1 Mann Iteration

Implemented the Mann iteration from the paper. The problem is that λ decreases with iterations so it's not really adaptive in the way we'd like it to be.

```
function res = AdaSolver4(wIn,wOut,wErr, wErrN, AbsErr,lambda, k, R

    p = 2;
    G = 10;

    A = p*k*(((k/G)*(R/AbsErr)).^(1/(p-1)));

    b1 = (1/(2*A))*(-1 + sqrt(1+4*A));
    b2 = (1/(2*A))*(-1 - sqrt(1+4*A));
    if b1 > 0
        b = b1;
    elseif b2 > 0
        b = b2;
    end

    lambda = (1/(p*k))*((1-b)/b);
    R = ((1/p) + (1-(1/p))*b)*R;

    wIn = (1-lambda)*wIn + lambda*wOut;

    k = k+1;
    res.R = R;
    res.k = k;
    res.lambda = lambda;
    res.wErr = wErr;
    res.wIn = wIn;
end
```

Figure 1: Mann Iteration

2 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:

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

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:

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

3 Adjoint 1

Taking the derivative with respect to ρ_a gives

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

And so:

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

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:

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

4 Adjoint 2

The second adjoint equation is equivalent to the first:

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

And the boundary condition is:

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

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

5 Gradient Equation

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

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

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:

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

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:

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

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:

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

6 Adjoint 1

Taking the derivative with respect to ρ_a gives

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

And so:

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

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:

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

7 Adjoint 2

The second adjoint equation is equivalent to the first:

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

And the boundary condition is:

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

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

8 Gradient Equation

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

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

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:

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

Additional Note

If we choose the problem to be:

$$J(\rho, \mathbf{w}) \coloneqq \frac{1}{2}||\rho - \widehat{\rho}||^2_{L_2(\Sigma)} + \frac{\beta}{2}||\kappa||^2_{L_2(\Sigma)}$$

subject to:

$$\frac{\partial \rho}{\partial t} = \nabla^2 \rho - \nabla \cdot (\rho \mathbf{w}) + D_a \nabla \cdot (\rho \nabla V_{ext}) + \kappa \nabla \cdot \int_\Omega \rho(r)\rho(r')\mathbf{K}(r, r')dr',$$

then the only thing that changes in our normal derivation is the gradient equation. This becomes:

$$\kappa = -\frac{1}{\beta}\nabla \int_\Omega \rho(r)\rho(r')\mathbf{K}(r, r')dr'.$$

However, I don't think we can make $\mathbf{K}$ the control (as I thought was possible) because we get:

$$\mathcal{L}_{\mathbf{K}}(\rho, \mathbf{K})h = \int_0^T \int_\Omega \left(\beta \mathbf{K}(r, r') \cdot \mathbf{h}(r, r') + \nabla \int_\Omega \rho(r)\rho(r')\mathbf{h}(r, r')dr'\right) dr dt,$$

for this setup:

$$J(\rho, \mathbf{w}) \coloneqq \frac{1}{2}||\rho - \widehat{\rho}||^2_{L_2(\Sigma)} + \frac{\beta}{2}||\mathbf{K}||^2_{L_2(\Sigma)}$$

subject to:

$$\frac{\partial \rho}{\partial t} = \nabla^2 \rho - \nabla \cdot (\rho \mathbf{w}) + D_a \nabla \cdot (\rho \nabla V_{ext}) + \kappa \nabla \cdot \int_\Omega \rho(r)\rho(r')\mathbf{K}(r, r')dr'.$$

Other

- DDFT background flow. I am not sure I am looking for the right thing. Poiseuille flow?