Shape derivative of a domain integral

We want to differentiate a domain integral with respect to a parameter that changes the domain itself, i.e., the parameter changes the shape of the domain. This is tricky when the quantities in the integrand of the domain integral are expressed in terms of the current domain. In the parlance of mechanics, we refer to the original domain as "material" domain and denote it by Ω_0; and the current domain as "spatial" domain and denote it by Ω. So, if we take a derivative of a quantity expressed in terms of original domain variable, we call it a *material derivative* and denote it with an over-dot as in $\dot{f} = \frac{df(\Omega_0)}{dp}$.

On the other hand, we use a prime for the *spatial derivative* as in $f' = \frac{df(\Omega)}{dp}$. There is a relation between the material and spatial derivatives: $\dot{f} = f' + \nabla f \cdot \mathbf{V}$ where $\mathbf{V} = \nabla_p \Omega = \frac{d\mathbf{x}}{dp} = \begin{Bmatrix} \partial x / \partial p \\ \partial y / \partial p \\ \partial z / \partial p \end{Bmatrix}$ is the "*shape velocity*" or "*design velocity*".

> Why is $\dot{f} = f' + \nabla f \cdot \mathbf{V}$ true?
>
> Note that $\dot{f} = \frac{df(\mathbf{X})}{dp}$ and $f' = \frac{df(\mathbf{x})}{dp}$.
>
> Generally, f is given or is known in terms of the spatial coordinates, which in turn depend on the material coordinates. Therefore,
>
> $\dot{f} = \frac{d}{dp}\{f(\mathbf{x}), \mathrm{p}\} = \frac{df(\mathbf{x}, p)}{dp} + \frac{\partial f(\mathbf{x}, p)}{\partial \mathbf{x}} \cdot \frac{d\mathbf{x}}{dp} = f' + \nabla f \cdot \mathbf{V}$
>
> Sometimes, we use the shorthand notation for the second term in the preceding equation: $\nabla f \cdot \mathbf{V} = f_{\mathrm{V}}$.

With this background, we want to compute:

$$\overline{\int_\Omega \dot{f}\, d\Omega} = \frac{d}{dp}\left(\int_\Omega f\, d\Omega\right) \tag{1}$$

when a parameter changes the domain from Ω_0 to Ω where f is the integrand of the domain integral of a performance measure that depends on the state variable and its derivatives. Notice that we used an over-dot here to indicate that we are taking a material derivative.

Note that we are taking the derivative w.r.t. to a parameter p of an integral where the integrand is integrated over the spatial domain, Ω. Since the spatial domain changes with the parameter, we cannot interchange differentiation and integration in Eq. (1). This is the tricky part. To overcome this difficulty, we change it to the material (original) domain, Ω_0, first, and then interchange the order of differentiation and integration.

Step 1:

$$\frac{d}{dp}\left(\int_{\Omega} f\, d\Omega\right) = \frac{d}{dp}\left(\int_{\Omega_0} f(\mathbf{X}, p)\left|\mathbf{J}(\mathbf{X}, p)\right| d\Omega_0\right) = \int_{\Omega_0} \frac{d}{dp}\left\{f(\mathbf{X}, p)\left|\mathbf{J}(\mathbf{X}, p)\right|\right\} d\Omega_0 \tag{2}$$

where $\mathbf{J}$ is the Jacobian of transformation from the material (original) domain to spatial (current) domain as in $d\mathbf{x} = \mathbf{J}\, d\mathbf{X}$ or $d\Omega = \left|\mathbf{J}\right| d\Omega_0$.

Now, we expand the integrand by differentiating using the product rule (Step 2) and then change the domain back to the spatial (current) domain (Step 3) to get

$$\text{Step 2: } \int_{\Omega_0} \frac{d}{dp}\left\{f(\mathbf{X}, p)\ \left|\mathbf{J}(\mathbf{X}, p)\right|\right\} d\Omega_0 = \int_{\Omega_0} \dot{\overline{f\left|\mathbf{J}\right|}}\ d\Omega_0 = \int_{\Omega_0}\left(\dot{f}\left|\mathbf{J}\right| + f\dot{\overline{\left|\mathbf{J}\right|}}\right) d\Omega_0 \tag{3a}$$

$$\text{Step 3: } \int_{\Omega_0}\left(\dot{f}\left|\mathbf{J}\right| + f\dot{\overline{\left|\mathbf{J}\right|}}\right) d\Omega_0 = \int_{\Omega}\left(\dot{f}\left|\mathbf{J}\right| + f\dot{\overline{\left|\mathbf{J}\right|}}\right)\frac{1}{\left|\mathbf{J}\right|} d\Omega \tag{3b}$$

By noting that $\dot{\overline{\left|\mathbf{J}\right|}} = \left|\mathbf{J}\right|\left(\nabla\cdot\mathbf{V}\right)$, we can simplify the preceding equation as

$$\begin{aligned} &\frac{d}{dp}\left(\int_{\Omega} f\, d\Omega\right) = \int_{\Omega}\left(\dot{f}\left|\mathbf{J}\right| + f\dot{\overline{\left|\mathbf{J}\right|}}\right)\frac{1}{\left|\mathbf{J}\right|} d\Omega = \int_{\Omega}\left\{\dot{f}\left|\mathbf{J}\right| + f\left|\mathbf{J}\right|\left(\nabla\cdot\mathbf{V}\right)\right\}\frac{1}{\left|\mathbf{J}\right|} d\Omega \\ &\Rightarrow \frac{d}{dp}\left(\int_{\Omega} f\, d\Omega\right) = \int_{\Omega}\left\{\dot{f} + f\left(\nabla\cdot\mathbf{V}\right)\right\} d\Omega \end{aligned} \tag{4}$$

