

1 Multishape OCP

(Note: MultiShapeFancyChannel3) Last week, there was an issue with the multishape OCP for small β in particular. I have found an alternative initial condition for the problem to work. Last week the initial condition was a Gaussian located in the first shape only. This causes the algorithm to converge to $wErr = 0.00$ in only a few iterations, while $J_{FW} < J_{Opt}$. I suspect this is happening because there is not enough mass in the system. When I ran the OCP on the last two shapes without changing the initial condition (by accident) the same mistake occurred, while it didn't occur when I ran it on the first shape. I now changed the initial condition to $\rho_0 = 0.5$. This works well with $\beta = 10^{-3}$ and $J_{FW} = 0.1218$, while $J_{Opt} = 0.0034$. The result can be seen in Figure 1.

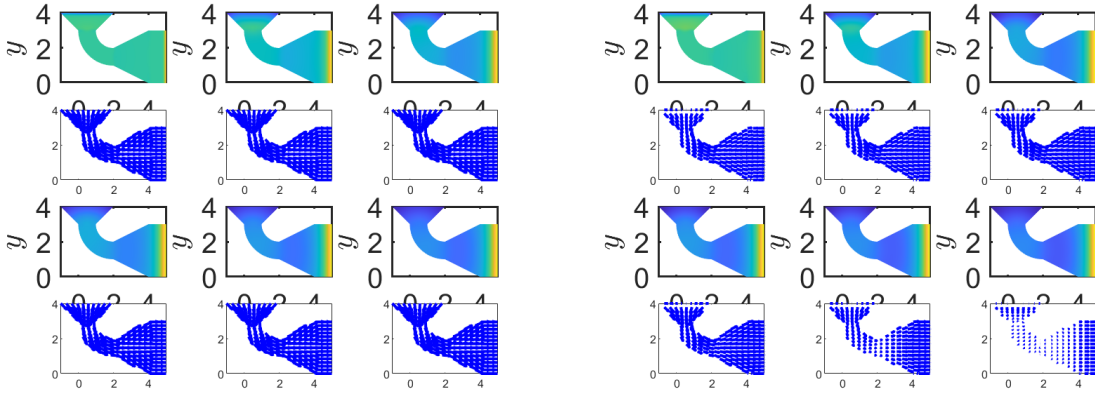


Figure 1: $\hat{\rho}$ and optimal ρ with corresponding \mathbf{w} .

I then tried to compute the sedimentation equations on the same geometry with a time independent control. The target was found by imposing gravity, while the initial guess for the problem was done without gravity. The result is a little unclear, because both J_{FW} and J_{Opt} are of order 10^{-6} and therefore too small to reliably compare. I am also unsure whether there is an artefact in the plots due to the number of points. However, in comparison to the example above, this one did have interactions included - so might just be that. I computed the problem with $N = 30$ for each shape and $n = 30$. Figure 2 shows the result.

2 Periodic Boundary Conditions

We consider the advection diffusion equation with periodic boundary conditions and a corresponding OCP:

$$\begin{aligned} & \min \frac{1}{2} \|\rho - \hat{\rho}\|^2 + \frac{\beta}{2} \|\mathbf{w}\|^2 \\ & \text{subject to:} \\ & \frac{\partial \rho}{\partial t} = \frac{\partial^2 \rho}{\partial x^2} - \frac{\partial \rho \mathbf{w}}{\partial x} \\ & \rho(a) = \rho(b) \\ & \frac{\partial \rho(a)}{\partial x} - \rho(a) \mathbf{w}(a) = \frac{\partial \rho(b)}{\partial x} - \rho(b) \mathbf{w}(b) \end{aligned}$$

The relevant part of the Lagrangian is then:

$$\begin{aligned} \mathcal{L} = & \dots - \int_0^T \int_{\Omega} \left(\frac{\partial \rho}{\partial t} - \frac{\partial^2 \rho}{\partial x^2} + \frac{\partial \rho \mathbf{w}}{\partial x} \right) q dr dt \\ & - \int_0^T \left(-\rho(b)q_1 + \rho(a)q_1 - \frac{\partial \rho(b)}{\partial x} q_2 + \rho(b) \mathbf{w}(b)q_2 + \frac{\partial \rho(a)}{\partial x} q_2 - \rho(a) \mathbf{w}(a)q_2 \right) dt. \end{aligned}$$

