+++++++++++++++Replace chapters with those from thesis ++++++++++

1 Introduction

At the point of the second year review, a good point was reached to develop both the models and the numerical methods further towards eventual industrial applications. At first, the implementation of the inertial equations, which were derived in the second year report, has been completed, and a few representative 1D examples were developed.

A large part of the efforts during this year has been put into the development of the 'Multi-Shape' implementation for PDE-constrained optimization problems. This is a spectral element method, which can be seen as an extension to the pseudospectral methods we have been using throughout this work.
This extension has been applied to problems

2 Inertial Equations Examples

++ Omitted?? ++

3 Multiple Species (tbc) Optimality Conditions

In this section we are interested in deriving the optimality conditions for two species, which are interacting through a non-local interaction term. 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 $D = \frac{1}{\gamma m}$. The interaction kernel $\mathbf{K}_{ij}$ are describing the effect of species i on species j. The function F_i describes a function of the control, which may be different for species $i = a$ and $i = b$. This generalization allows for effects such as that species a gets advected faster than species b, for example, due to size differences. We have the interaction strength κ, describing the effects within the species and the interaction strength $\tilde{\kappa}$, describing interaction strengths between species. The 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:

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

Therefore, the Lagrangian is:

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

3.1 Adjoint 1

Taking the derivative with respect to ρ_a gives

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

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 \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:

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

3.2 Adjoint 2

The second adjoint equation is derived in an equivalent manner to the first:

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

The boundary condition is:

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

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

3.3 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 second year 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:

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

4 Multishape Implementation

4.1 Validation of the different operators

4.2 Numerical Examples

4.2.1 Flow around Constriction

5 Derivation of Optimality Conditions with Periodic Boundary Conditions

+++++ Change notation for j ++++++ We consider the advection diffusion equation with periodic boundary conditions and a corresponding OCP:

$$\begin{aligned}
&\min \frac{1}{2}||\rho - \widehat{\rho}||^2 + \frac{\beta}{2}||\mathbf{w}||^2 \\
&\text{subject to:} \\
&\frac{\partial \rho}{\partial t} = \nabla \cdot (\nabla \rho - \rho \mathbf{w}) = -\nabla \cdot \mathbf{j} \\
&\rho|_{\partial \Omega_l} = \rho|_{\partial \Omega_r} \\
&\rho|_{\partial \Omega_t} = \rho|_{\partial \Omega_b} \\
&-\mathbf{j} \cdot \mathbf{n}|_{\partial \Omega_l} = -\mathbf{j} \cdot \mathbf{n}|_{\partial \Omega_r}
\end{aligned}$$

such that $\partial\Omega_l \cup \partial\Omega_r = \partial\Omega$ and the abbreviations corresponding to left and right respectively. Top and bottom boundaries are omitted, since, as shown in the previous section, they follow analogously and are independent of the results on the left and right boundary. Note that we could match first derivatives instead of the flux on the boundary. The relevant part of the Lagrangian is then:

$$\mathcal{L} = ... - \int_0^T \int_\Omega \left(\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} \right) q dr dt - \int_0^T \int_{\partial \Omega_l} (-\rho q_1 - \mathbf{j} \cdot \mathbf{n} q_2)\, dr + \int_{\partial \Omega_r} (\rho q_1 + \mathbf{j} \cdot \mathbf{n} q_2)\, dr.$$

Integrating by parts, and omitting terms in Ω, gives:

$$\mathcal{L} = ... - \int_0^T \int_{\partial \Omega} q \mathbf{j} \cdot \mathbf{n} + \mathbf{k}(\rho, q) \cdot \mathbf{n} dr dt - \int_0^T \int_{\partial \Omega_l} (-\rho q_1 - \mathbf{j} \cdot \mathbf{n} q_2)\, dr + \int_{\partial \Omega_r} (\rho q_1 + \mathbf{j} \cdot \mathbf{n} q_2)\, dr,$$

where $\mathbf{k}$ are any terms arising from integrating by parts a second time. We now need to take the Frechét derivative of $\mathbf{j}$ with respect to ρ. This cannot be done in general, because $\mathbf{j}$ does not only depend on ρ but also on $\mathbf{r}$. In each case we need to calculate:

$$\mathbf{j}'(h) := \mathbf{j}(\rho + h) - \mathbf{j}(\rho).$$

Similarly, we need to take the derivative of $\mathbf{k}$ and denote it by $\mathbf{k}'$. Denoting this Frechét derivative by $\mathbf{j}'(h)$ we can write out further terms as follows:

$$\mathcal{L}_\rho = ... - \int_0^T \int_{\partial\Omega} q\mathbf{j}'(h)\cdot\mathbf{n} + \mathbf{k}'\cdot\mathbf{n} drdt - \int_0^T \int_{\partial\Omega_l} \left(-hq_1 - \mathbf{j}'(h)\cdot\mathbf{n}q_2\right) dr + \int_{\partial\Omega_r} \left(hq_1 + \mathbf{j}'(h)\cdot\mathbf{n}q_2\right) drdt.$$

When writing out the terms explicitly we pay attention to the fact that $\mathbf{n}|_{\partial\Omega_l} = -\mathbf{n}|_{\partial\Omega_r}$ and $\mathbf{n}|_{\partial\Omega_t} = -\mathbf{n}|_{\partial\Omega_b}$.

$$\begin{aligned}\mathcal{L}_\rho = ... - \int_0^T \int_{\partial\Omega_l} &\left(-hq_1 + q\mathbf{j}'(h)\cdot\mathbf{n} + \mathbf{k}'\cdot\mathbf{n} - \mathbf{j}'(h)\cdot\mathbf{n}q_2\right) dr \\ + \int_{\partial\Omega_r} &\left(hq_1 - q\mathbf{j}'(h)\cdot\mathbf{n} - \mathbf{k}'\cdot\mathbf{n} + \mathbf{j}'(h)\cdot\mathbf{n}q_2\right) drdt.\end{aligned}$$