By recalling that $\dot{f} = f' + \nabla f\cdot\mathbf{V}$, we have

$$\begin{aligned} &\frac{d}{dp}\left(\int_{\Omega} f\, d\Omega\right) = \int_{\Omega}\left\{\dot{f} + f\left(\nabla\cdot\mathbf{V}\right)\right\} d\Omega = \int_{\Omega}\left\{f' + \nabla f\cdot\mathbf{V} + f\left(\nabla\cdot\mathbf{V}\right)\right\} d\Omega \\ &\Rightarrow \frac{d}{dp}\left(\int_{\Omega} f\, d\Omega\right) = \int_{\Omega}\left\{f' + \nabla\cdot\left(f\mathbf{V}\right)\right\} d\Omega \end{aligned} \tag{5}$$

The result in Eq. (5) is known as the *Reynolds Transport theorem* if the parameter p is interpreted as time. By using the divergence theorem, this theorem can also be written in its partial boundary form (Step 4) as follows.

$$\frac{d}{dp}\left(\int_{\Omega} f\, d\Omega\right) = \int_{\Omega}\left\{f' + \nabla\cdot\left(f\mathbf{V}\right)\right\} d\Omega = \int_{\Omega} f'\, d\Omega + \int_{\Gamma} f\left(\mathbf{V}\cdot\mathbf{n}\right) d\Gamma \tag{6}$$

As it happens in structural and multidisciplinary optimization, when f depends on state variable(s) that are governed by differential equations, the integrand of the first term of the last result in the preceding equation cannot be obtained analytically. Finite difference derivative will be computationally expensive and defeats the purpose of analytical sensitivity calculation. So, we need to reduce the first term in Eq. (6) to something that does not involve any derivative of the state variable. We consider that situation with a 1D example first and then generalize it for the diffusion and elasticity equations in 2D and 3D. Before we do that, we should talk briefly about the material derivative of a boundary integral as well. This is because our derivation of the material derivative of a domain integral needs some new results that we discuss next.

Material derivative of a boundary integral

Let us consider

$$\phi = \int_{\Gamma} f\, d\Gamma \tag{7a}$$

where Γ is the boundary of Ω. We repeat what we did for the material derivative of a domain integral: change to the material domain (Step 1); interchange the order of differentiation and integration; differentiate the integrand (Step 2); and change back to the spatial domain (Step 3).

$$\dot{\phi} = \frac{d}{dp}\left[\int_{\Gamma_0} f\,|\mathbf{J}|\,\left\|\mathbf{J}^{-T}\mathbf{n}_0\right\|\, d\Gamma_0\right] \tag{7b}$$

$$\dot{\phi} = \int_{\Gamma_0} \frac{d}{dp}\left(f\,|\mathbf{J}|\,\left\|\mathbf{J}^{-T}\mathbf{n}_0\right\|\right) d\Gamma_0 = \int_{\Gamma_0}\left(\dot{f}\,|\mathbf{J}|\,\left\|\mathbf{J}^{-T}\mathbf{n}_0\right\| + f\,\overset{\bullet}{\overline{|\mathbf{J}|\,\left\|\mathbf{J}^{-T}\mathbf{n}_0\right\|}}\right) d\Gamma_0$$

$$= \int_{\Gamma_0}\left(\dot{f}\,|\mathbf{J}|\,\left\|\mathbf{J}^{-T}\mathbf{n}_0\right\| + f\,\overset{\bullet}{\overline{|\mathbf{J}|}}\left\|\mathbf{J}^{-T}\mathbf{n}_0\right\| + f\,|\mathbf{J}|\,\overset{\bullet}{\overline{\left\|\mathbf{J}^{-T}\mathbf{n}_0\right\|}}\right) d\Gamma_0$$

By noting that $\overset{\bullet}{\overline{|\mathbf{J}|}} = |\mathbf{J}|\nabla\cdot\mathbf{V}$ and $\overset{\bullet}{\overline{\left\|\mathbf{J}^{-T}\mathbf{n}_0\right\|}} = -(\nabla\mathbf{V}\mathbf{n}\cdot\mathbf{n})\left\|\mathbf{J}^{-T}\mathbf{n}_0\right\|$, we can write

$$\dot{\phi} = \int_{\Gamma_0} \left\{ \dot{f} + f\left(\nabla\cdot\mathbf{V} - \nabla\mathbf{V}\mathbf{n}\cdot\mathbf{n}\right) \right\} |\mathbf{J}| \left\|\mathbf{J}^{-T}\mathbf{n}_0\right\| d\Gamma_0$$

$$\Rightarrow \dot{\phi} = \int_{\Gamma} \left\{ \dot{f} + f\left(\nabla\cdot\mathbf{V} - \nabla\mathbf{V}\mathbf{n}\cdot\mathbf{n}\right) \right\} d\Gamma \quad \left[\because |\mathbf{J}|\left\|\mathbf{J}^{-T}\mathbf{n}_0\right\| d\Gamma_0 = d\Gamma\right] \tag{7c}$$

Derivation of $\overset{\bullet}{\overbrace{\left\|\mathbf{J}^{-T}\mathbf{n}_0\right\|}}$ using indicial notation

$$\overset{\bullet}{\overbrace{\left\|\mathbf{J}^{-T}\mathbf{n}_0\right\|}} = \frac{d}{dp}\left(\left\|\mathbf{J}^{-T}\mathbf{n}_0\right\|\right) = \frac{d}{dp}\left(\left\langle \mathbf{J}^{-T}\mathbf{n}_0, \mathbf{J}^{-T}\mathbf{n}_0\right\rangle\right)^{1/2} \left[\because \left\|\mathbf{J}^{-T}\mathbf{n}_0\right\| = \left(\left\langle \mathbf{J}^{-T}\mathbf{n}_0, \mathbf{J}^{-T}\mathbf{n}_0\right\rangle\right)^{1/2}\right]$$

