

## Boundary Observation and Non-Constant Flux Boundary conditions

This set of notes is concerned with deriving non-zero (non-)constant flux boundary conditions, which are different for different parts of the boundary. Furthermore, the target distribution of particles  $\hat{\rho}$  is prescribed on parts of the boundary only, instead of on all of  $\Omega$ . Different parts of the boundary have different target distributions of particles.

+++ Boundary control correct here, since we don't directly apply the control on the boundary??+++

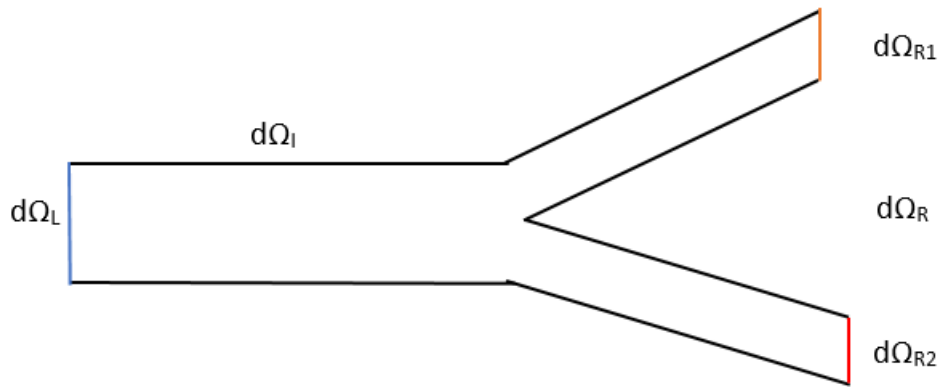


Figure 1: Boundary

The domain with the different parts of the boundary that are considered can be seen in Figure 1.

## 1 Distributed Observation and Constant Flux Boundary Conditions

The problem of interest is of the form:

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

subject to:

$$\begin{aligned} \partial_t \rho &= \nabla^2 \rho - \nabla \cdot (\rho \mathbf{w}_{Flow}) + \nabla \cdot (\rho \nabla V_{ext}) + \nabla \cdot \int_{\Omega} \rho(r) \rho(r') \nabla V_2(|r - r'|) dr' + f \quad \text{in } Q, \\ \rho &= \rho_0 \quad \text{at } t = 0 \\ -\mathbf{j} \cdot \mathbf{n} &= \mathbb{1}_{\partial\Omega_L} C_L + \mathbb{1}_{\partial\Omega_R} C_R + \mathbb{1}_{\partial\Omega_I} 0, \quad \text{on } \partial Q, \end{aligned}$$

where  $C_L, C_R$  are constants and  $\mathbb{1}$  is the indicator function of the set (the parts of the boundary) of interest. Furthermore,  $\mathbf{j}$  satisfies:

$$\mathbf{j} = \nabla \rho - (\rho \mathbf{w}_{Flow}) + (\rho \nabla V_{ext}) + \int_{\Omega} \rho(r) \rho(r') \nabla V_2(|r - r'|) dr'.$$

## The Lagrangian

The Lagrangian is of the form:

$$\begin{aligned} \mathcal{L}(\rho, f, p_Q, p_{\partial Q}) &= \int_0^T \int_{\Omega} \frac{1}{2} (\rho - \hat{\rho})^2 dr dt + \frac{\beta}{2} \int_0^T \int_{\Omega} f^2 dr dt \\ &+ \int_0^T \int_{\Omega} \left( \partial_t \rho - \nabla^2 \rho + \nabla \cdot (\rho \mathbf{w}_{Flow}) - \nabla \cdot (\rho \nabla V_{ext}) + \nabla \cdot \int_{\Omega} \rho(r) \rho(r') \nabla V_2(|r - r'|) dr' \right) p_Q dr dt \\ &+ \int_0^T \int_{\partial \Omega} \left( \left( -\nabla \rho + (\rho \mathbf{w}_{Flow}) - (\rho \nabla V_{ext}) - \int_{\Omega} \rho(r) \rho(r') \nabla V_2(|r - r'|) dr' \right) \cdot \mathbf{n} \right. \\ &\left. - \mathbb{1}_{\partial \Omega_L} C_L - \mathbb{1}_{\partial \Omega_R} C_R - \mathbb{1}_{\partial \Omega_I} 0 \right) p_{\partial Q} dr dt. \end{aligned}$$