In order to proceed further, we need to split up $\mathbf{j}'(h)$ into two parts as follows:

$$\mathbf{j}'(h) = \mathbf{j}'_1(h) + h\mathbf{j}'_2,$$

so that $\mathbf{j}'_1$ is applied to h, since it depends on $\mathbf{r}$ as well (e.g. the Frechét derivative of $\nabla\rho$) and $\mathbf{j}'_2$ is applied to another function and multiplied by h (e.g. h $\frac{\partial}{\partial n}$ applied to q). We do the same for $\mathbf{k}'$. We then have:

$$\begin{aligned}\mathcal{L}_\rho = ... - \int_0^T \int_{\partial\Omega_l} &\left(-hq_1 + q\mathbf{j}'_1(h)\cdot\mathbf{n} + \mathbf{k}'_1\cdot\mathbf{n} - \mathbf{j}'_1(h)\cdot\mathbf{n}q_2 + h\mathbf{j}'_2 q\cdot\mathbf{n} + h\mathbf{k}'_2\cdot\mathbf{n} - h\mathbf{j}'_2 q_2\cdot\mathbf{n}\right) dr \\ + \int_{\partial\Omega_r} &\left(hq_1 - q\mathbf{j}'_1(h)\cdot\mathbf{n} - \mathbf{k}'_1\cdot\mathbf{n} + \mathbf{j}'_1(h)\cdot\mathbf{n}q_2 - h\mathbf{k}'_2\cdot\mathbf{n} - h\mathbf{j}'_2 q\cdot\mathbf{n} + h\mathbf{j}'_2 q_2\cdot\mathbf{n}\right) drdt.\end{aligned}$$

Considering $\mathbf{j}'_1 \neq 0$, we get:

$$\int_0^T \int_{\partial\Omega_l} \left(q\mathbf{j}'_1(h)\cdot\mathbf{n} + \mathbf{k}'_1\cdot\mathbf{n} - \mathbf{j}'_1(h)\cdot\mathbf{n}q_2\right) dr + \int_{\partial\Omega_r} \left(-q\mathbf{j}'_1(h)\cdot\mathbf{n} - \mathbf{k}'_1\cdot\mathbf{n} + \mathbf{j}'_1(h)\cdot\mathbf{n}q_2\right) drdt = 0.$$

Note that if $\mathbf{k}'_1 = 0$, we can conclude that $q = q_2$ on both boundaries. In general, $q_2|_{\partial\Omega_l} = q_2|_{\partial\Omega_r}$, i.e. q_2 is constant on the boundary, and an equivalent statement holds for q_1. Therefore, we have that:

$$\int_0^T \int_{\partial\Omega_l} q\mathbf{j}'_1(h)\cdot\mathbf{n} + \mathbf{k}'_1\cdot\mathbf{n} drdt = \int_0^T \int_{\partial\Omega_r} q\mathbf{j}'_1(h)\cdot\mathbf{n} + \mathbf{k}'_1\cdot\mathbf{n} drdt.$$

Writing this in terms of the integrand only can be done for each specific case of $\mathbf{j}'_1$ and $\mathbf{k}'_1$. Now considering all terms such that $h \neq 0$ on each boundary separately, we get:

$$\begin{aligned}&\int_0^T \int_{\partial\Omega_l} \left(-hq_1 + h\mathbf{j}'_2 q\cdot\mathbf{n} + h\mathbf{k}'_2\cdot\mathbf{n} - h\mathbf{j}'_2 q_2\cdot\mathbf{n}\right) drdt = 0 \\ &\int_0^T \int_{\partial\Omega_r} \left(hq_1 - h\mathbf{j}'_2 q\cdot\mathbf{n} - h\mathbf{k}'_2\cdot\mathbf{n} + h\mathbf{j}'_2 q_2\cdot\mathbf{n}\right) drdt = 0,\end{aligned}$$

and so, as in the previous sections, we have:

$$q_1 = \mathbf{j}_2' q \cdot \mathbf{n} + \mathbf{k}_2' \cdot \mathbf{n} - \mathbf{j}_2' q_2 \cdot \mathbf{n}|_{\partial\Omega_l}$$
$$q_1 = \mathbf{j}_2' q \cdot \mathbf{n} + \mathbf{k}_2' \cdot \mathbf{n} - \mathbf{j}_2' q_2 \cdot \mathbf{n}|_{\partial\Omega_r},$$

which gives:

$$\mathbf{j}_2' q \cdot \mathbf{n} + \mathbf{k}_2' \cdot \mathbf{n} - \mathbf{j}_2' q_2 \cdot \mathbf{n}|_{\partial\Omega_l} = \mathbf{j}_2' q \cdot \mathbf{n} + \mathbf{k}_2' \cdot \mathbf{n} - \mathbf{j}_2' q_2 \cdot \mathbf{n}|_{\partial\Omega_r}.$$

If $\mathbf{k}_1' = 0$ and so $q = q_2$ as discussed above, the two terms involving $\mathbf{j}_2'$ cancel and we get

$$\mathbf{k}_2' \cdot \mathbf{n}|_{\partial\Omega_l} = \mathbf{k}_2' \cdot \mathbf{n}|_{\partial\Omega_r}.$$