$$= \frac{d}{dp}\left(\mathbf{J}_{ij}{}^{-T}\mathbf{n}_{0_j} \times \mathbf{J}_{ij}{}^{-T}\mathbf{n}_{0_j}\right)^{1/2}$$

$$= \frac{1}{2\left(\mathbf{J}_{ij}{}^{-T}\mathbf{n}_{0_j} \times \mathbf{J}_{ij}{}^{-T}\mathbf{n}_{0_j}\right)^{1/2}} \frac{d}{dp}\left(\mathbf{J}_{ij}{}^{-T}\mathbf{n}_{0_j} \times \mathbf{J}_{ij}{}^{-T}\mathbf{n}_{0_j}\right)$$

$$= \frac{2\times \mathbf{J}_{ij}{}^{-T}\mathbf{n}_{0_j}}{2\left\|\mathbf{J}^{-T}\mathbf{n}_0\right\|} \frac{d}{dp}\left(\mathbf{J}_{ij}{}^{-T}\mathbf{n}_{0_j}\right)$$

$$= \frac{\mathbf{J}_{ij}{}^{-T}\mathbf{n}_{0_j}}{\left\|J^{-T}n_0\right\|} \left(-\nabla\mathbb{V}_{ik}{}^{T}\mathbf{J}_{kj}{}^{-T}\mathbf{n}_{0_j}\right)$$

$$\left[\because \mathbf{n}_0 \text{ does not depend upon p and } \overset{\bullet}{\overline{\mathbf{J}^{-T}}} = \nabla\mathbf{V}^T\mathbf{J}^{-T}\right]$$

$$= \mathbf{n}_i \left(-\nabla\mathbb{V}_{ik}{}^{T}\mathbf{J}_{kj}{}^{-T}\mathbf{n}_{0_j}\right) \left[\because \quad n_i = \frac{J_{ij}{}^{-T}n_{0_j}}{\left\|J^{-T}n_0\right\|}\right]$$

$$= \frac{\mathbf{n}_i \left(-\nabla\mathbf{V}_{ik}{}^{T}\mathbf{J}_{kj}{}^{-T}\mathbf{n}_{0_j}\right)}{\left\|\mathbf{J}^{-T}\mathbf{n}_0\right\|} \times \left\|\mathbf{J}^{-T}\mathbf{n}_0\right\|$$

$$= \mathbf{n}_i \left(-\nabla\mathbf{V}_{ik}{}^{T}\mathbf{n}_k\right) \left\|\mathbf{J}^{-T}\mathbf{n}_0\right\| \left[\because \quad n_k = \frac{J_{kj}{}^{-T}n_{0_j}}{\left\|J^{-T}n_0\right\|}\right]$$

$$= \left\{ \mathbf{n} \bullet \left(-\nabla\mathbf{V}^T\mathbf{n}\right) \right\} \left\|\mathbf{J}^{-T}\mathbf{n}_0\right\|$$

$$= -(\nabla \mathbf{V}\mathbf{n} \bullet \mathbf{n})\left\|\mathbf{J}^{-T}\mathbf{n}_0\right\| \left[\because\ \mathbf{n} \bullet \mathbf{A}\mathbf{n} = \mathbf{A}^T\mathbf{n} \bullet \mathbf{n}\right]$$

$$\Rightarrow \quad \overbrace{\left\|\mathbf{J}^{-T}\mathbf{n}_0\right\|}^{\bullet} = -(\nabla \mathbf{V}\mathbf{n} \bullet \mathbf{n})\left\|\mathbf{J}^{-T}\mathbf{n}_0\right\|$$

Since only the normal component of the boundary needs to be considered while taking the derivative, we can replace $\mathbf{V}$ with $\mathbf{V} = V_n\,\mathbf{n}$. With some manipulation shown in the box, we get the compact final result:

$$\dot{\phi} = \int_{\Gamma} \left\{ \dot{f} + f\kappa V_n \right\} d\Gamma \tag{8}$$

where $\nabla \cdot \mathbf{n} = \kappa$, **the curvature.**

If $\mathbf{V} = V_n\,\mathbf{n}$ then

$$\nabla \mathbf{V} = \nabla(V_n \mathbf{n}) = \mathbf{n} \otimes \nabla V_n + V_n \nabla \mathbf{n}$$

$$\left(\nabla \mathbf{V}^T\right)\mathbf{n} = \left(\nabla V_n \otimes \mathbf{n}\right)\mathbf{n} + V_n \left(\nabla \mathbf{n}\right)^T \mathbf{n} \left[\mathit{But\ as}\ \nabla\left(\mathbf{n} \bullet \mathbf{n}\right) = 0 \ \Rightarrow \left(\nabla \mathbf{n}\right)^T \mathbf{n} = \mathbf{0}\right]$$

$$\left(\nabla \mathbf{V}^T\right)\mathbf{n} = \left(\nabla V_n \otimes \mathbf{n}\right)\mathbf{n}$$

$$\left(\nabla \mathbf{V}^T\right)\mathbf{n} = \left(\mathbf{n}.\mathbf{n}\right)\nabla V_n$$

$$\left(\nabla \mathbf{V}^T\right)\mathbf{n} = \nabla V_n$$

Now consider the 2nd expression in Eq. (35d). Then,

$$\left(\nabla \bullet \mathbf{V} - \nabla \mathbf{V}\mathbf{n} \bullet \mathbf{n}\right) = \nabla \bullet \left(V_n \mathbf{n}\right) - \mathbf{n} \bullet \left\{\left(\nabla \mathbf{V}\right)^T \mathbf{n}\right\} \quad \left[\because\ \mathbf{n} \bullet \mathbf{A}\mathbf{n} = \mathbf{A}^T\mathbf{n} \bullet \mathbf{n}\right]$$

