COMPUTE SHAPE DERIVATIVE - EXERCISE 2

This document is related to Exercise Sheet 7.

In order to compute the shape derivative we consider the Lagrangian. Since the Dirichlet boundary condition $T = T_1$ on $\partial\omega$ is defined on a moving boundary, we add it int the Lagrangian.

$$\begin{aligned}\mathcal{L}(\omega, S, q, \lambda) = &\int_{\Omega\setminus\omega} |S - T_0|^2 dx \\ &+ \int_{\Omega\setminus\omega} (-\Delta S + u \cdot \nabla S) q dx \\ &+ \int_{\partial\omega} (S - T_1)\lambda ds\end{aligned}$$

We now look at derivatives of $\mathcal{L}$ with respect to its variables:

Derivative w.r.t. q**:**

$$\frac{\partial \mathcal{L}}{\partial q}(\phi) = \int_{\Omega\setminus\omega} (-\Delta S + u \cdot \nabla S)\phi dx$$

Equating this derivative to zero gives the PDE inside the domain (take test functions with compact support):

$$-\Delta T + u \cdot \nabla T = 0$$

and the Neumann boundary condition on $\partial\Omega$ (take functions with general trace on $\partial\Omega$).

Derivative w.r.t. λ**:**

$$\frac{\partial \mathcal{L}}{\partial \lambda}(\phi) = \int_{\partial\omega} (S - T_1)\phi ds$$

Equating this derivative to zero gives the boundary condition on $\partial\omega$: $T = T_1$

Derivative w.r.t. S**:**

$$\frac{\partial \mathcal{L}}{\partial S}(\phi) = \int_{\Omega\setminus\omega} 2(S - T_0)\phi dx + \int_{\Omega\setminus\omega} (-\Delta\phi + u \cdot \nabla\phi) q dx$$

Equating this to zero gives the adjoint equation. In order to recover all the relevant information we should integrate by parts in order to get an expression without derivatives of ϕ. Here we use the fact that u is with divergence zero, in order to write the term $u \cdot \nabla\phi$ as $\operatorname{div}(\phi u)$.

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial S}(\phi) = &\int_{\Omega\setminus\omega} 2(S - T_0)\phi + \int_{\Omega\setminus\omega} \nabla\phi \cdot \nabla q dx - \int_{\partial\omega\cup\partial\Omega} \frac{\partial\phi}{\partial n} q ds - \int_{\Omega\setminus\omega} \phi u \cdot \nabla q ds \\ &+ \int_{\partial\omega\cup\partial\Omega} q\phi u \cdot n ds + \int_{\partial\omega} \phi\lambda ds \\ = &\int_{\Omega\setminus\omega} 2(S - T_0)\phi + \int_{\Omega\setminus\omega} (-\Delta q\phi) dx + \int_{\partial\Omega\cup\partial\omega} \phi\frac{\partial q}{\partial n} ds - \int_{\partial\omega\cup\partial\Omega} \frac{\partial\phi}{\partial n} q ds - \int_{\Omega\setminus\omega} \phi u \cdot \nabla q ds \\ &- \int_{\Omega\setminus\omega} \phi u \cdot \nabla q ds + \int_{\partial\omega\cup\partial\Omega} q\phi u \cdot n ds + \int_{\partial\omega} \phi\lambda ds\end{aligned}$$

Now equating the previous derivative to zero will give us the adjoint equation:

- for ϕ with compact support, all boundary terms vanish so we get

$$-\Delta p - u \cdot \nabla p + 2(T - T_0) = 0 \text{ in } \Omega \setminus \omega$$

- Next, for $\phi = 0$ on $\partial\Omega \cup \partial\omega$ with varying $\partial\phi/\partial n$ we get $p = 0$ on $\partial\Omega \cup \partial\omega$.

- Next, for general ϕ we find that

$$\frac{\partial p}{\partial n} + \lambda = 0 \text{ on } \partial\omega \qquad \frac{\partial p}{\partial n} = 0 \text{ on } \partial\Omega$$

Thus we have all information on the state T and on the adjoint p. When computing the partial derivative of $\mathcal{L}$ w.r.t. ω we get

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial \omega}(\theta) = &\int_{\partial\Omega} |S - T_0|^2 \theta.nds \\ &+ \int_{\partial\omega} (-\Delta S + u \cdot \nabla S) q\theta.nds \\ &+ \int_{\partial\omega} (\frac{\partial((S-T_1)\lambda)}{\partial n} + (S - T_1)\lambda\mathcal{H})\theta.nds\end{aligned}$$

Replacing $S = T$ and $q = p$ will cancel the second integral. Also, in the last integral $T - T_1 = 0$ on $\partial\omega$ **but not its gradient**. Therefore we are left with the following

$$J'(\Omega)(\theta) = \int_{\partial\omega} |T - T_0|^2 \theta.nds + \int_{\partial\omega} \frac{\partial T}{\partial n}\lambda\theta.nds$$

In the end we also use the fact that $\lambda = -\frac{\partial p}{\partial n}$ on $\partial\omega$ to have

(1)
$$J'(\Omega)(\theta) = \int_{\partial\omega} \left(|T - T_0|^2 - \frac{\partial T}{\partial n}\frac{\partial T}{\partial n} \right) \theta.nds$$

Please check the computations!!