Otherwise, since $q_2|_{\partial\Omega_l} = q_2|_{\partial\Omega_r}$, we can at least conclude that:

$$\mathbf{j}_2' q \cdot \mathbf{n} + \mathbf{k}_2' \cdot \mathbf{n}|_{\partial\Omega_l} = \mathbf{j}_2' q \cdot \mathbf{n} + \mathbf{k}_2' \cdot \mathbf{n}|_{\partial\Omega_r}.$$

An example: Let $\mathbf{j} = \nabla\rho - \rho\mathbf{w}$ as above. Then we have that $\mathbf{j}_1'(h) = \nabla h$ and $\mathbf{j}_2' = \mathbf{w}$. From integration by parts we will get that $\mathbf{k} = -\rho\nabla q$, so $\mathbf{k}_1' = 0$ and $\mathbf{k}_2' = -\nabla q$. We therefore get that:

$$\nabla q \cdot \mathbf{n}|_{\partial\Omega_l} = \nabla q \cdot \mathbf{n}|_{\partial\Omega_r},$$

and

$$\int_0^T \int_{\partial\Omega_l} q\nabla h \cdot \mathbf{n} dr dt = \int_0^T \int_{\partial\Omega_r} q\nabla h \cdot \mathbf{n} dr dt,$$

and so

$$q|_{\partial\Omega_l} = q|_{\partial\Omega_r},$$

as required.

6 Sedimentation

6.1 Forward Problem

We are interested in modelling sedimentation processes. In order to achieve this, the advection-diffusion equation with mean-field interaction term has to be modified to include an approximation to volume exclusion. Archer and Malijevský [1] have achieved this using the following model to describe sedimentation processes. The modelling equations are:

$$\frac{\partial\rho}{\partial t^*} = \Gamma\nabla \cdot \left(\rho\nabla\frac{\delta F[\rho]}{\delta\rho}\right),$$

where Γ is the diffusion coefficient. We can rescale this equation as done in [1] using the relationship $t = t^*/\tau_B$, where $\tau_B = \beta\sigma^2/\Gamma$ is the Brownian time scale. Applying this rescaling we get:

$$\frac{\partial \rho}{\partial t} = \beta\sigma^2 \nabla \cdot \left(\rho \nabla \frac{\delta F[\rho]}{\delta \rho}\right). \tag{1}$$

The free energy functional considered in [1] is:

$$F[\rho] = \frac{1}{\beta}\int \rho(\ln \Lambda^2\rho - 1) + f_{HDA}dr + \frac{1}{2}\int\int \rho(r)\rho(r')V_2(|r - r'|)drdr' + \int \rho V_{ext}dr,$$

where f_{HDA} the approximate free energy density describing the volume exclusion through hard disks. The external potential is defined as:

$$V_{ext} = cy, \quad \text{for} \quad 0 < y < L,$$

where c a constant and L is the height of a rectangular domain. Outside these bounds $V_{ext} = \infty$. Furthermore, we have the pair potential:

$$V_2 = exp(-r/\sigma),$$

where σ is the particle diameter of the hard sphere particle.

6.2 The Hard Disk Approximation

The part of the free energy functional, which accounts for the hard disk approximation, is:

$$F_{HDA}[\rho] = \frac{1}{\beta}\int f_{HDA}dr = \frac{1}{\beta}\int -\rho - \rho\ln(1-\eta) + \frac{\rho}{1-\eta}dr,$$

where $\eta = a\rho = \frac{\pi\sigma^2}{4}\rho$. This can be thought of as the bulk fluid, one species, two dimensional approximation of Fundamental Measure Theory (FMT) [2], which is a Density Functional Theory for hard sphere mixtures. The basis of this theory is that the excess free energy functional is of the form:

$$\beta F_{ex}[\rho_i] = \int \Phi(n_\alpha(r'))d^3r',$$

where i is the species count and Φ is a function of the weighted densities n_α. By now there are many different versions of Φ, yielding approximations of F_{ex} with different limitations, see [3]. Rosenfeld's original version is defined as:

$$\Phi = -n_0\ln(1-n_3) + \frac{n_1n_2 - \mathbf{n_1}\cdot\mathbf{n_2}}{1-n_3} + \frac{n_2^3 - 3n_2\mathbf{n_2}\cdot\mathbf{n_2}}{24\pi(1-n_3)^2}.$$

The weighted densities for ν species are:

$$n_\alpha(r) = \sum_{i=1}^{\nu} \int \rho_i(r')\omega_\alpha^i(r - r'). \tag{2}$$

The weight functions chosen by Rosenfeld are:

$$\omega_3^i = \Theta(R_i - r), \quad \omega_2^i = \delta(R_i - r), \quad \omega_{\mathbf{2}}^{\mathbf{i}} = \frac{\mathbf{r}}{r}\delta(R_i - r),$$
$$\omega_1^i = \omega_2^i/(4\pi R_i), \quad \omega_0^i = \omega_2^i/(4\pi R_i^2), \quad \omega_{\mathbf{1}}^{\mathbf{i}} = \omega_{\mathbf{2}}^{\mathbf{i}}/(4\pi R_i),$$

where R_i is the radius of the excluded volume, Θ is the Heaviside function and δ is the delta function. Integrating over ω_α, with $\alpha = 0, 1, 2, 3$, we get the fundamental measures of a sphere: volume, surface area, radius and the Euler characteristic [3] [2].