Using relation for $\left(\nabla \mathbf{V}^T\right)\mathbf{n}$ above Eq. reduces to

$$\left(\nabla \bullet \mathbf{V} - \nabla \mathbf{V}\mathbf{n} \bullet \mathbf{n}\right) = \nabla \bullet \left(V_n \mathbf{n}\right) - \mathbf{n} \bullet \nabla V_n$$

$$= \nabla V_n \bullet \mathbf{n} + V_n \nabla \bullet \mathbf{n} - \mathbf{n} \bullet \nabla V_n$$

$$\Rightarrow \left(\nabla \bullet \mathbf{V} - \nabla \mathbf{V}\mathbf{n} \bullet \mathbf{n}\right) = V_n \nabla \bullet \mathbf{n}$$

$$\Rightarrow \left(\nabla \bullet \mathbf{V} - \nabla \mathbf{V}\mathbf{n} \bullet \mathbf{n}\right) = V_n \kappa \left[\mathit{where}\ \nabla \bullet \mathbf{n} = \kappa\right]$$

Now, let us look at the material derivative of the domain integral in 1D and solve it using four different methods, as we had done for parameter sensitivity.

Example 1

Compute $\frac{d}{dl}\left(\int_0^l pu\,dx\right)$ at $l=L$ where the state variable $u(x)$ is governed by $EA\frac{d^2u}{dx^2}+p=0$ with the boundary conditions, $u_{x=0}=0$ and $\left.\frac{du}{dx}\right|_{x=L}=0$. Note that we want to compute the derivative of the mean compliance (work done by the external force) of an axially loaded bar with respect to the changed domain in one dimension. It is a 1D problem considered to understand the concept easily. Here, we are considering the case where the length of the bar is changed as shown in Fig. 1. We want to compute the derivative w.r.t. the length of the bar itself.

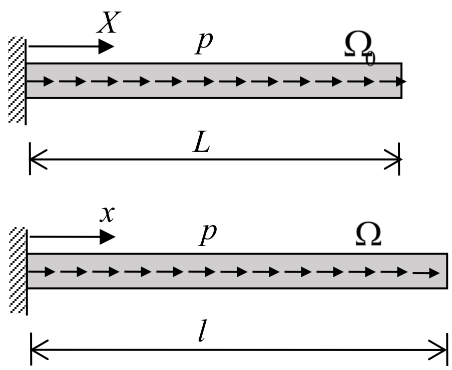

Fig. 1. A simple 1D problem of an axially loaded bar where the domain is elongated, not because of deformation but because of change of shape (or size here) of the domain.

Solution

Method A (direct closed-form)

The solution of $EA\frac{d^2u}{dx^2}+p=0$ with the boundary conditions, $u_{x=0}=0$ and $\left.\frac{du}{dx}\right|_{x=L}=0$ is given by $u=-\frac{px^2}{2EA}+\frac{pLx}{EA}$. Therefore, we have

$$\begin{aligned}&\frac{d}{dl}\left(\int_0^l pu\,dx\right)=\frac{d}{dl}\left\{\int_0^l p\left(-\frac{px^2}{2EA}+\frac{plx}{EA}\right)dx\right\}=\\&\frac{d}{dl}\left\{\left(\frac{p^2}{EA}\right)\left(-\frac{l^3}{6}+\frac{l^3}{2}\right)\right\}=\frac{d}{dl}\left(\frac{p^2l^3}{3EA}\right)=\frac{p^2l^2}{EA}\text{ or }\frac{p^2L^2}{EA}\end{aligned}\tag{9}$$

Method B (roundabout closed-form)

This will look like a roundabout method as this is a simple example, but it will prove to be useful for problems where the state variable can only be solved numerically.

In this method, we first change from the spatial to material domain. This allows us to interchange the order of differentiation and integration. Then, we change the domain back to spatial coordinates for further manipulation.

$$\frac{d}{dl}\left(\int_0^l pu\,dx\right) = \frac{d}{dl}\left(\int_0^L pu\frac{dx}{dX}dX\right) = \int_0^L \left\{\frac{d}{dl}\left(pu\frac{dx}{dX}\right)\right\}dX$$

$$= \int_0^l \left\{\frac{d}{dl}\left(pu\frac{dx}{dX}\right)\right\}\frac{dX}{dx}dx \tag{10}$$

$$= \int_0^l p\left\{\frac{du}{dl}\frac{dx}{dX} + u\frac{d}{dl}\left(\frac{dx}{dX}\right)\right\}\frac{dX}{dx}dx$$

We notice that

$$\frac{d}{dl}\left(\frac{dx}{dX}\right) = \frac{d}{dX}\left(\frac{dx}{dl}\right) = \frac{dV}{dX} = \frac{dV}{dx}\frac{dx}{dX} \tag{11a}$$

and $$\frac{du}{dl} = \frac{\partial u}{\partial l} + \frac{du}{dx}\frac{dx}{dl} = \frac{\partial u}{\partial l} + \frac{du}{dx}V \tag{11b}$$

The preceding step may be seen as the 1D equivalent of $\dot{f} = f' + \nabla f \cdot \mathbf{V}$ used in Eq. (5). Now, Eqs. (9a-b) into Eq. (8) lead to

$$\frac{d}{dl}\left(\int_0^l pu\,dx\right) = \int_0^l p\left\{\frac{du}{dl}\frac{dx}{dX} + u\frac{d}{dl}\left(\frac{dx}{dX}\right)\right\}\frac{dX}{dx}dx$$

$$= \int_0^l p\left\{\left(\frac{\partial u}{\partial l} + \frac{du}{dx}V\right)\frac{dx}{dX} + u\left(\frac{dV}{dx}\frac{dx}{dX}\right)\right\}\frac{dX}{dx}dx \tag{12}$$

$$= \int_0^l p\left\{\left(\frac{\partial u}{\partial l} + \frac{du}{dx}V\right) + u\frac{dV}{dx}\right\}dx = \int_0^l p\left\{\left(\frac{\partial u}{\partial l} + \frac{d}{dx}(uV)\right)\right\}dx$$