Taking partial derivatives, the relevant part of the Lagrangian is:

$$\mathcal{L} = \dots - \int_0^T \left[q \frac{\partial \rho}{\partial x} - \rho \frac{\partial q}{\partial x} - \rho \mathbf{w} q \right]_a^b - \left(-\rho(b)q_1 + \rho(a)q_1 - \frac{\partial \rho(b)}{\partial x} q_2 + \rho(b) \mathbf{w}(b)q_2 + \frac{\partial \rho(a)}{\partial x} q_2 - \rho(a) \mathbf{w}(a)q_2 \right) dt.$$

Taking the derivative with respect to ρ gives:

$$\begin{aligned} \mathcal{L}_{\rho} h = & \dots - \int_0^T \left[q \frac{\partial h}{\partial x} - h \frac{\partial q}{\partial x} - h \mathbf{w} q \right]_a^b \\ & - \left(-h(b)q_1 + h(a)q_1 - \frac{\partial h(b)}{\partial x} q_2 + h(b) \mathbf{w}(b)q_2 + \frac{\partial h(a)}{\partial x} q_2 - h(a) \mathbf{w}(a)q_2 \right) dt \end{aligned}$$

Writing all terms explicitly:

$$\begin{aligned} \mathcal{L}_{\rho} h = & \dots + \int_0^T \left(-q(b) \frac{\partial h(b)}{\partial x} + h(b) \frac{\partial q(b)}{\partial x} + h(b) \mathbf{w}(b)q(b) + q(a) \frac{\partial h(a)}{\partial x} - h(a) \frac{\partial q(a)}{\partial x} - h(a) \mathbf{w}(a)q(a) \right. \\ & \left. h(b)q_1 - h(a)q_1 + \frac{\partial h(b)}{\partial x} q_2 - h(b) \mathbf{w}(b)q_2 - \frac{\partial h(a)}{\partial x} q_2 + h(a) \mathbf{w}(a)q_2 \right) dt \end{aligned}$$

Then considering the terms that satisfy $\frac{\partial h}{\partial x} \neq 0$ at a and b separately we get:

$$\begin{aligned} \int_0^T -q(b) \frac{\partial h(b)}{\partial x} + \frac{\partial h(b)}{\partial x} q_2 dt &= 0 \\ \int_0^T q(a) \frac{\partial h(a)}{\partial x} - \frac{\partial h(a)}{\partial x} q_2 dt &= 0 \end{aligned}$$

And therefore we find $q(b) = q_2$ and $q(a) = q_2$ and so:

$$q(a) = q(b).$$

Then considering the terms where $h \neq 0$, again separately for a and b we get:

$$\begin{aligned} \int_0^T h(b) \frac{\partial q(b)}{\partial x} + h(b) \mathbf{w}(b) q(b) + h(b) q_1 - h(b) \mathbf{w}(b) q_2 dt &= 0 \\ \int_0^T -h(a) \frac{\partial q(a)}{\partial x} - h(a) \mathbf{w}(a) q(a) - h(a) q_1 + h(a) \mathbf{w}(a) q_2 dt &= 0 \end{aligned}$$

And using that $q(b) = q_2$ and $q(a) = q_2$ we get:

$$\begin{aligned} \frac{\partial q(b)}{\partial x} + \mathbf{w}(b) q(b) + q_1 - \mathbf{w}(b) q(b) &= 0 \\ -\frac{\partial q(a)}{\partial x} - \mathbf{w}(a) q(a) - q_1 + \mathbf{w}(a) q(a) &= 0 \end{aligned}$$

and so:

$$\frac{\partial q(b)}{\partial x} = \frac{\partial q(a)}{\partial x}.$$

Therefore, the two boundary conditions for the adjoint equation are:

$$q(a) = q(b) \quad \frac{\partial q(b)}{\partial x} = \frac{\partial q(a)}{\partial x},$$

as expected.

3 Periodic Boundary Conditions in a General Domain

We consider the advection diffusion equation with periodic boundary conditions and a corresponding OCP:

$$\min \frac{1}{2} \|\rho - \hat{\rho}\|^2 + \frac{\beta}{2} \|\mathbf{w}\|^2$$

subject to:

$$\frac{\partial \rho}{\partial t} = \frac{\partial^2 \rho}{\partial x^2} - \frac{\partial \rho \mathbf{w}}{\partial x}$$

$$\rho|_{\partial\Omega_l} = \rho|_{\partial\Omega_r}$$

$$\rho|_{\partial\Omega_t} = \rho|_{\partial\Omega_b}$$

$$\frac{\partial \rho}{\partial x} - \rho \mathbf{w}|_{\partial\Omega_l} = \frac{\partial \rho}{\partial x} - \rho \mathbf{w}|_{\partial\Omega_r}$$

$$\frac{\partial \rho}{\partial x} - \rho \mathbf{w}|_{\partial\Omega_t} = \frac{\partial \rho}{\partial x} - \rho \mathbf{w}|_{\partial\Omega_b},$$