Based on this theory for three dimensional spheres and the fact that the theory for hard rods is known exactly [4], Rosenfeld derived a version of this approach for two dimensional hard disks [5]. However, some additional approximations have to be made when choosing the weighted densities, which is not necessary in one and three dimensions. The resulting equation is:

$$\Phi = -n_0 \ln(1 - n_3) + \frac{1}{4\pi}\frac{n_2 n_2}{1 - n_3} + \frac{1}{4\pi}\frac{\mathbf{n_2} \cdot \mathbf{n_2}}{1 - n_3}.$$

In the uniform limit, for one particle species, we get that:

$$n_0 = \rho, \quad n_2 = 2\pi R\rho, \quad n_3 = \pi R^2 \rho,$$

by solving the integrals in (2), using spherical polar coordinates, with $\rho = \rho_{\text{bulk}}$, a constant. Substituting this in the 2D version of Φ gives:

$$\Phi = -\rho \ln(1 - \pi R^2 \rho) + \frac{1}{4\pi}\frac{4\pi^2 R^2 \rho^2}{1 - \pi R^2 \rho} + \frac{1}{4\pi}\frac{\mathbf{n_2} \cdot \mathbf{n_2}}{1 - \pi R^2 \rho},$$

where $\mathbf{n_2} = \mathbf{0}$ in the uniform limit, since the corresponding equation in (2) is an integral over an odd function. Noting that $R = \sigma/2$ and $\eta = \pi\sigma^2\rho/4$, we get that:

$$\Phi = -\rho \ln(1 - \eta) + \frac{\rho\eta}{1 - \eta} = \rho\left(-\ln(1 - \eta) + \frac{1}{1 - \eta} - 1\right). \tag{3}$$

This expression for the free energy for the bulk fluid is the same as derived by scaled particle theory (SPT) [6], [7], [8], which also coincides with the Percus-Yevic compressibility equation [9], as detailed in [10]. While the SPT approximation (3) and its three-dimensional equivalent are used in classical DFT, see [11], [12], [13], [14], [15], [16], and other statistical mechanics approaches, see [17], [18], [19], [20], in dynamical DFT it is not commonly applied and only the work of Archer et al. [1], [21], [22], [23], is known to us in this context.

6.3 Deriving the equation of motion

Since we are interested in the equation of motion, we need to calculate $\nabla \cdot \left(\rho \nabla \frac{\delta F_{HDA}[\rho]}{\delta \rho}\right)$. We combine F_{HDA} and $F_{ID} = \int_\Omega \rho(\ln \Lambda^2 \rho - 1) dr$ here so that we have:

$$F_N = F_{HDA} + F_{ID}.$$

Taking the functional derivative of F_N gives:

$$\begin{aligned}
\frac{\delta F_N[\rho]}{\delta \rho} &= \frac{1}{\beta}\left(1 + \ln \rho + \Lambda^2 - 2 - \ln(1-\eta) + a\frac{\rho}{1-\eta} + \frac{1}{1-\eta} + a\frac{\rho}{(1-\eta)^2}\right) \\
&= \frac{1}{\beta}\left(1 + \ln \rho + \Lambda^2 - 2 - \ln(1-\eta) + \frac{1}{(\eta-1)^2} - \frac{1}{\eta-1} - 1\right) \\
&= \frac{1}{\beta}\left(\ln \rho + \Lambda^2 - 2 - \ln(1-\eta) - \frac{\eta-2}{(\eta-1)^2}\right),
\end{aligned}$$

using partial fractions. Then:

$$\begin{aligned}
\nabla \frac{\delta F_N[\rho]}{\delta \rho} &= \frac{1}{\beta}\left(\nabla \ln \rho + \nabla(\Lambda^2 - 2) - \nabla \ln(1-\eta) - \nabla \frac{\eta-2}{(\eta-1)^2}\right) \\
&= \frac{1}{\beta}\left(\frac{\nabla \rho}{\rho} - \frac{\nabla(1-\eta)}{1-\eta} - \nabla \frac{\eta-2}{(\eta-1)^2}\right) \\
&= \frac{1}{\beta}\left(\frac{\nabla \rho}{\rho} + \frac{\nabla \eta}{1-\eta} - \nabla \frac{\eta-2}{(\eta-1)^2}\right).
\end{aligned}$$

Then multiplying by ρ gives:

$$\begin{aligned}
\rho \nabla \frac{\delta F_N[\rho]}{\delta \rho} &= \frac{1}{\beta}\left(\nabla \rho + \frac{\rho \nabla \eta}{1-\eta} - \rho \nabla \frac{\eta-2}{(\eta-1)^2}\right) \\
&= \frac{1}{\beta}\left(\nabla \rho + \frac{\eta \nabla \rho}{1-\eta} - \rho \nabla \frac{\eta-2}{(\eta-1)^2}\right) \\
&= \frac{1}{\beta}\left(\nabla \rho + \frac{\nabla \rho}{1-\eta} - \nabla \rho - \rho \nabla \frac{\eta-2}{(\eta-1)^2}\right) \\
&= \frac{1}{\beta}\left(\frac{\nabla \rho}{1-\eta} - \rho \nabla \frac{\eta-2}{(\eta-1)^2}\right).
\end{aligned}$$

Finally we take the divergence:

$$\begin{aligned}
\nabla \cdot \left(\rho \nabla \frac{\delta F_N[\rho]}{\delta \rho}\right) &= \frac{1}{\beta}\left(\nabla \cdot \left(\frac{\nabla \rho}{1-\eta}\right) - \nabla \cdot \left(\rho \nabla \frac{\eta-2}{(\eta-1)^2}\right)\right) \\
&= \frac{1}{\beta}\left(\frac{\nabla^2 \rho}{1-\eta} + \nabla \rho \cdot \nabla \frac{1}{1-\eta} - \nabla \rho \cdot \nabla \frac{\eta-2}{(\eta-1)^2} - \rho \nabla^2 \frac{\eta-2}{(\eta-1)^2}\right) \\
&= \frac{1}{\beta}\left(\frac{\nabla^2 \rho}{1-\eta} + \nabla \rho \cdot \nabla \frac{(3-2\eta)}{(1-\eta)^2} - \rho \nabla^2 \frac{\eta-2}{(\eta-1)^2}\right).
\end{aligned}$$

