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# Sensitivities of the Electroquasistatic Problem

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Supplementary material for the article “Adjoint Variable Method for Transient Nonlinear Electroquasistatic Problems” published in *Electrical Engineering* by Springer

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## 1 Electroquasistatic Problem

The nonlinear electroquasistatic (EQS) problem in time domain reads

$$\operatorname{div}(\mathbf{J}) + \operatorname{div}\left(\frac{\partial \mathbf{D}}{\partial t}\right) = 0 \quad t \in [0, T], \mathbf{r} \in \Omega; \quad (1a)$$

$$\mathbf{J} = \sigma \mathbf{E} \quad t \in [0, T], \mathbf{r} \in \Omega; \quad (1b)$$

$$\mathbf{D} = \varepsilon \mathbf{E} \quad t \in [0, T], \mathbf{r} \in \Omega; \quad (1c)$$

$$\mathbf{E} = -\operatorname{grad}(\phi) \quad t \in [0, T], \mathbf{r} \in \Omega; \quad (1d)$$

$$\phi = \phi_{\text{fixed}} \quad t \in [0, T], \mathbf{r} \in \Gamma_e; \quad (1e)$$

$$\left(\mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}\right) \cdot \mathbf{n} = 0 \quad t \in [0, T], \mathbf{r} \in \Gamma_m; \quad (1f)$$

$$\phi = \phi_0 \quad t = 0, \mathbf{r} \in \Omega, \quad (1g)$$

where  $\mathbf{J}$  is the current density,  $\mathbf{D}$  is the electric displacement field and  $\mathbf{E}$  is the electric field.  $\phi$  is the electric potential and  $\sigma$  and  $\varepsilon$  represent the electric conductivity and permittivity, respectively. The time variable is denoted by  $t$  and the position vector by  $\mathbf{r}$ .  $\Omega$  is the computational domain and  $T$  is the terminal simulation time.  $\phi_{\text{fixed}}$  are the fixed voltages at the electrodes,  $\Gamma_e \neq \emptyset$ , and  $\mathbf{n}$  is the unit vector at the magnetic boundaries,  $\Gamma_m = \partial\Omega \setminus \Gamma_e$ . The initial condition at  $t = 0$  is denoted by  $\phi_0$ . Eliminating  $\mathbf{J}$  and  $\mathbf{E}$  leads to

$$-\operatorname{div}(\sigma \operatorname{grad}(\phi)) - \operatorname{div}\left(\frac{\partial}{\partial t}(\varepsilon \operatorname{grad}(\phi))\right) = 0 \quad t \in [0, T], \mathbf{r} \in \Omega; \quad (2a)$$

$$\phi = \phi_{\text{fixed}} \quad t \in [0, T], \mathbf{r} \in \Gamma_e; \quad (2b)$$

$$\left(-\sigma \operatorname{grad}(\phi) - \frac{\partial}{\partial t}(\varepsilon \operatorname{grad}(\phi))\right) \cdot \mathbf{n} = 0 \quad t \in [0, T], \mathbf{r} \in \Gamma_m; \quad (2c)$$

$$\phi = \phi_0 \quad t = 0, \mathbf{r} \in \Omega. \quad (2d)$$

## 2 Sensitivities of the Nonlinear Electroquasistatic Problem

Sensitivities describe how a given quantity of interest (QoI),  $G(\phi(p), p)$ , is influenced by a design parameter,  $p$ , i.e.  $\frac{dG}{dp}(p_0)$ , where  $p_0$  is the currently active parameter value. In the following, two approaches for computing sensitivities of nonlinear EQS problems are presented, namely the direct sensitivity method (DSM) and the adjoint variable method (AVM). The derivations will focus on parameters that influence the material characteristics, i.e.  $\sigma(\mathbf{E}(p), p)$  and  $\varepsilon(\mathbf{E}(p), p)$ .

### 2.1 Direct Sensitivity Method for the Electroquasistatic Problem

One of the most common methods for sensitivity computation is the DSM [1]. For the DSM, the sensitivity is written in more detail using the chain rule,

$$\frac{dG}{dp}(p_0) = \frac{\partial G}{\partial p}(\phi(p_0), p_0) + \frac{\partial G}{\partial \phi}(\phi(p_0), p_0) \frac{d\phi}{dp}(p_0), \quad (3)$$

where the sensitivity of the electric potential,  $\frac{d\phi}{dp}(p_0)$ , is generally unknown. The DSM computes this unknown term by solving the linear sensitivity formulation, i.e. the derivative of (1) to  $p$ . The sensitivity formulation for nonlinear EQS problems in time domain reads

$$\operatorname{div}\left(\frac{d\mathbf{J}}{dp}\right) + \operatorname{div}\left(\frac{\partial}{\partial t} \frac{d\mathbf{D}}{dp}\right) = 0 \quad t \in [0, T], \mathbf{r} \in \Omega; \quad (4a)$$