such that $\partial\Omega_l \cup \partial\Omega_r \cup \partial\Omega_t \cup \partial\Omega_b = \partial\Omega$ and the abbreviations corresponding to left, right, top and bottom respectively. The relevant part of the Lagrangian is then:

$$\begin{aligned}\mathcal{L} = & \dots - \int_0^T \int_{\Omega} \left(\frac{\partial \rho}{\partial t} - \frac{\partial^2 \rho}{\partial x^2} + \frac{\partial \rho \mathbf{w}}{\partial x} \right) q dr dt \\ & - \int_0^T \int_{\partial\Omega_l} (-\rho q_1 - \nabla \rho q_2 \cdot \mathbf{n} + \rho \mathbf{w} q_2 \cdot \mathbf{n}) dr + \int_{\partial\Omega_r} (\rho q_1 + \nabla \rho q_2 \cdot \mathbf{n} - \rho \mathbf{w} q_2 \cdot \mathbf{n}) dr \\ & + \int_{\partial\Omega_t} (-\rho q_3 - \nabla \rho q_4 \cdot \mathbf{n} + \rho \mathbf{w} q_4 \cdot \mathbf{n}) dr + \int_{\partial\Omega_b} (\rho q_3 + \nabla \rho q_4 \cdot \mathbf{n} - \rho \mathbf{w} q_4 \cdot \mathbf{n}) dr dt.\end{aligned}$$

Taking partial derivatives, the relevant part of the Lagrangian is:

$$\begin{aligned}\mathcal{L} = & \dots - \int_0^T \int_{\partial\Omega} (q \nabla \rho - \rho \nabla q - \rho \mathbf{w} q) \cdot \mathbf{n} dr dt \\ & - \int_0^T \int_{\partial\Omega_l} (-\rho q_1 - \nabla \rho q_2 \cdot \mathbf{n} + \rho \mathbf{w} q_2 \cdot \mathbf{n}) dr + \int_{\partial\Omega_r} (\rho q_1 + \nabla \rho q_2 \cdot \mathbf{n} - \rho \mathbf{w} q_2 \cdot \mathbf{n}) dr \\ & + \int_{\partial\Omega_t} (-\rho q_3 - \nabla \rho q_4 \cdot \mathbf{n} + \rho \mathbf{w} q_4 \cdot \mathbf{n}) dr + \int_{\partial\Omega_b} (\rho q_3 + \nabla \rho q_4 \cdot \mathbf{n} - \rho \mathbf{w} q_4 \cdot \mathbf{n}) dr dt.\end{aligned}$$

Taking the derivative with respect to ρ gives:

$$\begin{aligned}\mathcal{L} = & \dots - \int_0^T \int_{\partial\Omega} q \frac{\partial h}{\partial n} - h \frac{\partial q}{\partial n} - \rho \mathbf{w} q \cdot \mathbf{n} dr dt \\ & - \int_0^T \int_{\partial\Omega_l} \left(-h q_1 - \frac{\partial h}{\partial n} q_2 + h \mathbf{w} q_2 \cdot \mathbf{n} \right) dr + \int_{\partial\Omega_r} \left(h q_1 + \frac{\partial h}{\partial n} q_2 - h \mathbf{w} q_2 \cdot \mathbf{n} \right) dr \\ & + \int_{\partial\Omega_t} \left(-h q_3 - \frac{\partial h}{\partial n} q_4 + h \mathbf{w} q_4 \cdot \mathbf{n} \right) dr + \int_{\partial\Omega_b} \left(h q_3 + \frac{\partial h}{\partial n} q_4 - h \mathbf{w} q_4 \cdot \mathbf{n} \right) dr dt.\end{aligned}$$

Writing all terms explicitly:

$$\begin{aligned}\mathcal{L} = & \dots - \int_0^T \int_{\partial\Omega_l} \left(q \frac{\partial h}{\partial n} - h \frac{\partial q}{\partial n} - h \mathbf{w} q \cdot \mathbf{n} - h q_1 - \frac{\partial h}{\partial n} q_2 + h \mathbf{w} q_2 \cdot \mathbf{n} \right) dr \\ & + \int_{\partial\Omega_r} \left(-q \frac{\partial h}{\partial n} + h \frac{\partial q}{\partial n} + h \mathbf{w} q \cdot \mathbf{n} + h q_1 + \frac{\partial h}{\partial n} q_2 - h \mathbf{w} q_2 \cdot \mathbf{n} \right) dr \\ & + \int_{\partial\Omega_t} \left(q \frac{\partial h}{\partial n} - h \frac{\partial q}{\partial n} - h \mathbf{w} q \cdot \mathbf{n} - h q_3 - \frac{\partial h}{\partial n} q_4 + h \mathbf{w} q_4 \cdot \mathbf{n} \right) dr \\ & + \int_{\partial\Omega_b} \left(-q \frac{\partial h}{\partial n} + h \frac{\partial q}{\partial n} + h \mathbf{w} q \cdot \mathbf{n} + h q_3 + \frac{\partial h}{\partial n} q_4 - h \mathbf{w} q_4 \cdot \mathbf{n} \right) dr dt.\end{aligned}$$