$$= \int_0^l p\frac{\partial u}{\partial l}dx + p(uV)\Big|_0^l$$

Up to this point, it is a general procedure. Here onwards, we use the known solution of $u = -\frac{px^2}{2EA} + \frac{pLx}{EA}$ to get

$$\frac{d}{dl}\left(\int_0^l pu\,dx\right) = \int_0^l p\frac{\partial u}{\partial l}dx + p(uV)\Big|_0^l$$

$$= \int_0^l p\left(\frac{px}{EA}\right)dx + pu_{x=l} = \frac{p^2l^2}{2EA} + p\left(-\frac{pl^2}{2EA} + \frac{pl^2}{EA}\right) = \frac{p^2l^2}{EA} \text{ or } \frac{p^2L^2}{EA} \tag{13}$$

The last line of the preceding equation needs explanation for the boundary term. First, we note that both u and V are zero at $x=0$. At $x=l$, $V=\dfrac{dx}{dl}=1$.

So, we got the same answer in Eq. (13) that we got in Eq. (9). But what if we pretend that we do not know the analytical solution for $u(x)$ that satisfies the differential equation and the boundary conditions? Then, we will be stuck with the end result of Eq. (12). We will continue from there in what follows, first by using the adjoint method (which avoids computing $\dfrac{\partial u}{\partial l}$) and the direct method (which solves the sensitivity equation to solve for $\dfrac{\partial u}{\partial l}$).

<u>Method 1 (adjoint method)</u>

In the adjoint method, we add the governing equation multiplied by $\lambda(x)$ to the domain integral whose sensitivity we want to find, and then differentiate it. This, although may seem like a clever trick, is perfectly logical because we are only adding something that is identically zero. In fact, it is logical if we think in terms of the Lagrangian used in optimization where we add Lagrange multiplier times the constraint expression.

<u>Step 1</u> (add the governing equation multiplied by λ.

$$\frac{d\psi}{dl}=\frac{d}{dl}\left[\int_0^l\left\{pu+\lambda\left(EA\frac{d^2u}{dx^2}+p\right)\right\}dx\right]=\left\{\frac{d}{dl}\left(\int_0^l pu\,dx\right)\right\}+\frac{d}{dl}\left[\int_0^l\left\{\lambda\left(EA\frac{d^2u}{dx^2}+p\right)\right\}dx\right] \tag{14}$$

By doing integration by parts for the second term of Eq. (14), we write:

$$\frac{d\psi}{dl}=\left\{\frac{d}{dl}\left(\int_0^l pu\,dx\right)\right\}+\frac{d}{dl}\left\{\left(\lambda EA\frac{du}{dx}\right)\Big|_0^l\right\}+\frac{d}{dl}\left\{\int_0^l\left(-EA\frac{d\lambda}{dx}\frac{du}{dx}+\lambda p\right)dx\right\} \tag{15}$$

<u>Step 2</u> (Reynolds Transport Theorem)

By applying the Reynolds Transport Theorem (RTP) to the first term of the preceding equation, we get

$$\frac{d}{dl}\left(\int_0^l pu\,dx\right)=\int_0^l\left\{pu'+\frac{d}{dx}\left(puV\right)\right\}dx=\int_0^l pu'\,dx+\left(puV\right)\Big|_0^l \tag{16a}$$

where $u'=\dfrac{du}{dl}$ is the spatial derivative.

By applying the Reynolds Transport Theorem to the third term of Eq. (15), we have

$$\frac{d}{dl}\left\{\int_0^l\left(-EA\frac{d\lambda}{dx}\frac{du}{dx}+\lambda p\right)dx\right\}=\int_0^l\left(-EA\frac{d\lambda}{dx}\frac{du}{dx}+\lambda p\right)'dx+\left(-EA\frac{d\lambda}{dx}\frac{du}{dx}V+\lambda pV\right)\Big|_0^l \tag{16b}$$

Now, we expand the first term of the preceding equation by taking spatial derivative to get

$$\begin{aligned}&\frac{d}{dl}\left\{\int_0^l\left(-EA\frac{d\lambda}{dx}\frac{du}{dx}+\lambda p\right)'dx\right\}\\&=\int_0^l\left(-EA\frac{d\lambda'}{dx}\frac{du}{dx}-EA\frac{d\lambda}{dx}\frac{du'}{dx}+\lambda' p\right)dx+\left(-EA\frac{d\lambda}{dx}\frac{du}{dx}V+\lambda pV\right)\Bigg|_0^l\end{aligned}\tag{16c}$$

We also expand the second term of Eq. (15).

$$\begin{aligned}&\frac{d}{dl}\left\{\left(\lambda EA\frac{du}{dx}\right)\Bigg|_0^l\right\}=\left(EA\frac{d\lambda}{dl}\frac{du}{dx}\right)\Bigg|_0^l+\left(EA\lambda\frac{d\left(\frac{du}{dx}\right)}{dl}\right)\Bigg|_0^l\\&=\left(EA\lambda'\frac{du}{dx}\right)\Bigg|_0^l+\left(EA\lambda\frac{du'}{dx}\right)\Bigg|_0^l\end{aligned}\tag{16d}$$

Now, by adding terms in Eqs. (16a), (16c), and (16d), we get

$$\begin{aligned}&\frac{d\psi}{dl}=\int_0^l pu'\,dx+\left(puV\right)\Big|_0^l+\left(EA\lambda'\frac{du}{dx}\right)\Bigg|_0^l+\left(EA\lambda\frac{du'}{dx}\right)\Bigg|_0^l\\&+\int_0^l\left(-EA\frac{d\lambda'}{dx}\frac{du}{dx}-EA\frac{d\lambda}{dx}\frac{du'}{dx}+\lambda' p\right)dx+\left(-EA\frac{d\lambda}{dx}\frac{du}{dx}V+\lambda pV\right)\Bigg|_0^l\end{aligned}\tag{17}$$

Step 3 (Re-grouping terms to simplify by analogy with the weak form)

Note that the weak form of the governing equation.

$$\begin{aligned}&EA\frac{d^2u}{dx^2}+p=0\Rightarrow\int_0^l\left(EA\frac{d^2u}{dx^2}+p\right)v\,dx=0\\&\Rightarrow EAv\frac{du}{dx}\Bigg|_0^l-\int_0^l\left(EA\frac{dv}{dx}\frac{du}{dx}-pv\right)dx=0\end{aligned}\tag{18}$$

where v is the weak variable and p is the load. We solve for u using this equation.