6.4 Derivation of Optimality Conditions

One optimal control problem to consider is:

$$
\begin{aligned}
&J = \frac{1}{2}\int_0^T \int_\Omega (\rho - \widehat{\rho})^2 dr dt + \frac{\beta}{2}\int_0^T \int_\Omega \mathbf{w}(r)^2 dr \\
&\text{subject to:} \\
&\frac{\partial \rho}{\partial t} = \beta\sigma^2\Bigg(\nabla\cdot(\rho\nabla V_{ext}) - \nabla(\rho\mathbf{w}) + \nabla\cdot\left(\rho\nabla\frac{\delta F_N[\rho]}{\delta\rho}\right) + \kappa\int_\Omega \rho(r)\rho(r')\mathbf{K}(r,r')dr\Bigg),
\end{aligned}
\tag{4}
$$

where $\mathbf{K}(r,r') = \nabla V_2$. We consider the terms of the PDE and the boundary conditions separately here.

6.4.1 Calculating Frechét Derivatives

In order to derive the optimalty conditions for the above OCP, we need to calculate the Frechét derivatives of the following terms:

$$
\nabla\cdot\left(\rho\nabla\frac{\delta F_N[\rho]}{\delta\rho}\right) = \frac{1}{\beta}\left(\frac{\nabla^2\rho}{1-\eta} + \nabla\rho\cdot\nabla\frac{(3-2\eta)}{(1-\eta)^2} - \rho\nabla^2\frac{\eta-2}{(\eta-1)^2}\right),
$$

where $\eta = a\rho$ and $a = \pi\sigma^2/4$. Consider:

$$
\begin{aligned}
F_1(\rho) &= \nabla^2\rho\frac{1}{1-a\rho}, \\
F_2(\rho) &= \nabla\rho\cdot\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right), \\
F_3(\rho) &= \rho\nabla^2\left(\frac{a\rho-2}{(a\rho-1)^2}\right).
\end{aligned}
$$

Then

$$
F_1(\rho+h) - F_1(\rho) = \nabla(\rho+h)\frac{1}{1-a(\rho+h)} - \nabla\rho\frac{1}{1-a\rho}.
$$

Using the expansion:

$$
\frac{1}{c-x} = \frac{1}{c} + \frac{1}{c^2}x + O(x^2),
$$

where $c = 1 - a\rho$, we get:

$$
\begin{aligned}
F_1(\rho+h) - F_1(\rho) &= \nabla^2(\rho+h)\left(\frac{1}{1-a\rho} + \frac{a}{(1-a\rho)^2}h\right) - \nabla^2\rho\frac{1}{1-a\rho} \\
&= \nabla^2 h\left(\frac{1}{1-a\rho}\right) + \nabla^2\rho\left(\frac{a}{(1-a\rho)^2}h\right),
\end{aligned}
$$

not considering higher order terms of h. For F_2 we consider the expansion:

$$
\frac{1}{(c-x)^2} = \frac{1}{c^2} + \frac{2}{c^3}x + O(x^2),
$$

and get:

$$
\begin{aligned}
F_2(\rho+h)-F_2(\rho) &= \nabla(\rho+h)\cdot\nabla\left(\frac{3-2a(\rho+h)}{(1-a(\rho+h))^2}\right)-\nabla\rho\cdot\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right)\\
&= \nabla(\rho+h)\cdot\nabla\left(\frac{3-2a(\rho+h)}{(1-a\rho)^2}+\frac{3-2a(\rho+h)}{(1-a\rho)^3}2ah\right)-\nabla\rho\cdot\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right)\\
&= \nabla h\cdot\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right)+\nabla\rho\cdot\nabla\left(h\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right)\right)\\
&= \nabla h\cdot\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right)+(\nabla h\cdot\nabla\rho)\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right)\\
&+h\nabla\rho\cdot\nabla\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right).
\end{aligned}
$$

Finally, we have:

$$
\begin{aligned}
F_3(\rho+h)-F_3(\rho) &= (\rho+h)\nabla^2\left(\frac{a(\rho+h)-2}{(a(\rho+h)-1)^2}\right)-\rho\nabla^2\left(\frac{a\rho-2}{(a\rho-1)^2}\right)\\
&= (\rho+h)\nabla^2\left(\frac{a(\rho+h)-2}{(1-a\rho)^2}+\frac{a(\rho+h)-2}{(1-a\rho)^3}2ah\right)-\rho\nabla^2\left(\frac{a\rho-2}{(a\rho-1)^2}\right)\\
&= h\nabla^2\left(\frac{a\rho-2}{(a\rho-1)^2}\right)+\rho\nabla^2\left(h\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\right)\\
&= h\nabla^2\left(\frac{a\rho-2}{(a\rho-1)^2}\right)+\rho\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\nabla^2 h\\
&+2\rho\nabla\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\cdot\nabla h+\rho h\nabla^2\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right).
\end{aligned}
$$

