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 drdt + \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) 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_a F_a(\mathbf{w}) h q_a \cdot \mathbf{n} + D_a \nabla V_{ext,a} h q_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 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} 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;

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

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. If F is a function of $\mathbf{w}$ only and not of the position variable r, we can do the following. Otherwise, we will have to work with the definition of the Frechét derivative and derive the gradient equation like that. We consider the first order term of the Taylor expansion, so that we have:

$$F(\mathbf{w} + \mathbf{h}) - F(\mathbf{w}) = \left(\nabla_{\mathbf{w}} F(\mathbf{w})^T \right) \mathbf{h}$$

Then:

$$
\begin{aligned}
\mathcal{L}_{\mathbf{w}}(\rho_a,\rho_b,\mathbf{w},q_a,q_b)\mathbf{h} &= \int_0^T \int_\Omega \Big(\beta\mathbf{w}\cdot\mathbf{h} - D_a\nabla\cdot(\rho_a\left(\nabla_{\mathbf{w}}F_a(\mathbf{w})^T\right)\mathbf{h})q_a - D_b\nabla\cdot(\rho_b\left(\nabla_{\mathbf{w}}F_b(\mathbf{w})^T\right)\mathbf{h})q_b\Big)drdt \\
&+ \int_0^T \int_{\partial\Omega}\Big(D_a\rho_a\left(\nabla_{\mathbf{w}}F_a(\mathbf{w})^T\right)\mathbf{h}q_{a,\partial\Omega} + D_b\rho_b\left(\nabla_{\mathbf{w}}F_b(\mathbf{w})^T\right)\mathbf{h}q_{b,\partial\Omega}\Big)\cdot\mathbf{n}drdt \\
&= \int_0^T \int_\Omega \Big(\beta\mathbf{w}\cdot\mathbf{h} + D_a\rho_a\Big(\left(\nabla_{\mathbf{w}}F_a(\mathbf{w})^T\right)\mathbf{h}\Big)\cdot\nabla q_a \\
&+ D_b\rho_b\Big(\left(\nabla_{\mathbf{w}}F_b(\mathbf{w})^T\right)\mathbf{h}\Big)\cdot\nabla q_b\Big)drdt \\
&- \int_0^T \int_{\partial\Omega}\Big(D_a\rho_a\left(\nabla_{\mathbf{w}}F_a(\mathbf{w})^T\right)\mathbf{h}q_a + D_b\rho_b\left(\nabla_{\mathbf{w}}F_b(\mathbf{w})^T\right)\mathbf{h}q_b\Big)\cdot\mathbf{n}drdt \\
&+ \int_0^T \int_{\partial\Omega}\Big(D_a\rho_a\left(\nabla_{\mathbf{w}}F_a(\mathbf{w})^T\right)\mathbf{h}q_{a,\partial\Omega} + D_b\rho_b\left(\nabla_{\mathbf{w}}F_b(\mathbf{w})^T\right)\mathbf{h}q_{b,\partial\Omega}\Big)\cdot\mathbf{n}drdt \\
&= \int_0^T \int_\Omega \Big(\beta\mathbf{w}\cdot\mathbf{h} + D_a\rho_a\Big(\left(\nabla_{\mathbf{w}}F_a(\mathbf{w})^T\right)\mathbf{h}\Big)\cdot\nabla q_a \\
&+ D_b\rho_b\Big(\left(\nabla_{\mathbf{w}}F_b(\mathbf{w})^T\right)\mathbf{h}\Big)\cdot\nabla q_b\Big)drdt,
\end{aligned}
$$

since $q_a = q_{a,\partial\Omega}$ and $q_b = q_{b,\partial\Omega}$ from the adjoint derivation.
Now we use the relation $((\nabla\mathbf{a})^T)\mathbf{b})\cdot\mathbf{c} = ((\mathbf{c}\cdot\nabla)\mathbf{a})\cdot\mathbf{b}$ (from year end review) to find that:

$$
\begin{aligned}
\mathcal{L}_{\mathbf{w}}(\rho_a,\rho_b,\mathbf{w},q_a,q_b)\mathbf{h} = \int_0^T \int_\Omega \Big(&\beta\mathbf{w}\cdot\mathbf{h} + D_a\rho_a\left(\left(\nabla_r q_a\cdot\nabla_{\mathbf{w}}\right)F_a(\mathbf{w})\right)\cdot\mathbf{h} \\
&+ D_b\rho_b\left(\left(\nabla_r q_b\cdot\nabla_{\mathbf{w}}\right)F_b(\mathbf{w})\right)\cdot\mathbf{h}\Big)drdt,
\end{aligned}
$$

Setting this to zero and since this holds for all permissible $\mathbf{h}$, we get:

$$
\beta\mathbf{w} + D_a\rho_a\left(\left(\nabla_r q_a\cdot\nabla_{\mathbf{w}}\right)F_a(\mathbf{w})\right) + D_b\rho_b\left(\left(\nabla_r q_b\cdot\nabla_{\mathbf{w}}\right)F_b(\mathbf{w})\right) = 0.
$$

Using that $\nabla\cdot(\mathbf{b}\mathbf{a}^T) = \mathbf{a}(\nabla\cdot\mathbf{b}) + (\mathbf{b}\cdot\nabla)\mathbf{a}$, and observing that $\nabla_{\mathbf{w}}\cdot(\nabla_r q) = 0$, we get:

$$
\beta\mathbf{w} + D_a\rho_a\nabla_{\mathbf{w}}\cdot\left(\nabla q_a F_a(\mathbf{w})^T\right) + D_b\rho_b\nabla_{\mathbf{w}}\cdot\left(\nabla q_b F_b(\mathbf{w})^T\right) = 0.
$$

Since $\nabla_r q$ does not depend on $\mathbf{w}$ we can rearrange this to get:

$$
\beta\mathbf{w} + D_a\rho_a\left(\nabla_{\mathbf{w}}F_a(\mathbf{w})\right)^T\nabla q_a + D_b\rho_b\left(\nabla_{\mathbf{w}}F_b(\mathbf{w})\right)^T\nabla q_b = 0.
$$

And finally we have:

$$
\mathbf{w} = -\frac{1}{\beta}\left(D_a\rho_a\left(\nabla_{\mathbf{w}}F_a(\mathbf{w})\right)^T\nabla q_a + D_b\rho_b\left(\nabla_{\mathbf{w}}F_b(\mathbf{w})\right)^T\nabla q_b\right).
$$

As an example, take $F_a(\mathbf{w}) = c_a\mathbf{w}$ and $F_b(\mathbf{w}) = c_b\mathbf{w}$. We get:

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