By considering the preceding equation, we re-group the terms of Eq. (17):

$$\frac{d\psi}{dl} = \left\{ \int_0^l \left(-EA\frac{d\lambda}{dx}\frac{du'}{dx} + pu' \right) dx \right\} + \left\{ \int_0^l \left(-EA\frac{d\lambda'}{dx}\frac{du}{dx} + \lambda' p \right) dx + \left(EA\lambda'\frac{du}{dx} \right)\Bigg|_0^l \right\} + \left(puV \right)\Big|_0^l + \left(EA\lambda\frac{du'}{dx} \right)\Bigg|_0^l + \left(-EA\frac{d\lambda}{dx}\frac{du}{dx}V + \lambda pV \right)\Bigg|_0^l \tag{19}$$

The first bracketed expression is replaced with $EAu'\frac{d\lambda}{dx}\Big|_0^l$ by virtue of the weak form with u' as the weak variable to get

$$\frac{d\psi}{dl} = \left\{ EAu'\frac{d\lambda}{dx}\Bigg|_0^l \right\} + \left\{ \int_0^l \left(-EA\frac{d\lambda'}{dx}\frac{du}{dx} + \lambda' p \right) dx + \left(EA\lambda'\frac{du}{dx} \right)\Bigg|_0^l \right\} + \left(puV \right)\Big|_0^l + \left(EA\lambda\frac{du'}{dx} \right)\Bigg|_0^l + \left(-EA\frac{d\lambda}{dx}\frac{du}{dx}V + \lambda pV \right)\Bigg|_0^l \tag{20}$$

The second bracketed expression is zero as it is the weak form of the governing equation with λ' as the weak variable. Then, we are left with the following terms:

$$\frac{d\psi}{dl} = \left(puV \right)\Big|_0^l + EA\lambda\frac{du'}{dx}\Bigg|_0^l + \left(-EA\frac{d\lambda}{dx}\frac{du}{dx}V + \lambda pV \right)\Bigg|_0^l + EAu'\frac{d\lambda}{dx}\Bigg|_0^l \tag{21}$$

Notice that all the terms on the right hand side of the preceding equation are to be evaluated at only the boundary. In this example, since we take $\lambda = u$ as the first bracketed expression in Eq. (19) actually means that with $EAu'\frac{d\lambda}{dx}\Big|_0^l$ added.

Now, let us evaluate each term in Eq. (21) assuming the fixed-free bar conditions.

$$\left(puV \right)\Big|_0^l = pu_l \text{ because } u_0 = 0 \text{ and } V_l = \frac{dx}{dl}\Bigg|_l = 1 \tag{22a}$$

$$EAu\frac{du'}{dx}\Bigg|_0^l = 0 \text{ because } u_0 = 0 \text{ and } \frac{du'}{dx}\Bigg|_l = \frac{d}{dl}\left(\frac{du}{dx} \right)_l = 0 \tag{22b}$$

$$\left(-EA\frac{d\lambda}{dx}\frac{du}{dx}V + upV \right)\Bigg|_0^l = \left(-EA\frac{du}{dx}\frac{du}{dx}V + upV \right)\Bigg|_l = pu_l \tag{22c}$$

because $V_0 = 0$ and $\left(\frac{du}{dx}\right)\Big|_l = 0\,; V_l = \frac{dx}{dl}\Big|_l = 1$.

$EAu'\frac{d\lambda}{dx}\Big|_0^l = 0$ because $u'\big|_{x=0} = \frac{du}{dl}\Big|_{x=0} = 0$ as u is specified there; and $\frac{d\lambda}{dx}\Big|_{x=l} = \frac{du}{dx}\Big|_{x=l} = 0$. (22d)

Thus, we finally get

$$\frac{d}{dl}\left(\int_0^l pu\,dx\right) = 2\,pu_l = \frac{p^2 l^2}{EA} = \frac{p^2 L^2}{EA} \tag{23}$$

which is the same result we got earlier in Eqs. (9) and (13).

The adjoint method proved to be somewhat tedious in this example. But it is actually the most convenient in practice as we can reduce the material derivative to the computation of the boundary terms after solving the adjoint equation. The three steps need to be kept in mind as we consider other examples.

<u>Method 2 (direct method)</u>

We begin with $\frac{d}{dl}\left(\int_0^l pu\,dx\right) = \int_0^l p\left\{\left(\frac{du}{dl} + \frac{d}{dx}(uV)\right)\right\}dx$. In order to compute $\frac{du}{dl} = u'$, which we avoid in the adjoint method, we use the governing differential equation and differentiate it with respect to the parameter to get the sensitivity equation. That is,

$$\begin{aligned} &\frac{d}{dl}\left(EA\frac{d^2u}{dx^2} + p\right) = EA\frac{d}{dl}\left(\frac{d^2u}{dx^2}\right) = EA\frac{d^2}{dx^2}\left(\frac{du}{dl}\right) = 0 \\ &\Rightarrow \left(\frac{du}{dl}\right) = C_1 x + C_2 \end{aligned} \tag{24}$$