## The Adjoint Equation

The derivative of  $\mathcal{L}$  with respect to  $\rho$  is, as taken from the extended project:

$$\begin{aligned} \mathcal{L}_{\rho}(\rho, \mathbf{w}, p_{\Omega}, p_{\partial \Omega}) h &= \int_{\Omega} h(T) p_Q(T) dr \\ &+ \int_0^T \int_{\Omega} \left( (\rho - \hat{\rho}) - \partial_t p_Q - \nabla p_Q \cdot \mathbf{w}_{Flow} - \nabla^2 p_Q + \nabla p_Q \cdot \nabla V_{ext} \right. \\ &+ \int_{\Omega} (\nabla p_Q(r) + \nabla p_Q(r')) \rho(r') \nabla V_2(|r - r'|) dr' + \int_{\partial \Omega} (p_{\partial Q}(r') - p_Q(r')) \rho(r') \frac{\partial V_2(|r - r'|)}{\partial n} dr' \left. \right) h dr dt \\ &+ \int_0^T \int_{\partial \Omega} \left( \left( \frac{\partial p_Q}{\partial n} + p_Q \mathbf{w} \cdot \mathbf{n} - p_{\partial Q} \mathbf{w}_{Flow} \cdot \mathbf{n} + p_{\partial Q} \frac{\partial V_{ext}}{\partial n} - p_Q \frac{\partial V_{ext}}{\partial n} + (p_{\partial Q} - p_Q) \int_{\Omega} \rho(r') \frac{\partial V_2(|r - r'|)}{\partial n} dr' \right) h \right. \\ &\left. + \left( p_{\partial Q} - p_Q \right) \frac{\partial h}{\partial n} \right) dr dt = 0. \end{aligned}$$

Then, from appropriate analysis we find that:

$$p_{\partial Q} = p_Q,$$

and therefore we get:

$$\begin{aligned} (\rho - \hat{\rho}) - \partial_t p_Q - \nabla p_Q \cdot \mathbf{w}_{Flow} - \nabla^2 p_Q + \nabla p_Q \cdot \nabla V_{ext} \\ + \int_{\Omega} (\nabla p_Q(r) + \nabla p_Q(r')) \rho(r') \nabla V_2(|r - r'|) dr' &= 0, \quad \text{in } Q, \\ \frac{\partial p_Q}{\partial n} &= 0, \quad \text{on } \partial Q. \end{aligned}$$

## 2 Distributed Observation and Non-Constant Flux Boundary Conditions

The problem of interest is of the form:

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

subject to:

$$\begin{aligned} \partial_t \rho &= \nabla^2 \rho - \nabla \cdot (\rho \mathbf{w}_{Flow}) + \nabla \cdot (\rho \nabla V_{ext}) + \nabla \cdot \int_{\Omega} \rho(r) \rho(r') \nabla V_2(|r - r'|) dr' + f \quad \text{in } Q, \\ \rho &= \rho_0 \quad \text{at } t = 0 \\ -\mathbf{j} \cdot \mathbf{n} &= \mathbb{1}_{\partial\Omega_L} (C_{L1} + C_{L2}\rho) + \mathbb{1}_{\partial\Omega_R} (C_{R1} + C_{R2}\rho) + \mathbb{1}_{\partial\Omega_I} 0, \quad \text{on } \partial Q \end{aligned}$$

where  $C_{L1}, C_{L2}, C_{R1}, C_{R2}$  are constants and  $\mathbb{1}$  is the indicator function of the set (the parts of the boundary) of interest. Furthermore,  $\mathbf{j}$  satisfies:

$$\mathbf{j} = \nabla \rho - (\rho \mathbf{w}_{Flow}) + (\rho \nabla V_{ext}) + \int_{\Omega} \rho(r) \rho(r') \nabla V_2(|r - r'|) dr'$$