6.4.2 Adjoint Equation

In order to derive the adjoint equation, we need to consider the Lagrangian of the above OCP and take the derivative with respect to ρ. Given that most of the analysis has been done in a different chapter, we only consider the terms derived from F_N. The Frechét derivatives of the relevant terms have been taken and are combined to give:

$$
\begin{aligned}
\mathcal{L}_\rho(\rho,\mathbf{w},q)h = \ldots - \frac{1}{\beta}\int_0^T\int_\Omega & q\nabla^2 h\left(\frac{1}{1-a\rho}\right) + q\nabla^2\rho\left(\frac{a}{(1-a\rho)^2}h\right) \\
& + q\nabla h\cdot\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right) + q\left(\nabla h\cdot\nabla\rho\right)\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right) \\
& + qh\nabla\rho\cdot\nabla\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right) \\
& - qh\nabla^2\left(\frac{a\rho-2}{(a\rho-1)^2}\right) - q\rho\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\nabla^2 h \\
& - q\rho\nabla\left(\frac{2a}{(1-a\rho)^2}+\frac{4a^2\rho-8a}{(1-a\rho)^3}\right)\cdot\nabla h - q\rho h\nabla^2\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right).
\end{aligned}
$$

Rearranging gives:

$$
\begin{aligned}
\mathcal{L}_\rho(\rho,\mathbf{w},q)h = \ldots - \frac{1}{\beta}\int_0^T\int_\Omega & h\Bigg(q\nabla^2\rho\left(\frac{a}{(1-a\rho)^2}\right) + q\nabla\rho\cdot\nabla\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right) - q\nabla^2\left(\frac{a\rho-2}{(a\rho-1)^2}\right) \\
& - q\rho\nabla^2\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\Bigg) \\
& + \nabla h\cdot\Bigg(q\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right) + q\nabla\rho\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right) - q\rho\nabla\left(\frac{2a}{(1-a\rho)^2}+\frac{4a^2\rho-8a}{(1-a\rho)^3}\right)\Bigg) \\
& + \nabla^2 h\Bigg(q\left(\frac{1}{1-a\rho}\right) - q\rho\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\Bigg).
\end{aligned}
$$

Integration by parts gives:

$$
\begin{aligned}
\mathcal{L}_\rho(\rho,\mathbf{w},q)h = \ldots - \frac{1}{\beta}\int_0^T\int_\Omega & h\Bigg(q\nabla^2\rho\left(\frac{a}{(1-a\rho)^2}\right) + q\nabla\rho\cdot\nabla\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right) - q\nabla^2\left(\frac{a\rho-2}{(a\rho-1)^2}\right) \\
& - q\rho\nabla^2\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\Bigg) \\
& - h\nabla\Bigg(q\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right) + q\nabla\rho\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right) - q\rho\nabla\left(\frac{2a}{(1-a\rho)^2}+\frac{4a^2\rho-8a}{(1-a\rho)^3}\right)\Bigg) \\
& + h\nabla^2\Bigg(q\left(\frac{1}{1-a\rho}\right) - q\rho\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\Bigg).
\end{aligned}
$$

So we have:

$$
\begin{aligned}
\mathcal{L}_\rho(\rho,\mathbf{w},q)h = ... - \frac{1}{\beta}\int_0^T\int_\Omega h\bigg[& q\nabla^2\rho\left(\frac{a}{(1-a\rho)^2}\right) + q\nabla\rho\cdot\nabla\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right) - q\nabla^2\left(\frac{a\rho-2}{(a\rho-1)^2}\right) \\
& - q\rho\nabla^2\left(\frac{a}{(1-a\rho)^2}\right) - q\rho\nabla^2\left(\frac{2a^2\rho-4a}{(1-a\rho)^3}\right) \\
& - \nabla\cdot\left(q\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right)\right) - \nabla\cdot\left(q\nabla\rho\left(\frac{-2a}{(1-a\rho)^2}\right)\right) - \nabla\cdot\left(q\nabla\rho\left(\frac{6a-4a^2\rho}{(1-a\rho)^3}\right)\right) \\
& + \nabla\cdot\left(q\rho\nabla\left(\frac{2a}{(1-a\rho)^2}\right)\right) + \nabla\cdot\left(q\rho\nabla\left(\frac{4a^2\rho-8a}{(1-a\rho)^3}\right)\right) \\
& + \nabla^2\left(q\left(\frac{1}{1-a\rho}\right)\right) - \nabla^2\left(q\rho\left(\frac{a}{(1-a\rho)^2}\right)\right) - \nabla^2\left(q\rho\left(\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\right)\bigg]drdt.
\end{aligned}
$$

Combining fractions gives:

$$
\begin{aligned}
\mathcal{L}_\rho(\rho,\mathbf{w},q)h = ... - \frac{1}{\beta}\int_0^T\int_\Omega h\bigg[& q\nabla^2\rho\left(\frac{a}{(1-a\rho)^2}\right) + q\nabla\rho\cdot\nabla\left(\frac{2a(a\rho-2)}{(1-a\rho)^3}\right) - q\nabla^2\left(\frac{a\rho-2}{(a\rho-1)^2}\right) \\
& - q\rho\nabla^2\left(\frac{a(3-a\rho)}{(1-a\rho)^3}\right) - \nabla\cdot\left(q\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right)\right) - \nabla\cdot\left(q\nabla\rho\left(\frac{2a(a\rho-2)}{(1-a\rho)^3}\right)\right) \\
& + \nabla\cdot\left(q\rho\nabla\left(\frac{-2a(a\rho-3)}{(1-a\rho)^3}\right)\right) + \nabla^2\left(q\left(\frac{1}{1-a\rho}\right)\right) - \nabla^2\left(q\rho\left(\frac{-a(a\rho-3)}{(1-a\rho)^3}\right)\right)\bigg]drdt.
\end{aligned}
$$

According to Mathematica this is:

$$
\mathcal{L}_\rho(\rho,\mathbf{w},q)h = ... - \frac{1}{\beta}\int_0^T\int_\Omega h\left[\frac{1}{(a\rho-1)^3}\left(4a\nabla\rho\cdot\nabla q + 2a(-1+a\rho)q\nabla^2\rho + (-1+5a\rho-2a^2\rho^2)\nabla^2 q\right)\right]drdt.
$$

