Periodic Boundary Conditions for OCPs

1 Periodic Boundary Conditions 1D Advection-Diffusion

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

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

The relevant part of the Lagrangian is then:

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

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

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

Taking the derivative with respect to ρ gives:

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

Writing all terms explicitly:

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

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:

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

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

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

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.

2 Periodic Boundary Conditions in a General Domain

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

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

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:

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

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

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

Taking the derivative with respect to ρ gives:

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

Writing all terms explicitly:

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

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:

$$\int_0^T \int_{\partial\Omega_l} q\frac{\partial h}{\partial x} - \frac{\partial h}{\partial x}q_2 drdt = 0 \qquad \int_0^T \int_{\partial\Omega_r} -q\frac{\partial h}{\partial x} + \frac{\partial h}{\partial x}q_2 drdt = 0$$
$$\int_0^T \int_{\partial\Omega_t} q\frac{\partial h}{\partial x} - \frac{\partial h}{\partial x}q_4 drdt = 0 \qquad \int_0^T \int_{\partial\Omega_b} -q\frac{\partial h}{\partial x} + \frac{\partial h}{\partial x}q_4 drdt = 0.$$

Therefore we have

$$q = q_2|_{\partial\Omega_l} \quad q = q_2|_{\partial\Omega_r}$$
$$q = q_4|_{\partial\Omega_t} \quad q = q_4|_{\partial\Omega_b},$$

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:

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

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

$$\int_0^T \int_{\partial\Omega_l} -h\frac{\partial q}{\partial n} - hq_1 drdt = 0 \qquad \int_0^T \int_{\partial\Omega_r} h\frac{\partial q}{\partial n} + hq_1 drdt = 0$$
$$\int_0^T \int_{\partial\Omega_t} -h\frac{\partial q}{\partial n} - hq_3 drdt = 0 \qquad \int_0^T \int_{\partial\Omega_b} h\frac{\partial q}{\partial n} + hq_3 drdt = 0.$$

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:

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

as required.