### The Lagrangian

The Lagrangian is of the form:

$$\begin{aligned} \mathcal{L}(\rho, f, p_Q, p_{\partial Q}) &= \int_0^T \int_{\Omega} \frac{1}{2} (\rho - \hat{\rho})^2 dr dt + \frac{\beta}{2} \int_0^T \int_{\Omega} f^2 dr dt \\ &+ \int_0^T \int_{\Omega} \left( \partial_t \rho - \nabla^2 \rho + \nabla \cdot (\rho \mathbf{w}_{Flow}) - \nabla \cdot (\rho \nabla V_{ext}) + \nabla \cdot \int_{\Omega} \rho(r) \rho(r') \nabla V_2(|r - r'|) dr' \right) p_Q dr dt \\ &+ \int_0^T \int_{\partial\Omega} \left( \left( -\nabla \rho + (\rho \mathbf{w}_{Flow}) - (\rho \nabla V_{ext}) - \int_{\Omega} \rho(r) \rho(r') \nabla V_2(|r - r'|) dr' \right) \cdot \mathbf{n} \right. \\ &\quad \left. - \mathbb{1}_{\partial\Omega_L} (C_{L1} + C_{L2}\rho) - \mathbb{1}_{\partial\Omega_R} (C_{R1} + C_{R2}\rho) - \mathbb{1}_{\partial\Omega_I} 0 \right) p_{\partial Q} dr dt. \end{aligned}$$

## The Adjoint Equation

The derivative of  $\mathcal{L}$  with respect to  $\rho$  is, as taken from the extended project:

$$\begin{aligned}
\mathcal{L}_\rho(\rho, \mathbf{w}, p_\Omega, p_{\partial\Omega})h &= \int_\Omega h(T)p_Q(T)dr \\
&+ \int_0^T \int_\Omega \left( (\rho - \hat{\rho}) - \partial_t p_Q - \nabla p_Q \cdot \mathbf{w}_{Flow} - \nabla^2 p_Q + \nabla p_Q \cdot \nabla V_{ext} \right. \\
&+ \int_\Omega (\nabla p_Q(r) + \nabla p_Q(r'))\rho(r')\nabla V_2(|r - r'|)dr' + \int_{\partial\Omega} (p_{\partial Q}(r') - p_Q(r'))\rho(r')\frac{\partial V_2(|r - r'|)}{\partial n}dr' \Big) h dr dt \\
&+ \int_0^T \int_{\partial\Omega} \left( \left( \frac{\partial p_Q}{\partial n} + p_Q \mathbf{w} \cdot \mathbf{n} - p_{\partial Q} \mathbf{w}_{Flow} \cdot \mathbf{n} + p_{\partial Q} \frac{\partial V_{ext}}{\partial n} - p_Q \frac{\partial V_{ext}}{\partial n} + (p_{\partial Q} - p_Q) \int_\Omega \rho(r')\frac{\partial V_2(|r - r'|)}{\partial n}dr' \right. \right. \\
&- \mathbb{1}_{\partial\Omega_L} C_{L2} p_{\partial Q} - \mathbb{1}_{\partial\Omega_R} C_{R2} p_{\partial Q} \Big) h \\
&+ \left( p_{\partial Q} - p_Q \right) \frac{\partial h}{\partial n} \Big) dr dt = 0.
\end{aligned}$$

Then, from appropriate analysis we find that:

$$p_{\partial Q} = p_Q,$$

and therefore we get:

$$\begin{aligned}
(\rho - \hat{\rho}) - \partial_t p_Q - \nabla p_Q \cdot \mathbf{w}_{Flow} - \nabla^2 p_Q + \nabla p_Q \cdot \nabla V_{ext} \\
+ \int_\Omega (\nabla p_Q(r) + \nabla p_Q(r'))\rho(r')\nabla V_2(|r - r'|)dr' &= 0, \quad \text{in } Q, \\
\frac{\partial p_Q}{\partial n} - \mathbb{1}_{\partial\Omega_L} C_{L2} p_Q - \mathbb{1}_{\partial\Omega_R} C_{R2} p_Q &= 0, \quad \text{on } \partial Q.
\end{aligned}$$