$$\frac{d\mathbf{J}}{dp} = \frac{\partial \sigma}{\partial p} \mathbf{E} + \sigma_d \frac{d\mathbf{E}}{dp} \quad t \in [0, T], \mathbf{r} \in \Omega; \quad (4b)$$

$$\frac{d\mathbf{D}}{dp} = \frac{\partial \varepsilon}{\partial p} \mathbf{E} + \varepsilon_d \frac{d\mathbf{E}}{dp} \quad t \in [0, T], \mathbf{r} \in \Omega; \quad (4c)$$

$$\frac{d\mathbf{E}}{dp} = -\operatorname{grad}\left(\frac{d\phi}{dp}\right) \quad t \in [0, T], \mathbf{r} \in \Omega; \quad (4d)$$

$$\frac{d\phi}{dp} = 0 \quad t \in [0, T], \mathbf{r} \in \Gamma_e; \quad (4e)$$

$$\left( \frac{d\mathbf{J}}{dp} + \frac{\partial}{\partial t} \frac{d\mathbf{D}}{dp} \right) \cdot \mathbf{n} = 0 \quad t \in [0, T], \mathbf{r} \in \Gamma_m; \quad (4f)$$

$$\frac{d\phi}{dp} = \frac{d\phi_0}{dp} \quad t = 0, \mathbf{r} \in \Omega, \quad (4g)$$

with the differential material tensors [2]

$$\begin{aligned} \boldsymbol{\sigma}_d(\mathbf{E}) &= \sigma(\mathbf{E}) \mathbf{1} + \mathbf{E} 2 \frac{d\sigma}{dE^2}(\mathbf{E}) \mathbf{E}^T, \\ \boldsymbol{\varepsilon}_d(\mathbf{E}) &= \varepsilon(\mathbf{E}) \mathbf{1} + \mathbf{E} 2 \frac{d\varepsilon}{dE^2}(\mathbf{E}) \mathbf{E}^T, \end{aligned}$$

where  $E$  is the absolute value of the electric field strength and  $\mathbf{1}$  is the identity tensor. Eliminating  $\frac{d\mathbf{J}}{dp}$ ,  $\frac{d\mathbf{E}}{dp}$  and  $\frac{d\mathbf{D}}{dp}$  brings up

$$\begin{aligned} & -\operatorname{div} \left( \boldsymbol{\sigma}_d \operatorname{grad} \left( \frac{d\phi}{dp} \right) \right) - \operatorname{div} \left( \frac{\partial}{\partial t} \left( \boldsymbol{\varepsilon}_d \operatorname{grad} \left( \frac{d\phi}{dp} \right) \right) \right) \\ & = -\operatorname{div} \left( \frac{\partial \sigma}{\partial p} \mathbf{E} \right) - \operatorname{div} \left( \frac{\partial}{\partial t} \left( \frac{\partial \varepsilon}{\partial p} \mathbf{E} \right) \right) \quad t \in [0, T], \mathbf{r} \in \Omega; \end{aligned} \quad (5a)$$

$$\frac{d\phi}{dp} = 0 \quad t \in [0, T], \mathbf{r} \in \Gamma_e; \quad (5b)$$

$$\begin{aligned} & \left( -\boldsymbol{\sigma}_d \operatorname{grad} \left( \frac{d\phi}{dp} \right) - \frac{\partial}{\partial t} \left( \boldsymbol{\varepsilon}_d \operatorname{grad} \left( \frac{d\phi}{dp} \right) \right) \right) \cdot \mathbf{n} \\ & = \left( -\frac{\partial \sigma}{\partial p} \mathbf{E} - \frac{\partial}{\partial t} \left( \frac{\partial \varepsilon}{\partial p} \mathbf{E} \right) \right) \cdot \mathbf{n} \quad t \in [0, T], \mathbf{r} \in \Gamma_m; \end{aligned} \quad (5c)$$

$$\frac{d\phi}{dp} = \frac{d\phi_0}{dp} \quad t = 0, \mathbf{r} \in \Omega, \quad (5d)$$

where  $\sigma_d(p_0)$ ,  $\varepsilon_d(p_0)$ ,  $\frac{\partial \mathbf{J}}{\partial p}(p_0)$ ,  $\frac{d\phi_0}{dp}(p_0)$  and  $\frac{\partial \mathbf{D}}{\partial p}(p_0)$  are evaluated at the active parameter value  $p_0$ .

