## Optimality Conditions for Two Species

We have the following set of forward equations:

$$\begin{aligned}\frac{\partial \rho_a}{\partial t} =& D_a \nabla^2 \rho_a - D_a \nabla \cdot (\rho_a F_a(\mathbf{w})) + D_a \nabla \cdot (\rho_a \nabla V_{ext,a}) + D_a \kappa \nabla \cdot \int_\Omega \rho_a(r)\rho_a(r')\mathbf{K}_{aa}(r,r')dr' \\ &+ D_a \tilde{\kappa} \nabla \cdot \int_\Omega \rho_a(r)\rho_b(r')\mathbf{K}_{ab}(r,r')dr' \\ \frac{\partial \rho_b}{\partial t} =& D_b \nabla^2 \rho_b - D_b \nabla \cdot (\rho_b F_b(\mathbf{w})) + D_b \nabla \cdot (\rho_b \nabla V_{ext,b}) + D_b \kappa \nabla \cdot \int_\Omega \rho_b(r)\rho_b(r')\mathbf{K}_{bb}(r,r')dr' \\ &+ D_b \tilde{\kappa} \nabla \cdot \int_\Omega \rho_b(r)\rho_a(r')\mathbf{K}_{ba}(r,r')dr',\end{aligned}$$

where $D = \frac{1}{\gamma m}$. No flux boundary conditions are:

$$\begin{aligned}&\Big(D_a \nabla \rho_a - D_a \rho_a F_a(\mathbf{w}) + D_a \rho_a \nabla V_{ext,a} + D_a \kappa \int_\Omega \rho_a(r)\rho_a(r')\mathbf{K}_{aa}(r,r')dr' \\ &+ D_a \tilde{\kappa} \int_\Omega \rho_a(r)\rho_b(r')\mathbf{K}_{ab}(r,r')dr'\Big) \cdot \mathbf{n} = 0 \\ &\Big(D_b \nabla \rho_b - D_b \rho_b F_b(\mathbf{w}) + D_b \rho_b \nabla V_{ext,b} + D_b \kappa \int_\Omega \rho_b(r)\rho_b(r')\mathbf{K}_{bb}(r,r')dr' \\ &+ D_b \tilde{\kappa} \int_\Omega \rho_b(r)\rho_a(r')\mathbf{K}_{ba}(r,r')dr'\Big) \cdot \mathbf{n} = 0\end{aligned}$$

The cost functional is:

$$J(\rho_a, \rho_b, \mathbf{w}) := \frac{1}{2}||\rho_a - \widehat{\rho_a}||^2_{L_2(\Sigma)} + \frac{\alpha}{2}||\rho_b - \widehat{\rho_b}||^2_{L_2(\Sigma)} + \frac{\beta}{2}||\mathbf{w}||^2_{L_2(\Sigma)}.$$

The Lagrangian is then:

$$
\begin{aligned}
\mathcal{L}(\rho_a,\rho_b,\mathbf{w},q_a,q_b) =& \frac{1}{2}\int_0^T\int_\Omega(\rho_a-\widehat{\rho_a})^2drdt+\frac{\alpha}{2}\int_0^T\int_\Omega(\rho_b-\widehat{\rho_b})^2drdt+\frac{\beta}{2}\int_0^T\int_\Omega \mathbf{w}^2drdt\\
&-\int_0^T\int_\Omega\bigg(\frac{\partial\rho_a}{\partial t}-D_a\nabla^2\rho_a+D_a\nabla\cdot(\rho_aF_a(\mathbf{w}))-D_a\nabla\cdot(\rho_a\nabla V_{ext,a})\\
&-D_a\kappa\nabla\cdot\int_\Omega\rho_a(r)\rho_a(r')\mathbf{K}_{aa}(r,r')dr'-D_a\tilde{\kappa}\nabla\cdot\int_\Omega\rho_a(r)\rho_b(r')\mathbf{K}_{ab}(r,r')dr\bigg)q_adrdt\\
&-\int_0^T\int_\Omega\bigg(\frac{\partial\rho_b}{\partial t}-D_b\nabla^2\rho_b+D_b\nabla\cdot(\rho_bF_b(\mathbf{w}))-D_b\nabla\cdot(\rho_b\nabla V_{ext,b})\\
&-D_b\kappa\nabla\cdot\int_\Omega\rho_b(r)\rho_b(r')\mathbf{K}_{bb}(r,r')dr'-D_b\tilde{\kappa}\nabla\cdot\int_\Omega\rho_b(r)\rho_a(r')\mathbf{K}_{ba}(r,r')dr'\bigg)q_bdrdt\\
&-\int_0^T\int_{\partial\Omega}\bigg(D_a\nabla\rho_a-D_a\rho_aF_a(\mathbf{w})+D_a\rho_a\nabla V_{ext,a}+D_a\kappa\int_\Omega\rho_a(r)\rho_a(r')\mathbf{K}_{aa}(r,r')dr'\\
&+D_a\tilde{\kappa}\int_\Omega\rho_a(r)\rho_b(r')\mathbf{K}_{ab}(r,r')dr'\bigg)\cdot\mathbf{n}q_{a,\partial\Omega}drdt\\
&-\int_0^T\int_{\partial\Omega}\bigg(D_b\nabla\rho_b-D_b\rho_bF_b(\mathbf{w})+D_b\rho_b\nabla V_{ext,b}+D_b\kappa\int_\Omega\rho_b(r)\rho_b(r')\mathbf{K}_{bb}(r,r')dr'\\
&+D_b\tilde{\kappa}\int_\Omega\rho_b(r)\rho_a(r')\mathbf{K}_{ba}(r,r')dr'\bigg)\cdot\mathbf{n}q_{b,\partial\Omega}drdt
\end{aligned}
$$