And rewriting this is:

$$
\mathcal{L}_\rho(\rho,\mathbf{w},q)h = ... - \frac{1}{\beta}\int_0^T\int_\Omega h\left[\frac{4a\nabla\rho\cdot\nabla q}{(a\rho-1)^3} + \frac{2aq\nabla^2\rho}{(a\rho-1)^2} + \frac{(-1+5a\rho-2a^2\rho^2)\nabla^2 q}{(a\rho-1)^3}\right]drdt.
$$

Adding the other terms of the adjoint found in previous analysis, the adjoint equation is:

$$
\begin{aligned}
\frac{\partial q}{\partial t} =& \frac{1}{\beta}\frac{(-1+5a\rho-2a^2\rho^2)}{(a\rho-1)^3}\nabla^2 q + \frac{1}{\beta}\frac{4a\nabla\rho}{(a\rho-1)^3}\cdot\nabla q + \frac{1}{\beta}\frac{2a\nabla^2\rho}{(a\rho-1)^2}q \\
& - \mathbf{w}\cdot\nabla q + \nabla V_{ext}\cdot\nabla q - \rho + \widehat{\rho} + \int\left(\nabla_r q(r) - \nabla_{r'}q(r')\right)\rho(r').\mathbf{K}(r,r')dr'
\end{aligned}
$$

6.4.3 Frechét Derivatives for Boundary Terms

When considering no-flux boundary conditions, we have the equation:

$$
-\mathbf{j}\cdot\mathbf{n} = ... - \rho\nabla\frac{\delta F_N[\rho]}{\delta\rho}\cdot\mathbf{n} = ... - \frac{1}{\beta}\left(\frac{\nabla\rho}{1-\eta} - \rho\nabla\frac{\eta-2}{(\eta-1)^2}\right)\cdot\mathbf{n},
$$

omitting the other terms, as done in the previous section. The Frechét derivatives of the following terms have to be taken, similarly to the section above:

$$
\begin{aligned}
F_4(\rho) &= \frac{\nabla\rho}{1-a\rho},\\
F_5(\rho) &= \rho\nabla\frac{a\rho-2}{(a\rho-1)^2}.
\end{aligned}
$$

Then for F_4 we have:

$$
\begin{aligned}
F_4(\rho+h)-F_4(\rho) &= \nabla(\rho+h)\frac{1}{1-a(\rho+h)} - \nabla\rho\frac{1}{1-a\rho}\\
&= \nabla(\rho+h)\left(\frac{1}{1-a\rho}+\frac{a}{(1-a\rho)^2}h\right)\\
&= \nabla h\left(\frac{1}{1-a\rho}\right)+\nabla\rho\left(\frac{a}{(1-a\rho)^2}h\right).
\end{aligned}
$$

For F_5 we get:

$$
\begin{aligned}
F_5(\rho+h)-F_5(\rho) &= (\rho+h)\nabla\frac{a(\rho+h)-2}{(a(\rho+h)-1)^2} - \rho\nabla\frac{a\rho-2}{(a\rho-1)^2}\\
&= (\rho+h)\nabla\left(\frac{a(\rho+h)-2}{(1-a\rho)^2}+\frac{a(\rho+h)-2}{(1-a\rho)^3}2ah\right) - \rho\nabla\frac{a\rho-2}{(a\rho-1)^2}\\
&= h\nabla\left(\frac{a\rho-2}{(1-a\rho)^2}\right)+\rho\nabla\left(h\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\right)\\
&= h\nabla\left(\frac{a\rho-2}{(1-a\rho)^2}\right)+h\rho\nabla\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)+\nabla h\left(\rho\frac{a}{(1-a\rho)^2}+\rho\frac{2a^2\rho-4a}{(1-a\rho)^3}\right).
\end{aligned}
$$

6.4.4 Boundary Terms

Given the Frechét derivatives, the relevant boundary terms for the Lagrangian are:

$$
\begin{aligned}
\mathcal{L}_{\rho,1}(\rho,\mathbf{w},q)h = ..-\frac{1}{\beta}\int_0^T\int_{\partial\Omega}\Bigg(&-q_{\partial\Omega}\nabla h\left(\frac{1}{1-a\rho}\right)-q_{\partial\Omega}\nabla\rho\left(\frac{a}{(1-a\rho)^2}h\right)+q_{\partial\Omega}h\nabla\left(\frac{a\rho-2}{(1-a\rho)^2}\right)\\
&+hq_{\partial\Omega}\rho\nabla\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)+q_{\partial\Omega}\nabla h\left(\rho\frac{a}{(1-a\rho)^2}+\rho\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\Bigg)\cdot\mathbf{n}dr.dt
\end{aligned}
$$

From the integration by parts of the terms within the domain (in the previous section) we get:

$$\mathcal{L}_{\rho,2}(\rho,\mathbf{w},q)h = ... - \frac{1}{\beta}\int_0^T\int_{\partial\Omega}\Bigg(h\Bigg(q\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right) + q\nabla\rho\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right)$$
$$- q\rho\nabla\left(\frac{2a}{(1-a\rho)^2}+\frac{4a^2\rho-8a}{(1-a\rho)^3}\right)\Bigg)$$
$$+ \nabla h\Bigg(q\left(\frac{1}{1-a\rho}\right) - q\rho\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\Bigg)$$
$$- h\nabla\Bigg(q\left(\frac{1}{1-a\rho}\right) - q\rho\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\Bigg)\Bigg)\cdot\mathbf{n}drdt.$$

