

Optimality Conditions for Two Species

We have the following set of forward equations:

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

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

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

The cost functional is:

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

The Lagrangian is then:

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

1 Adjoint 1

Taking the derivative with respect to ρ_a gives

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

And so:

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

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

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

$$q_a = q_{a,\partial\Omega}$$

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:

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

2 Adjoint 2

The second adjoint equation is equivalent to the first:

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

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

The derivative of the Lagrangian with respect to \mathbf{w} is:

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

since $q_a = q_{a, \partial\Omega}$ and $q_b = q_{b, \partial\Omega}$ from the adjoint derivation.

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:

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