## 3 Boundary Observation and Constant Flux Boundary Conditions

The problem of interest is of the form:

$$\min_{\rho, f} \quad \frac{1}{2} \|\rho - \hat{\rho}\|_{L_2(\partial Q_R)}^2 + \frac{\beta}{2} \|f\|_{L_2(Q)}^2$$

subject to:

$$\begin{aligned}
\partial_t \rho &= \nabla^2 \rho - \nabla \cdot (\rho \mathbf{w}_{Flow}) + \nabla \cdot (\rho \nabla V_{ext}) + \nabla \cdot \int_\Omega \rho(r)\rho(r')\nabla V_2(|r - r'|)dr' + f \quad \text{in } Q, \\
\rho &= \rho_0 \quad \text{at } t = 0 \\
-\mathbf{j} \cdot \mathbf{n} &= \mathbb{1}_{\partial\Omega_L} C_L + \mathbb{1}_{\partial\Omega_R} C_R + \mathbb{1}_{\partial\Omega_I} 0, \quad \text{on } \partial Q,
\end{aligned}$$

where  $C_L, C_R$  are constants and  $\mathbb{1}$  is the indicator function of the set (the parts of the boundary) of interest. Furthermore,  $\mathbf{j}$  satisfies:

$$\mathbf{j} = \nabla \rho - (\rho \mathbf{w}_{Flow}) + (\rho \nabla V_{ext}) + \int_{\Omega} \rho(r) \rho(r') \nabla V_2(|r - r'|) dr'.$$

Moreover, let  $\hat{\rho}$  be defined such that:

$$\hat{\rho} = \mathbb{1}_{\partial\Omega_{R1}} \tilde{\rho} + \mathbb{1}_{\partial\Omega_{R2}} 0.$$

## The Lagrangian

The Lagrangian is of the form:

$$\begin{aligned} \mathcal{L}(\rho, f, p_Q, p_{\partial Q}) &= \int_0^T \int_{\partial\Omega_R} \frac{1}{2} (\rho - \hat{\rho})^2 dr dt + \frac{\beta}{2} \int_0^T \int_{\Omega} f^2 dr dt \\ &+ \int_0^T \int_{\Omega} \left( \partial_t \rho - \nabla^2 \rho + \nabla \cdot (\rho \mathbf{w}_{Flow}) - \nabla \cdot (\rho \nabla V_{ext}) + \nabla \cdot \int_{\Omega} \rho(r) \rho(r') \nabla V_2(|r - r'|) dr' \right) p_Q dr dt \\ &+ \int_0^T \int_{\partial\Omega} \left( \left( -\nabla \rho + (\rho \mathbf{w}_{Flow}) - (\rho \nabla V_{ext}) - \int_{\Omega} \rho(r) \rho(r') \nabla V_2(|r - r'|) dr' \right) \cdot \mathbf{n} \right. \\ &\left. - \mathbb{1}_{\partial\Omega_L} C_L - \mathbb{1}_{\partial\Omega_R} C_R - \mathbb{1}_{\partial\Omega_I} 0 \right) p_{\partial Q} dr dt. \end{aligned}$$

## The Adjoint Equation

The derivative of  $\mathcal{L}$  with respect to  $\rho$  is, as taken from the extended project:

$$\begin{aligned} \mathcal{L}_{\rho}(\rho, \mathbf{w}, p_{\Omega}, p_{\partial\Omega}) h &= \int_{\Omega} h(T) p_Q(T) dr \\ &+ \int_0^T \int_{\Omega} \left( -\partial_t p_Q - \nabla p_Q \cdot \mathbf{w}_{Flow} - \nabla^2 p_Q + \nabla p_Q \cdot \nabla V_{ext} \right. \\ &+ \int_{\Omega} (\nabla p_Q(r) + \nabla p_Q(r')) \rho(r') \nabla V_2(|r - r'|) dr' + \int_{\partial\Omega} (p_{\partial Q}(r') - p_Q(r')) \rho(r') \frac{\partial V_2(|r - r'|)}{\partial n} dr' \Big) h dr dt \\ &+ \int_0^T \int_{\partial\Omega} \left( \left( \frac{\partial p_Q}{\partial n} + p_Q \mathbf{w} \cdot \mathbf{n} - p_{\partial Q} \mathbf{w}_{Flow} \cdot \mathbf{n} + p_{\partial Q} \frac{\partial V_{ext}}{\partial n} - p_Q \frac{\partial V_{ext}}{\partial n} + (p_{\partial Q} - p_Q) \int_{\Omega} \rho(r') \frac{\partial V_2(|r - r'|)}{\partial n} dr' \right. \right. \\ &\left. \left. (\rho - \hat{\rho}) \mathbb{1}_{\partial\Omega_R} \right) h + \left( p_{\partial Q} - p_Q \right) \frac{\partial h}{\partial n} \right) dr dt = 0. \end{aligned}$$