Combining all of these give all boundary terms for the Lagrangian:

$$\mathcal{L}_{\rho}(\rho,\mathbf{w},q)h = ... - \frac{1}{\beta}\int_0^T\int_{\partial\Omega}\Bigg(h\Bigg(-q_{\partial\Omega}\nabla\rho\left(\frac{a}{(1-a\rho)^2}\right) + q_{\partial\Omega}\nabla\left(\frac{a\rho-2}{(1-a\rho)^2}\right)$$
$$+ q_{\partial\Omega}\rho\nabla\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right) + \Bigg(q\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right) + q\nabla\rho\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right)$$
$$- q\rho\nabla\left(\frac{2a}{(1-a\rho)^2}+\frac{4a^2\rho-8a}{(1-a\rho)^3}\right)\Bigg) - \nabla\Bigg(q\left(\frac{1}{1-a\rho}\right) - q\rho\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\Bigg)\Bigg)$$
$$+ \nabla h\Bigg(-q_{\partial\Omega}\left(\frac{1}{1-a\rho}\right) + q_{\partial\Omega}\left(\rho\frac{a}{(1-a\rho)^2}+\rho\frac{2a^2\rho-4a}{(1-a\rho)^3}\right) + q\left(\frac{1}{1-a\rho}\right)$$
$$- q\rho\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\Bigg)\Bigg)\cdot\mathbf{n}drdt.$$

Comparing terms in ∇h:

$$\Bigg[-q_{\partial\Omega}\left(\frac{1}{1-a\rho}\right) + q_{\partial\Omega}\left(\rho\frac{a}{(1-a\rho)^2}+\rho\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)$$
$$+ q\left(\frac{1}{1-a\rho}\right) - q\rho\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\Bigg]\cdot\mathbf{n} = 0.$$

This holds when $q_{\partial\Omega} = q$. Then for $h \neq 0$ we get:

$$\Bigg[-q\nabla\rho\left(\frac{a}{(1-a\rho)^2}\right) + q\nabla\left(\frac{a\rho-2}{(1-a\rho)^2}\right)$$
$$+ q\rho\nabla\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right) + q\nabla\left(\frac{3-2a\rho}{(1-a\rho)^2}\right) + q\nabla\rho\left(\frac{-2a}{(1-a\rho)^2}+\frac{6a-4a^2\rho}{(1-a\rho)^3}\right)$$
$$- q\rho\nabla\left(\frac{2a}{(1-a\rho)^2}+\frac{4a^2\rho-8a}{(1-a\rho)^3}\right) - \nabla\Bigg(q\left(\frac{1}{1-a\rho}\right) - q\rho\left(\frac{a}{(1-a\rho)^2}+\frac{2a^2\rho-4a}{(1-a\rho)^3}\right)\Bigg)\Bigg]\cdot\mathbf{n} = 0$$

According to Mathematica this reduces to:

$$\frac{(1+a\rho)\nabla q}{(a\rho-1)^3}\cdot\mathbf{n} = 0$$

Since $a\rho > 0$ by definition, this is:

$$\frac{\partial q}{\partial n} = 0.$$

Note that the other terms of the PDE are not entering this expression, as they cancel out during the derivation. This has been shown in the derivation of a simpler set of equations and since this derivation is additive, the result remains unchanged.
Furthermore, the gradient equation remains unchanged by this equation, since F_N does not contain terms involving $\mathbf{w}$, compare to (5), and is:

$$\mathbf{w} = -\frac{1}{\beta}\rho\nabla q.$$

6.4.5 Derivation of Time-Independent Control

While the gradient equation is unchanged by the sedimentation equation, as compared to an advection diffusion equation, it is changed when we consider a time independent control. We choose the problem:

$$J = \frac{1}{2}\int_0^T \int_\Omega (\rho - \widehat{\rho})^2 dr dt + \frac{\beta}{2}\int_\Omega \mathbf{w}(r)^2 dr$$

subject to:

$$\frac{\partial \rho}{\partial t} = \beta\sigma^2\left(\nabla \cdot (\rho \nabla V_{ext}) - \nabla(\rho \mathbf{w}) + \nabla \cdot \left(\rho \nabla \frac{\delta F_N[\rho]}{\delta \rho}\right) + \kappa \int_\Omega \rho(r)\rho(r')\mathbf{K}(r, r')dr\right),$$

where $\mathbf{K}(r, r') = \nabla V_2$. Taking derivatives of the Lagrangian with respect to $\mathbf{w}$ gives:

$$\mathcal{L}_{\mathbf{w}}(\rho, \mathbf{w}, q)h = \int_\Omega \beta \mathbf{w}(r) \cdot \mathbf{h}(r)dt + \int_0^T \int_\Omega \rho \mathbf{h}(r) \cdot \nabla q dr dt. \tag{5}$$

Since $\mathbf{w}$ does not depend on t, neither does $\mathbf{h}$ and so this can be taken out of the time integral:

$$\mathcal{L}_{\mathbf{w}}(\rho, \mathbf{w}, q)h = \int_\Omega \left(\beta \mathbf{w}(r) \cdot \mathbf{h}(r) + \mathbf{h}(r) \cdot \int_0^T \rho \nabla q dt\right) dr.$$

Then we get:

$$\beta \mathbf{w}(r) + \int_0^T \rho \nabla q dt = 0,$$

and finally:

$$\mathbf{w}(r) = -\frac{1}{\beta}\int_0^T \rho \nabla q dt.$$

6.5 Numerical Examples

7 Newton-Krylov

8 Some other stuff

8.1 Sparse to Fine Grid Stuff

8.2 Final time target derivation

8.3 Averaging 3D to 2D

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