Since $u_{x=0}$ is specified, $\left(\frac{\partial u}{\partial l}\right)_{x=0} = 0 \Rightarrow C_2 = 0$ in the preceding equation. Since we know $u(x) = -\frac{px^2}{2EA} + \frac{plx}{EA}$, we find that $C_1 = \frac{p}{EA}$. By substituting $\left(\frac{du}{dl}\right) = \frac{p}{EA}x$ into $\frac{d}{dl}\left(\int_0^l pu\,dx\right) = \int_0^l p\left\{\left(\frac{\partial u}{\partial l} + \frac{d}{dx}(uV)\right)\right\}dx$, we get

$$\frac{d}{dl}\left(\int_0^l pu\,dx\right)=\int_0^l p\left\{\left(\frac{du}{dl}+\frac{d}{dx}(uV)\right)\right\}dx=\int_0^l \frac{p^2x}{EA}dx+(uV)\Big|_0^l$$
$$=\frac{p^2l^2}{2EA}+pu_{x=l}=\frac{p^2l^2}{2EA}+p\left(-\frac{pl^2}{2EA}+\frac{pl^2}{EA}\right)=\frac{p^2l^2}{EA}\text{ or }\frac{p^2L^2}{EA} \tag{25}$$

Note that in the last step of the preceding equation, we have used the analytical expression for $u_{x=l}$ even though we pretended that we did not know the analytical solution. We did this only to show that we get the same correct answer with this method. In practice, we will simply substitute the numerical solution that we already know in order to compute the numerical value of the domain-parameter sensitivity.

Example 2

Compute $\frac{d}{dl}\left(\int_0^l u^2\,dx\right)$ at $l=L$ where the state variable $u(x)$ is governed by $EA\frac{d^2u}{dx^2}+p=0$ with the boundary conditions, $u_{x=0}=0$ and $\left.\frac{du}{dx}\right|_{x=L}=0$. Use the adjoint method.

Solution

In this simple problem, we can get the solution in closed-form. Let us do it so that it will serve the purpose of verifying the solution obtained with the step-wise procedure of the adjoint method.

<u>Closed-form solution:</u>

Since we know $u=\frac{-px^2}{2EA}+\frac{plx}{EA}$, we get

$$\frac{d}{dl}\left[\int_0^l \{u^2\}\,dx\right]=\frac{d}{dl}\left[\int_0^l\left(\frac{-px^2}{2EA}+\frac{plx}{EA}\right)^2dx\right]=\frac{2p^2l^4}{3E^2A^2} \tag{26}$$

We follow the three steps of the adjoint method as we did in Example 1.

<u>Step 1</u> (add the governing equation multiplied by λ.

$$\frac{d\psi}{dl}=\frac{d}{dl}\left[\int_0^l\left\{u^2+\lambda\left(EA\frac{d^2u}{dx^2}+p\right)\right\}dx\right]=\left\{\frac{d}{dl}\left(\int_0^l u^2\,dx\right)\right\}+\frac{d}{dl}\left[\int_0^l\left\{\lambda\left(EA\frac{d^2u}{dx^2}+p\right)\right\}dx\right] \tag{27}$$

By doing integration by parts for the second term of Eq. (27), we write:

$$\frac{d\psi}{dl}=\left\{\frac{d}{dl}\left(\int_0^l u^2\,dx\right)\right\}+\frac{d}{dl}\left\{\left(\lambda EA\frac{du}{dx}\right)\Big|_0^l\right\}+\frac{d}{dl}\left\{\int_0^l\left(-EA\frac{d\lambda}{dx}\frac{du}{dx}+\lambda p\right)dx\right\} \tag{28}$$

Step 2 (Reynolds Transport Theorem)

By applying the Reynolds Transport Theorem (RTP) to the first term of the preceding equation, we get

$$\frac{d}{dl}\left(\int_0^l u^2\,dx\right)=\int_0^l 2uu'\,dx+\left(u^2V\right)\Big|_0^l \tag{29a}$$

where $u'=\dfrac{du}{dl}$ is the spatial derivative.

By applying the Reynolds Transport Theorem to the third term of Eq. (28), we have

$$\frac{d}{dl}\left\{\int_0^l\left(-EA\frac{d\lambda}{dx}\frac{du}{dx}+\lambda p\right)dx\right\}=\int_0^l\left(-EA\frac{d\lambda}{dx}\frac{du}{dx}+\lambda p\right)'dx+\left(-EA\frac{d\lambda}{dx}\frac{du}{dx}V+\lambda pV\right)\Bigg|_0^l \tag{29b}$$

Now, we expand the first term of the preceding equation by taking spatial derivative to get

$$\begin{aligned}&\frac{d}{dl}\left\{\int_0^l\left(-EA\frac{d\lambda}{dx}\frac{du}{dx}+\lambda p\right)'dx\right\}\\&=\int_0^l\left(-EA\frac{d\lambda'}{dx}\frac{du}{dx}-EA\frac{d\lambda}{dx}\frac{du'}{dx}+\lambda' p\right)dx+\left(-EA\frac{d\lambda}{dx}\frac{du}{dx}V+\lambda pV\right)\Bigg|_0^l\end{aligned} \tag{29c}$$

We also expand the second term of Eq. (27).

$$\begin{aligned}&\frac{d}{dl}\left\{\left(\lambda EA\frac{du}{dx}\right)\Bigg|_0^l\right\}=\left(EA\frac{d\lambda}{dl}\frac{du}{dx}\right)\Bigg|_0^l+\left(EA\lambda\frac{d\left(\frac{du}{dx}\right)}{dl}\right)\Bigg|_0^l\\&=\left(EA\lambda'\frac{du}{dx}\right)\Bigg|_0^l+\left(EA\lambda\frac{du'}{dx}\right)\Bigg|_0^l\end{aligned} \tag{29d}$$

