} - \nabla \cdot \mathbf{p} - \nabla q \cdot \mathbf{v} + \int_\Omega e^{s(r')}(\mathbf{p}(r) - \mathbf{p}(r')) \cdot \nabla V_2(|r - r'|) dr'$$

The second adjoint equation 4 was:

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

Rewriting terms in the new variable $s$ gives:

$$\begin{aligned}
-\eta\nabla^2(\rho\mathbf{p}) &= -e^s\Big(2\eta\nabla\mathbf{p}\cdot\nabla s + \eta\mathbf{p}\cdot(\nabla s)^2 + \eta\mathbf{p}\cdot\nabla^2 s + \eta\nabla^2\mathbf{p}\Big) \\
\frac{\partial \rho}{\partial t} &= e^s\frac{\partial s}{\partial t} \\
m(\mathbf{v}\cdot\nabla\rho)\mathbf{p} &= e^s m(\mathbf{v}\cdot\nabla s)\mathbf{p}.
\end{aligned}$$

+++ Note: I am not sure about these calculations in terms of vector notation, since, for example, $\eta\mathbf{p}\cdot(\nabla s)^2$ doesn't really make sense in 2D (trying to compute a dot product between three terms). However, that shouldn't matter in 1D and the application of the product rule in 1D should be correct! +++ And therefore the new adjoint equation is:

$$\begin{aligned}
\frac{\partial \mathbf{p}}{\partial t} =& -\frac{2\eta}{m}\nabla\mathbf{p}\cdot\nabla s - \frac{\eta}{m}\mathbf{p}\cdot(\nabla s)^2 - \frac{\eta}{m}\mathbf{p}\cdot\nabla^2 s - \frac{\eta}{m}\nabla^2\mathbf{p} \\
&- \frac{\partial s}{\partial t}\mathbf{p} + \gamma\mathbf{p} - \frac{1}{m}\nabla q + (\nabla\mathbf{v})^\top\mathbf{p} \\
&- (\mathbf{v}\cdot\nabla)\mathbf{p} - (\nabla\cdot\mathbf{v})\mathbf{p} - (\mathbf{v}\cdot\nabla s)\mathbf{p} \qquad \text{in} \quad \Sigma.
\end{aligned}$$

Substituting the definition of $\frac{\partial s}{\partial t}$ from Equation 6:

$$\begin{aligned}
\frac{\partial \mathbf{p}}{\partial t} =& -\frac{2\eta}{m}\nabla\mathbf{p}\cdot\nabla s - \frac{\eta}{m}\mathbf{p}\cdot(\nabla s)^2 - \frac{\eta}{m}\mathbf{p}\cdot\nabla^2 s - \frac{\eta}{m}\nabla^2\mathbf{p} \\
&- \Big(-\mathbf{v}\cdot\nabla s - \nabla\cdot\mathbf{v}\Big)\mathbf{p} + \gamma\mathbf{p} - \frac{1}{m}\nabla q + (\nabla\mathbf{v})^\top\mathbf{p} \\
&- (\mathbf{v}\cdot\nabla)\mathbf{p} - (\nabla\cdot\mathbf{v})\mathbf{p} - (\mathbf{v}\cdot\nabla s)\mathbf{p} \qquad \text{in} \quad \Sigma.
\end{aligned}$$

Cancellations result in the adjoint equation:

$$\begin{aligned}
\frac{\partial \mathbf{p}}{\partial t} =& -\frac{2\eta}{m}\nabla\mathbf{p}\cdot\nabla s - \frac{\eta}{m}\mathbf{p}\cdot(\nabla s)^2 - \frac{\eta}{m}\mathbf{p}\cdot\nabla^2 s - \frac{\eta}{m}\nabla^2\mathbf{p} \\
&+ \gamma\mathbf{p} - \frac{1}{m}\nabla q + (\nabla\mathbf{v})^\top\mathbf{p} - (\mathbf{v}\cdot\nabla)\mathbf{p} \qquad \text{in} \quad \Sigma.
\end{aligned}$$

Finally, in both adjoints, time is reversed due to the negative Laplacian term and the final time conditions. The first adjoint equation becomes:

$$\frac{\partial q}{\partial \tau} = -(e^s - \hat{\rho}) + \nabla s\cdot\mathbf{p} + \nabla\cdot\mathbf{p} + \nabla q\cdot\mathbf{v} - \int_\Omega e^{s(r')}(\mathbf{p}(r) - \mathbf{p}(r'))\cdot\nabla V_2(|r-r'|)dr'$$

The second adjoint equation is:

$$\begin{aligned}\frac{\partial \mathbf{p}}{\partial \tau} =& \frac{2\eta}{m}\nabla \mathbf{p} \cdot \nabla s + \frac{\eta}{m}\mathbf{p} \cdot (\nabla s)^2 + \frac{\eta}{m}\mathbf{p} \cdot \nabla^2 s + \frac{\eta}{m}\nabla^2 \mathbf{p} \\ & - \gamma \mathbf{p} + \frac{1}{m}\nabla q - (\nabla \mathbf{v})^\top \mathbf{p} + (\mathbf{v} \cdot \nabla)\mathbf{p}\end{aligned}$$