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:

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

1 Adjoint 1

Taking the derivative with respect to ρ_a gives

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

And so:

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

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

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

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:

$$
F(\mathbf{w} + \mathbf{h}) - F(\mathbf{w}) = F'(\mathbf{w}) \cdot \mathbf{h} = h_1 \frac{\partial}{\partial w_1} F(\mathbf{w}) + h_2 \frac{\partial}{\partial w_2} F(\mathbf{w}).
$$

This is only valid if F is a function of $\mathbf{w}$. If F is a function of the position r, we would need to work with the definition of the Frechét derivative. Assuming that the above holds we can do some further calculations:

$$
\begin{aligned}
\mathcal{L}_{\mathbf{w}}(\rho_a, \rho_b, \mathbf{w}, q_a, q_b)\mathbf{h} = &\int_0^T \int_\Omega \Big(\beta \mathbf{w} \cdot \mathbf{h} - D_a \nabla \cdot (\rho_a F_a'(\mathbf{w}) \cdot \mathbf{h}) q_a - D_b \nabla \cdot (\rho_b F_b'(\mathbf{w}) \cdot \mathbf{h}) q_b \Big) drdt \\
&+ \int_0^T \int_{\partial\Omega} \Big(D_a \rho_a q_{a,\partial\Omega} F_a'(\mathbf{w}) \cdot \mathbf{h} + D_b \rho_b q_{b,\partial\Omega} F_b'(\mathbf{w}) \cdot \mathbf{h} \Big) \cdot \mathbf{n} drdt \\
&= \int_0^T \int_\Omega \Big(\beta \mathbf{w} \cdot \mathbf{h} + D_a \nabla q_a \cdot (\rho_a F_a'(\mathbf{w}) \cdot \mathbf{h}) + D_b \nabla q_b \cdot (\rho_b F_b'(\mathbf{w}) \cdot \mathbf{h}) \Big) drdt \\
&- \int_0^T \int_{\partial\Omega} \Big(D_a \rho_a q_{a,\partial\Omega} F_a'(\mathbf{w}) \cdot \mathbf{h} + D_b \rho_b q_{b,\partial\Omega} F_b'(\mathbf{w}) \cdot \mathbf{h} \Big) \cdot \mathbf{n} drdt \\
&+ \int_0^T \int_{\partial\Omega} \Big(D_a \rho_a q_a F_a'(\mathbf{w}) \cdot \mathbf{h} + D_b \rho_b q_b F_b'(\mathbf{w}) \cdot \mathbf{h} \Big) \cdot \mathbf{n} drdt \\
&= \int_0^T \int_\Omega \Big(\beta \cdot \mathbf{w}\mathbf{h} + D_a \nabla q_a \cdot (\rho_a F_a'(\mathbf{w}) \cdot \mathbf{h}) + D_b \nabla q_b \cdot (\rho_b F_b'(\mathbf{w}) \cdot \mathbf{h}) \Big) drdt,
\end{aligned}
$$

since $q_a = q_{a,\partial\Omega}$ and $q_b = q_{b,\partial\Omega}$ from the adjoint derivation.
Since this holds for all permissible $\mathbf{h}$, we get:

$$\mathbf{w} = -\frac{1}{\beta} \Big(D_a \nabla q_a \cdot (\rho_a F_a'(\mathbf{w})) + D_b \nabla q_b \cdot (\rho_b F_b'(\mathbf{w})) \Big).$$

This we can only solve if we know about F_a and F_b (I guess technically I can't even write $F(\mathbf{h})$, maybe only if I assume F to be linear?). Assume $F_a(x) = c_a x$ and $F_b(x) = c_b x$, we get:

$$\mathbf{w} = \frac{1}{\beta} \Big(D_a c_a \rho_a \nabla q_a + D_b c_b \rho_b \nabla q_b \Big).$$