Then, from appropriate analysis we find that:

$$p_{\partial Q} = p_Q,$$

and therefore we get:

$$\begin{aligned} &-\partial_t p_Q - \nabla p_Q \cdot \mathbf{w}_{Flow} - \nabla^2 p_Q + \nabla p_Q \cdot \nabla V_{ext} \\ &+ \int_{\Omega} (\nabla p_Q(r) + \nabla p_Q(r')) \rho(r') \nabla V_2(|r - r'|) dr' = 0, \quad \text{in } Q, \\ &\frac{\partial p_Q}{\partial n} + \mathbb{1}_{\partial\Omega_R} (\rho - \hat{\rho}) = 0, \quad \text{on } \partial Q. \end{aligned}$$

In particular, the boundary condition is:

$$\frac{\partial p_Q}{\partial n} + \mathbb{1}_{\partial\Omega_{R1}}(\rho - \tilde{\rho}) + \mathbb{1}_{\partial\Omega_{R2}}\rho = 0, \quad \text{on } \partial Q.$$

## 4 Boundary Observation and Non-Constant Flux Boundary Conditions

The problem of interest is of the form:

$$\min_{\rho, f} \quad \frac{1}{2} \|\rho - \hat{\rho}\|_{L_2(\partial Q_R)}^2 + \frac{\beta}{2} \|f\|_{L_2(Q)}^2$$

subject to:

$$\begin{aligned} \partial_t \rho &= \nabla^2 \rho - \nabla \cdot (\rho \mathbf{w}_{Flow}) + \nabla \cdot (\rho \nabla V_{ext}) + \nabla \cdot \int_{\Omega} \rho(r) \rho(r') \nabla V_2(|r - r'|) dr' + f \quad \text{in } Q, \\ \rho &= \rho_0 \quad \text{at } t = 0 \\ -\mathbf{j} \cdot \mathbf{n} &= \mathbb{1}_{\partial\Omega_L}(C_{L1} + C_{L2}\rho) + \mathbb{1}_{\partial\Omega_R}(C_{R1} + C_{R2}\rho) + \mathbb{1}_{\partial\Omega_I}0, \quad \text{on } \partial Q, \end{aligned}$$

where  $C_{L1}, C_{L2}, C_{R1}, C_{R2}$  are constants and  $\mathbb{1}$  is the indicator function of the set (the parts of the boundary) of interest. Furthermore,  $\mathbf{j}$  satisfies:

$$\mathbf{j} = \nabla \rho - (\rho \mathbf{w}_{Flow}) + (\rho \nabla V_{ext}) + \int_{\Omega} \rho(r) \rho(r') \nabla V_2(|r - r'|) dr'.$$

Moreover, let  $\hat{\rho}$  be defined such that:

$$\hat{\rho} = \mathbb{1}_{\partial\Omega_{R1}}\tilde{\rho} + \mathbb{1}_{\partial\Omega_{R2}}0.$$