For the second type of boundary condition (point 5) the shape derivative changes... First, note that we do not have a Dirichlet boundary condition on the inclusion $\partial\omega$, therefore we don't need an additional Lagrange multiplier for this!

First we should write the variational formulation for this boundary condition. The space of definition are functions in $H^1(\mathbb{R}^d)$ that are zero on $\partial\Omega$. Note that this does not poses a problem in our case, since $\partial\Omega$ does not move. As before, we have

$$\begin{aligned}0 = &\int_{\Omega\setminus\omega} (-\Delta T + u \cdot \nabla T)\phi = \int_{\Omega\setminus\omega} \nabla T \cdot \nabla\phi dx - \int_{\partial\omega} \frac{\partial T}{\partial n}\phi ds \\ &- \int_{\Omega\setminus\omega} T u \cdot \nabla\phi dx + \int_{\partial\omega} T\phi u \cdot nds \\ &= \int_{\Omega\setminus\omega} (\nabla T \cdot \nabla\phi) dx - \int_{\Omega\setminus\omega} T u \cdot \nabla\phi dx - \int_{\partial\omega} \Phi_1 \phi ds\end{aligned}$$

where we have used the fact that $\frac{\partial T}{\partial n} - u \cdot nT = \Phi_1$ on $\partial\omega$ and the fact that $\phi = 0$ on $\partial\Omega$. It is not hard to see that this formulation is indeed equivalent to the initial PDE by performing the integration by parts in the backwards direction.

Therefore, the associated Lagrangian for our problem is:

$$\begin{aligned}\mathcal{L}(\omega, S, q) = &\int_{\Omega\setminus\omega} |S - T_0|^2 dx \\ &+ \int_{\Omega\setminus\omega} (\nabla S \cdot \nabla q) dx - \int_{\Omega\setminus\omega} S u \cdot \nabla q dx - \int_{\partial\omega} \Phi_1 q ds\end{aligned}$$

defined for shapes ω included in Ω, and for S and q in H^1 which are zero on $\partial\Omega$.

Now we are in the position to compute the partial derivatives with respect to all variables:

- Derivative w.r.t. q:

$$\frac{\partial \mathcal{L}}{\partial q}(\phi) = \int_{\Omega\setminus\omega} (\nabla S \cdot \nabla\phi) dx - \int_{\Omega\setminus\omega} S u \cdot \nabla\phi dx - \int_{\partial\omega} \Phi_1 \phi ds$$

Equating this derivative to zero we get the initial state equation for T.

- Derivative w.r.t. S:

$$\frac{\partial \mathcal{L}}{\partial S}(\phi) = \int_{\Omega\setminus\omega} 2(S-T_0)\phi dx + \int_{\Omega\setminus\omega} (\nabla\phi\cdot\nabla q)dx - \int_{\Omega\setminus\omega} \phi u\cdot\nabla q dx$$

Equating this derivative to zero gives the adjoint state. In order to find the boundary information we eliminate the derivatives on ϕ so we get for $S = T$

$$0 = \int_{\Omega\setminus\omega} 2(S-T_0)\phi dx + \int_{\Omega\setminus\omega} (-\Delta p)\phi + \int_{\partial\omega} \frac{\partial p}{\partial n}\phi - \int_{\Omega\setminus\omega} \phi u\cdot\nabla p$$

Now, for ϕ wit compact support we get the PDE in $\Omega\setminus\omega$:

$$-\Delta p - u\cdot\nabla p + 2(S-T_0) = 0$$

For general ϕ we get the boundary condition on $\partial\omega$:

$$\frac{\partial p}{\partial n} = 0$$

- Derivative w.r.t ω:

$$\begin{aligned}\frac{\partial L}{\partial \omega} &= \int_{\partial\omega} |S-T_0|^2\theta.nds \\ &+ \int_{\partial\omega} \nabla S\cdot\nabla q\theta.nds \\ &- \int_{\partial\omega} Su\cdot\nabla q\theta.nds \\ &- \int_{\partial\omega}\left(\frac{\partial(\Phi_1 q)}{\partial n} + \Phi_1 q\mathcal{H}\right)\theta.n \qquad (2)\end{aligned}$$

In order to get the shape derivative you should replace $S = T$ and $q = p$ in the previous formula.

Homework questions:

For question 1 we are in the first case, with Dirichlet boundary condition $T = T_1$ on $\partial\omega$. You just need to write the state and adjoint problems in `FreeFem++` and use the formula (1).

In the homework question for question 2 things are SIMPLE since $\Phi_1 = 0$ and $u = 0$. Therefore from all the above terms in Formula (2) only the first two remain. In particular, the term with the mean curvature $\mathcal{H}$ (which is not immediate from a numerical point of view) vanishes.

For question 3 the mean curvature is just the inverse of the radius of the circle, so everything in the above formula (2) can be easily computed in `FreeFem++`.

As recalled above: please check the computations. Some errors may have slipped through! You should be able to redo the computations yourself.