# 1 Adjoint 1

Taking the derivative with respect to $\rho_a$ gives

$$
\begin{aligned}
\mathcal{L}_{\rho_a}(\rho_a,\rho_b,\mathbf{w},q_a,q_b)h =& \int_0^T\int_\Omega(\rho_a-\widehat{\rho_a})hdrdt+\int_0^T\int_\Omega\bigg(-\frac{\partial h}{\partial t}q_a+D_a\nabla^2hq_a-D_a\nabla\cdot(hF_a(\mathbf{w}))q_a\\
&+D_a\nabla\cdot(h\nabla V_{ext,a})q_a+D_a\kappa q_a\nabla\cdot\int_\Omega h(r)\rho_a(r')\mathbf{K}_{aa}(r,r')dr'\\
&+D_a\kappa q_a\nabla\cdot\int_\Omega\rho_a(r)h(r')\mathbf{K}_{aa}(r,r')dr'+D_a\tilde{\kappa}q_a\nabla\cdot\int_\Omega h(r)\rho_b(r')\mathbf{K}_{ab}(r,r')dr\\
&+D_b\tilde{\kappa}q_b\nabla\cdot\int_\Omega\rho_b(r)h(r')\mathbf{K}_{ba}(r,r')dr'\bigg)drdt\\
&-\int_0^T\int_{\partial\Omega}\bigg(D_a\nabla h-D_ahF_a(\mathbf{w})+D_ah\nabla V_{ext,a}+D_a\kappa\int_\Omega h(r)\rho_a(r')\mathbf{K}_{aa}(r,r')dr'\\
&+D_a\kappa\int_\Omega\rho_a(r)h(r')\mathbf{K}_{aa}(r,r')dr'+D_a\tilde{\kappa}\int_\Omega h(r)\rho_b(r')\mathbf{K}_{ab}(r,r')dr'\bigg)\cdot\mathbf{n}q_{a,\partial\Omega}drdt\\
&-\int_0^T\int_{\partial\Omega}D_b\tilde{\kappa}\int_\Omega\rho_b(r)h(r')\mathbf{K}_{ba}(r,r')dr'\cdot\mathbf{n}q_{b,\partial\Omega}drdt
\end{aligned}
$$

And so:

$$
\begin{aligned}
\mathcal{L}_{\rho_a}(\rho_a, \rho_b, \mathbf{w}, q_a, q_b)h = & \int_0^T \int_\Omega (\rho_a - \widehat{\rho_a}) h dr dt + \int_0^T \int_\Omega \Bigg( \frac{\partial q_a}{\partial t} h + D_a \nabla^2 q_a h + D_a \nabla q_a \cdot (h F_a(\mathbf{w})) \\
& - D_a \nabla q_a \cdot (h \nabla V_{ext,a}) - D_a \kappa \nabla q_a(r) h(r) \int_\Omega \rho_a(r') \mathbf{K}_{aa}(r, r') dr' \\
& - D_a \kappa h(r) \int_\Omega \nabla q_a(r') \rho_a(r') \mathbf{K}_{aa}(r', r) dr' - D_a \tilde{\kappa} \nabla q_a h(r) \int_\Omega \rho_b(r') \mathbf{K}_{ab}(r, r') dr \\
& - D_b \tilde{\kappa} h(r) \int_\Omega \nabla q_b(r') \rho_b(r') \mathbf{K}_{ba}(r', r) dr' \Bigg) dr dt \\
& + \int_\Omega q_a(T) h(T) - q_a(0) h(0) dr \\
& + \int_0^T \int_\Omega \Bigg( D_a \kappa h(r) \int_{\partial\Omega} q_a(r') \rho_a(r') \mathbf{K}_{aa}(r', r) dr' \cdot \mathbf{n} \\
& + D_b \tilde{\kappa} h(r) \int_{\partial\Omega} q_b(r') \rho_b(r') \mathbf{K}_{ba}(r', r) dr' \cdot \mathbf{n} \Bigg) dr dt \\
& + \int_0^T \int_{\partial\Omega} D_a \frac{\partial h}{\partial n} q_a - D_a \frac{\partial q_a}{\partial n} h - D_a F_a(\mathbf{w}) h q_a \cdot \mathbf{n} + D_a \nabla V_{ext,a} h q_a \cdot \mathbf{n} dr dt \\
& + \int_0^T \int_{\partial\Omega} \Bigg( D_a \kappa h(r) q_a(r) \int_\Omega \rho_a(r') \mathbf{K}_{aa}(r, r') \cdot \mathbf{n} dr' \\
& + D_a \tilde{\kappa} q_a(r) h(r) \int_\Omega \rho_b(r') \mathbf{K}_{ab}(r, r') \cdot \mathbf{n} dr' \Bigg) dr dt \\
& - \int_0^T \int_{\partial\Omega} \Bigg( D_a \nabla h q_{a,\partial\Omega} - D_a h F_a(\mathbf{w}) q_{a,\partial\Omega} + D_a h \nabla V_{ext,a} q_{a,\partial\Omega} \\
& + D_a \kappa q_{a,\partial\Omega}(r) h(r) \int_\Omega \rho_a(r') \mathbf{K}_{aa}(r, r') dr' + D_a \tilde{\kappa} q_{a,\partial\Omega} h(r) \int_\Omega \rho_b(r') \mathbf{K}_{ab}(r, r') dr' \Bigg) \cdot \mathbf{n} dr dt \\
& - \int_0^T \int_\Omega \Bigg( D_a \kappa h(r) \int_{\partial\Omega} q_{a,\partial\Omega}(r') \rho_a(r') \mathbf{K}_{aa}(r', r) dr' \\
& + D_b \tilde{\kappa} h(r) \int_\Omega q_{b,\partial\Omega}(r') \rho_b(r') \mathbf{K}_{ba}(r', r) dr' \Bigg) \cdot \mathbf{n} dr dt
\end{aligned}
$$