### The Lagrangian

The Lagrangian is of the form:

$$\begin{aligned} \mathcal{L}(\rho, f, p_Q, p_{\partial Q}) &= \int_0^T \int_{\partial\Omega_R} \frac{1}{2}(\rho - \hat{\rho})^2 dr dt + \frac{\beta}{2} \int_0^T \int_{\Omega} f^2 dr dt \\ &+ \int_0^T \int_{\Omega} \left( \partial_t \rho - \nabla^2 \rho + \nabla \cdot (\rho \mathbf{w}_{Flow}) - \nabla \cdot (\rho \nabla V_{ext}) + \nabla \cdot \int_{\Omega} \rho(r) \rho(r') \nabla V_2(|r - r'|) \right) p_Q dr dt \\ &+ \int_0^T \int_{\partial\Omega} \left( \left( -\nabla \rho + (\rho \mathbf{w}_{Flow}) - (\rho \nabla V_{ext}) - \int_{\Omega} \rho(r) \rho(r') \nabla V_2(|r - r'|) dr' \right) \cdot \mathbf{n} \right. \\ &\left. - \mathbb{1}_{\partial\Omega_L}(C_{L1} + C_{L2}\rho) - \mathbb{1}_{\partial\Omega_R}(C_{R1} + C_{R2}\rho) - \mathbb{1}_{\partial\Omega_I}0 \right) p_{\partial Q} dr dt. \end{aligned}$$

## The Adjoint Equation

The derivative of  $\mathcal{L}$  with respect to  $\rho$  is, as taken from the extended project:

$$\begin{aligned}
\mathcal{L}_\rho(\rho, \mathbf{w}, p_\Omega, p_{\partial\Omega})h &= \int_\Omega h(T)p_Q(T)dr \\
&+ \int_0^T \int_\Omega \left( -\partial_t p_Q - \nabla p_Q \cdot \mathbf{w}_{Flow} - \nabla^2 p_Q + \nabla p_Q \cdot \nabla V_{ext} \right. \\
&+ \int_\Omega (\nabla p_Q(r) + \nabla p_Q(r'))\rho(r')\nabla V_2(|r - r'|)dr' + \int_{\partial\Omega} (p_{\partial Q}(r') - p_Q(r'))\rho(r')\frac{\partial V_2(|r - r'|)}{\partial n}dr' \Big) h dr dt \\
&+ \int_0^T \int_{\partial\Omega} \left( \left( \frac{\partial p_Q}{\partial n} + p_Q \mathbf{w} \cdot \mathbf{n} - p_{\partial Q} \mathbf{w}_{Flow} \cdot \mathbf{n} + p_{\partial Q} \frac{\partial V_{ext}}{\partial n} - p_Q \frac{\partial V_{ext}}{\partial n} + (p_{\partial Q} - p_Q) \int_\Omega \rho(r') \frac{\partial V_2(|r - r'|)}{\partial n} dr' \right. \right. \\
&\left. \left. \mathbb{1}_{\partial\Omega_R}(\rho - \hat{\rho}) - \mathbb{1}_{\partial\Omega_L} C_{L2} p_{\partial Q} - \mathbb{1}_{\partial\Omega_R} C_{R2} p_{\partial Q} \right) h + \left( p_{\partial Q} - p_Q \right) \frac{\partial h}{\partial n} \right) dr dt = 0.
\end{aligned}$$

Then, from appropriate analysis we find that:

$$p_{\partial Q} = p_Q,$$

and therefore we get:

$$\begin{aligned}
&-\partial_t p_Q - \nabla p_Q \cdot \mathbf{w}_{Flow} - \nabla^2 p_Q + \nabla p_Q \cdot \nabla V_{ext} \\
&+ \int_\Omega (\nabla p_Q(r) + \nabla p_Q(r'))\rho(r')\nabla V_2(|r - r'|)dr' = 0, \quad \text{in } Q, \\
&\frac{\partial p_Q}{\partial n} + \mathbb{1}_{\partial\Omega_R}(\rho - \hat{\rho}) - \mathbb{1}_{\partial\Omega_L} C_{L2} p_Q - \mathbb{1}_{\partial\Omega_R} C_{R2} p_Q = 0, \quad \text{on } \partial Q.
\end{aligned}$$

Again, in particular the boundary condition is:

$$\frac{\partial p_Q}{\partial n} + \mathbb{1}_{\partial\Omega_{R1}}(\rho - \tilde{\rho} - C_{R2} p_Q) + \mathbb{1}_{\partial\Omega_{R2}}(\rho - C_{R2} p_Q) - \mathbb{1}_{\partial\Omega_L} C_{L2} p_Q = 0, \quad \text{on } \partial Q.$$