When writing out the terms explicitly we pay attention to the fact that $n|_{\partial\Omega_l} = -n|_{\partial\Omega_r}$ and $n|_{\partial\Omega_t} = -n|_{\partial\Omega_b}$. Then considering the terms that satisfy $\frac{\partial h}{\partial x}$ on each boundary separately, we

get:

$$\begin{aligned} \int_0^T \int_{\partial\Omega_l} q \frac{\partial h}{\partial x} - \frac{\partial h}{\partial x} q_2 dr dt &= 0 & \int_0^T \int_{\partial\Omega_r} -q \frac{\partial h}{\partial x} + \frac{\partial h}{\partial x} q_2 dr dt &= 0 \\ \int_0^T \int_{\partial\Omega_t} q \frac{\partial h}{\partial x} - \frac{\partial h}{\partial x} q_4 dr dt &= 0 & \int_0^T \int_{\partial\Omega_b} -q \frac{\partial h}{\partial x} + \frac{\partial h}{\partial x} q_4 dr dt &= 0. \end{aligned}$$

Therefore we have

$$\begin{aligned} q &= q_2|_{\partial\Omega_l} & q &= q_2|_{\partial\Omega_r} \\ q &= q_4|_{\partial\Omega_t} & q &= q_4|_{\partial\Omega_b}, \end{aligned}$$

and so:

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

as expected. Now, considering $h \neq 0$ on each separate boundary gives:

$$\begin{aligned} \int_0^T \int_{\partial\Omega_l} -h \frac{\partial q}{\partial n} - hq\mathbf{w} \cdot \mathbf{n} - hq_1 + hq_2\mathbf{w} \cdot \mathbf{n} dr dt &= 0 \\ \int_0^T \int_{\partial\Omega_r} h \frac{\partial q}{\partial n} + hq\mathbf{w} \cdot \mathbf{n} + hq_1 - hq_2\mathbf{w} \cdot \mathbf{n} dr dt &= 0 \\ \int_0^T \int_{\partial\Omega_t} -h \frac{\partial q}{\partial n} - hq\mathbf{w} \cdot \mathbf{n} - hq_3 + hq_4\mathbf{w} \cdot \mathbf{n} dr dt &= 0 \\ \int_0^T \int_{\partial\Omega_b} h \frac{\partial q}{\partial n} + hq\mathbf{w} \cdot \mathbf{n} + hq_3 - hq_4\mathbf{w} \cdot \mathbf{n} dr dt &= 0. \end{aligned}$$

Using the relationships of q , q_2 and q_4 from above, the terms involving \mathbf{w} cancel and we get:

$$\begin{aligned} \int_0^T \int_{\partial\Omega_l} -h \frac{\partial q}{\partial n} - hq_1 dr dt &= 0 & \int_0^T \int_{\partial\Omega_r} h \frac{\partial q}{\partial n} + hq_1 dr dt &= 0 \\ \int_0^T \int_{\partial\Omega_t} -h \frac{\partial q}{\partial n} - hq_3 dr dt &= 0 & \int_0^T \int_{\partial\Omega_b} h \frac{\partial q}{\partial n} + hq_3 dr dt &= 0. \end{aligned}$$

This results in the four relationships:

$$\frac{\partial q}{\partial n} = -q_1|_{\partial\Omega_l}, \quad \frac{\partial q}{\partial n} = -q_1|_{\partial\Omega_r}, \quad \frac{\partial q}{\partial n} = -q_3|_{\partial\Omega_t}, \quad \frac{\partial q}{\partial n} = -q_3|_{\partial\Omega_b},$$

And therefore, we get:

$$\frac{\partial q}{\partial n}|_{\partial\Omega_l} = \frac{\partial q}{\partial n}|_{\partial\Omega_r}, \quad \frac{\partial q}{\partial n}|_{\partial\Omega_t} = \frac{\partial q}{\partial n}|_{\partial\Omega_b},$$

as required.