Then for $\frac{\partial h}{\partial n} \neq 0$ we get;

$$
\begin{aligned}
&(D_a q_a - D_a q_{a,\partial\Omega}) \mathbf{n} = \mathbf{0} \\
&q_a = q_{a,\partial\Omega}
\end{aligned}
$$

And all boundary terms cancel so that we get:

$$
\frac{\partial q_a}{\partial n} = 0 \quad \text{on} \quad \partial\Omega.
$$

And we also get $q_a(T) = 0$.

We get:

$$
\begin{aligned}
\frac{\partial q_a}{\partial t} =& - D_a \nabla^2 q_a - \rho_a + \widehat{\rho_a} - D_a \nabla q_a \cdot F_a(\mathbf{w}) + D_a \nabla q_a \cdot \nabla V_{ext,a} \\
&+ D_a \kappa \nabla q_a(r) \int_\Omega \rho_a(r') \mathbf{K}_{aa}(r, r') dr' + D_a \kappa \int_\Omega \nabla q_a(r') \rho_a(r') \mathbf{K}_{aa}(r', r) dr' \\
&+ D_a \tilde{\kappa} \nabla q_a(r) \int_\Omega \rho_b(r') \mathbf{K}_{ab}(r, r') dr' + D_b \tilde{\kappa} \int_\Omega \nabla q_b(r') \rho_b(r') \mathbf{K}_{ba}(r', r) dr'.
\end{aligned}
$$

## 2 Adjoint 2

The second adjoint equation is almost equivalent to the first:

$$
\begin{aligned}
\frac{\partial q_b}{\partial t} =& - D_b \nabla^2 q_b - \alpha \rho_b + \alpha \widehat{\rho_b} - D_b \nabla q_b \cdot F_b(\mathbf{w}) + D_b \nabla q_b \cdot \nabla V_{ext,b} \\
&+ D_b \kappa \nabla q_b(r) \int_\Omega \rho_b(r') \mathbf{K}_{bb}(r, r') dr' + D_b \kappa \int_\Omega \nabla q_b(r') \rho_b(r') \mathbf{K}_{bb}(r', r) dr' \\
&+ D_b \tilde{\kappa} \nabla q_b \int_\Omega \rho_a(r') \mathbf{K}_{ba}(r, r') dr' + D_a \tilde{\kappa} \int_\Omega \nabla q_a(r') \rho_a(r') \mathbf{K}_{ab}(r', r) dr'.
\end{aligned}
$$

And the boundary condition is:

$$
\frac{\partial q_b}{\partial n} = 0 \quad \text{on} \quad \partial \Omega.
$$

And we also get $q_b(T) = 0$.

## 3 Gradient Equation

We consider the derivative of the Lagrangian with respect to $\mathbf{w}$. However, we will need to consider the Frechét derivative of terms involving $F(\mathbf{w})$ first. From the definition from the Frechét derivative, we know that we have to consider the first order term of the Taylor expansion, so that we have:

$$
F(\mathbf{w} + \mathbf{h}) - F(\mathbf{w}) = \nabla F(\mathbf{w}) \cdot \mathbf{h}.
$$

However, this doesn't seem quite right. Consider from year end review: $F(\rho) = \nabla \ln(\rho)$. The resulting Frechét derivative was $\nabla(\frac{h}{\rho})$, which doesn't match with the above definition.