Now, by adding terms in Eqs. (29a), (29c), and (29d), we get

$$\begin{aligned}\frac{d\psi}{dl}&=\int_0^l 2uu'\,dx+\left(u^2V\right)\Big|_0^l+\left(EA\lambda'\frac{du}{dx}\right)\Bigg|_0^l+\left(EA\lambda\frac{du'}{dx}\right)\Bigg|_0^l\\&+\int_0^l\left(-EA\frac{d\lambda'}{dx}\frac{du}{dx}-EA\frac{d\lambda}{dx}\frac{du'}{dx}+\lambda' p\right)dx+\left(-EA\frac{d\lambda}{dx}\frac{du}{dx}V+\lambda pV\right)\Bigg|_0^l\end{aligned} \tag{30}$$

Step 3 (Re-grouping terms to simplify by analogy with the weak form)

$$\frac{d\psi}{dl} = \left\{ \int_0^l \left(-EA\frac{d\lambda}{dx}\frac{du'}{dx} + 2uu' \right) dx \right\} + \left\{ \int_0^l \left(-EA\frac{d\lambda'}{dx}\frac{du}{dx} + \lambda' p \right) dx + \left(EA\lambda'\frac{du}{dx} \right)\Bigg|_0^l \right\} + \left(u^2 V \right)\Big|_0^l + \left(EA\lambda\frac{du'}{dx} \right)\Bigg|_0^l + \left(-EA\frac{d\lambda}{dx}\frac{du}{dx}V + \lambda p V \right)\Bigg|_0^l \tag{31}$$

Now, by virtue of the weak form with u' as the weak variable, we can solve for $\lambda(x)$ using the first bracketed expression after adding its boundary conditions ($EAu'\frac{d\lambda}{dx}\Big|_0^l$, which is assumed to be zero). The second bracketed expression is zero as it is the weak form of the governing equation with λ' as the weak variable. Then, we are left with the following terms:

$$\frac{d\psi}{dl} = \left(u^2 V \right)\Big|_0^l + EA\lambda\frac{du'}{dx}\Bigg|_0^l + \left(-EA\frac{d\lambda}{dx}\frac{du}{dx}V + \lambda p V \right)\Bigg|_0^l + EAu'\frac{d\lambda}{dx}\Bigg|_0^l \tag{32}$$

Notice that all the terms on the right hand side of the preceding equation are to be evaluated only at the boundary. Now, let us evaluate each term in Eq. (32) assuming a fixed-free bar.

$$\left(u^2 V \right)\Big|_0^l = u_l^2 \text{ because } u_0 = 0 \text{ and } V_l = \frac{dx}{dl}\Big|_l = 1 \tag{33a}$$

$$EA\lambda\frac{du'}{dx}\Bigg|_0^l = EA\lambda\frac{du'}{dx}\Bigg|_l \text{ because } \left(\frac{du}{dx} \right)\Bigg|_l = 0 \tag{33b}$$

$$\left(-EA\frac{d\lambda}{dx}\frac{du}{dx}V + \lambda p V \right)\Bigg|_0^l = p\lambda_l \text{ because } V_0 = 0 \text{ and} \left(\frac{du}{dx} \right)\Bigg|_l = 0\, ; V_l = \frac{dx}{dl}\Big|_l = 1\,. \tag{33c}$$

$$EAu'\frac{d\lambda}{dx}\Bigg|_0^l = 0 \text{ because } u'\big|_{x=0} = \frac{du}{dl}\Bigg|_{x=0} = 0 \text{ as } u \text{ is specified there; and } \frac{d\lambda}{dx}\Bigg|_{x=l} = 0\,. \tag{33d}$$

Thus, we finally get

$$\frac{d}{dl}\left[\int_0^l \left\{ u^2 \right\} dx \right] = u_l^2 + \lambda EA\frac{du'}{dx}\Bigg|_0 + p\lambda\big|_l \tag{34}$$

Here, we note that assuming $\lambda_{x=0} = 0$ is useful as u (state variable) and λ (adjoint variable) often have the same boundary conditions. For the purpose of verification, we note that $u_{x=l} = \dfrac{pl^2}{2EA}$ and $\lambda_{x=l} = \dfrac{5pl^4}{12E^2A^2}$, and get the final answer:

$$\frac{d}{dl}\left[\int_0^l \left\{u^2\right\} dx\right] = u_{x=l}^2 + \left(\lambda p\right)_{x=l} = \left(\frac{p^2l^4}{4E^2A^2}\right) + \left(\frac{5p^2l^4}{12E^2A^2}\right) = \frac{2p^2l^4}{3E^2A^2}$$

Now by comparing with the closed-form solution given in Eq. (26), we find that we got the same result by adjoint method. The nice thing about the adjoint method is that the material derivative depends only on the boundary quantities.

Example 3

Compute $\dfrac{d}{dl}\left(\int_0^l f(u, \dfrac{du}{dx})\, dx\right)$ at $l = L$ where the state variable $u(x)$ is governed by $EA\dfrac{d^2u}{dx^2} + p = 0$ with the boundary conditions, $u_{x=0} = 0$ and $\left.\dfrac{du}{dx}\right|_{x=L} = 0$. Use the adjoint method.

Solution (steps left as an exercise)

This example is identical to the last two examples except that the functional is different. In the equation used to solve for $\lambda(x)$, in Example 1, the adjoint load was p; that in Example 2 was $2u$. If notice, the adjoint load is simply the derivative of the integrand of the functional w.r.t. to the state variable. So, in this third example, the adjoint load will be $\dfrac{\partial f}{\partial u} - \dfrac{\partial}{\partial x}\left\{\dfrac{\partial f}{\partial\left(du/dx\right)}\right\}$. And there will be one more boundary term.

Now, it becomes clear that computing the material derivative of a domain integral entails solving the adjoint equation and then evaluating the terms only at the boundary.