4 Questions

How do we get the results for the uniform limit? We have:

$$n_1 = \int \rho \delta(|\mathbf{r} - \mathbf{r}'| - R) dr = 4\pi R^2 \rho$$
$$\mathbf{n}_1 = \int \rho \frac{\mathbf{r}}{r} \delta(|\mathbf{r} - \mathbf{r}'| - R) dr = 0.$$

Do I have to explain averaging from 3D to 2D FMT? Or even 3D FMT?

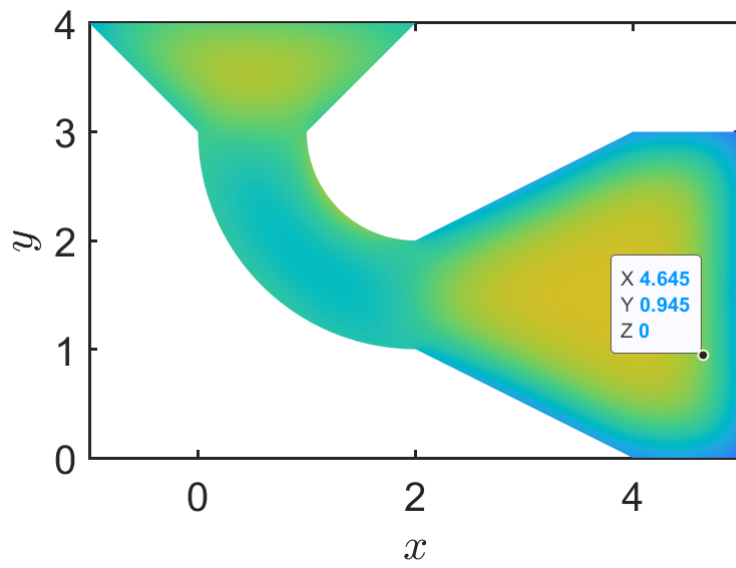
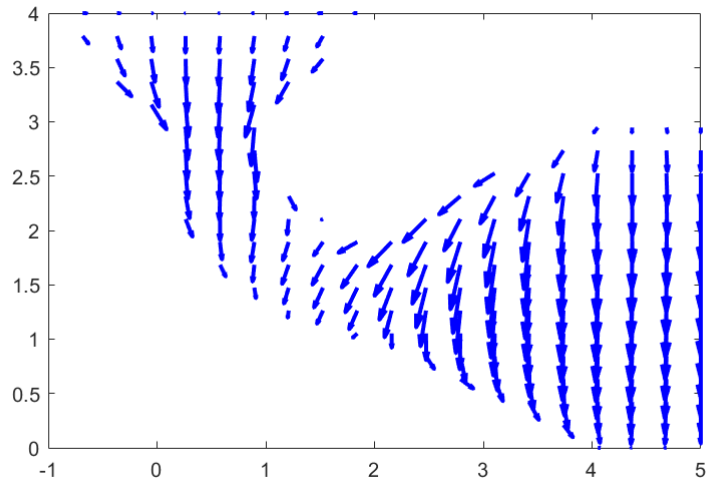
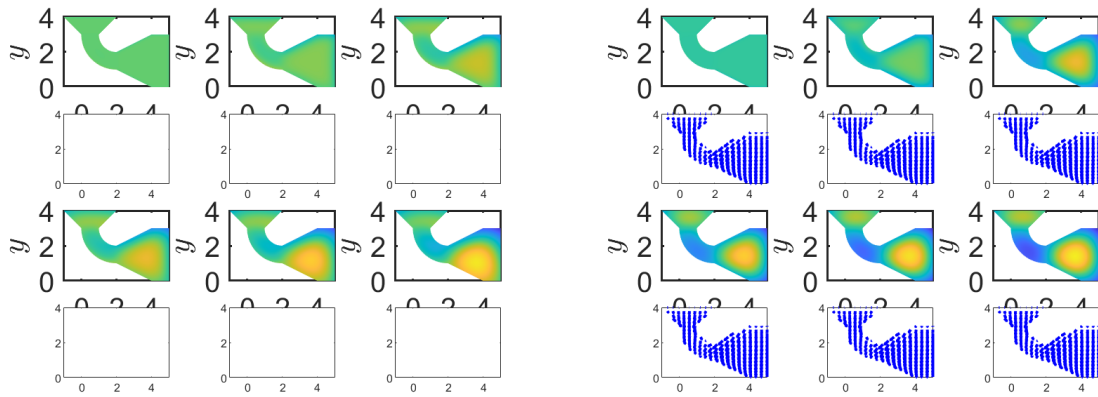


Figure 2: $\hat{\rho}$ and optimal ρ with corresponding \mathbf{w} , one \mathbf{w} for illustration.