## 2.2 Adjoint Method for the Electroquasistatic Problem

The first step in deriving the adjoint formulation is a modified notation of the QoI. Since the derivation of the adjoint formulation requires partial integration in space and time, the QoI is written in terms of a functional,  $g$ , that is integrated over the spatial and temporal computational domain [3, 4], i.e.,

$$G(\phi(p), p) = \int_0^T \int_{\Omega} g(\phi(p), \mathbf{r}, t, p) \, d\Omega dt$$

Furthermore, the QoI is extended by subtracting the EQS equation multiplied by a test function,  $w(\mathbf{r}, t)$ , i.e.

$$\begin{aligned} G(\phi(p), p) &= \int_0^T \int_{\Omega} g(\phi(p), \mathbf{r}, t, p) \, d\Omega dt \\ &\quad - \int_0^T \int_{\Omega} w \operatorname{div} \left( \underbrace{\mathbf{J}(p) + \frac{\partial \mathbf{D}}{\partial t}(p)}_{\stackrel{\text{(1a)}}{=} \mathbf{0}} \right) \, d\Omega dt. \end{aligned} \quad (6)$$

The sensitivity of the extended QoI reads

$$\begin{aligned} \frac{dG}{dp}(p_0) &= \underbrace{\int_0^T \int_{\Omega} \frac{\partial g}{\partial p}(\phi(p_0), \mathbf{r}, t, p_0) + \frac{\partial g}{\partial \phi}(\phi(p_0), \mathbf{r}, t, p_0) \frac{d\phi}{dp}(p_0) \, d\Omega dt}_{=:\textcircled{1}} \\ &\quad - \underbrace{\int_0^T \int_{\Omega} w \operatorname{div} \left( \frac{d\mathbf{J}}{dp}(p_0) \right) \, d\Omega dt}_{=:\textcircled{2}} - \underbrace{\int_0^T \int_{\Omega} w \operatorname{div} \left( \frac{\partial}{\partial t} \left( \frac{d\mathbf{D}}{dp}(p_0) \right) \right) \, d\Omega dt}_{=:\textcircled{3}}. \end{aligned} \quad (7)$$

Here  $\frac{d\phi}{dp}(p_0)$ ,  $\frac{d\mathbf{J}}{dp}(p_0)$  and  $\frac{d\mathbf{D}}{dp}(p_0)$  are unknown, however  $\frac{d\mathbf{J}}{dp}(p_0)$  and  $\frac{d\mathbf{D}}{dp}(p_0)$  can be expressed by means of  $\frac{d\phi}{dp}(p_0)$ . The goal is to factor  $\frac{d\phi}{dp}(p_0)$  out and choose  $w$  such that all unknown terms vanish.

From now on, the evaluation at  $p_0$  is omitted for the sake of readability. First, the second integral ② is unravelled. This is done by repeatedly applying integration by parts and equation (4), i.e.,

$$\begin{aligned} \textcircled{2} &= - \int_0^T \int_{\Omega} w \operatorname{div} \left( \frac{d\mathbf{J}}{dp} \right) d\Omega dt \\ &= \int_0^T \int_{\Omega} \operatorname{grad}(w) \cdot \frac{d\mathbf{J}}{dp} d\Omega dt - \int_0^T \oint_{\partial\Omega} w \frac{d\mathbf{J}}{dp} \cdot d\mathbf{S} dt \end{aligned} \quad (8)$$

$$\begin{aligned} &\stackrel{(4b),(4d)}{=} \int_0^T \int_{\Omega} \operatorname{grad}(w) \cdot \frac{\partial\sigma}{\partial p} \mathbf{E} d\Omega dt - \int_0^T \int_{\Omega} \operatorname{grad}(w) \cdot \boldsymbol{\sigma}_d \operatorname{grad} \left( \frac{d\phi}{dp} \right) d\Omega dt \\ &\quad - \int_0^T \oint_{\partial\Omega} w \frac{d\mathbf{J}}{dp} \cdot d\mathbf{S} dt \end{aligned} \quad (9)$$

$$\begin{aligned} &= \int_0^T \int_{\Omega} \operatorname{grad}(w) \cdot \frac{\partial\sigma}{\partial p} \mathbf{E} d\Omega dt - \int_0^T \oint_{\partial\Omega} w \frac{d\mathbf{J}}{dp} \cdot d\mathbf{S} dt \\ &\quad + \int_0^T \int_{\Omega} \operatorname{div}(\boldsymbol{\sigma}_d \operatorname{grad}(w)) \frac{d\phi}{dp} d\Omega dt - \int_0^T \oint_{\partial\Omega} \frac{d\phi}{dp} \boldsymbol{\sigma}_d \operatorname{grad}(w) \cdot d\mathbf{S} dt. \end{aligned} \quad (10)$$

Second, the third integral ③ is investigated. The differential operator is shifted from  $\frac{\partial}{\partial t} \left( \frac{d\mathbf{D}}{dp} \right)$  to the test function,  $w$ , using integration by parts,

$$\textcircled{3} = - \int_0^T \int_{\Omega} w \operatorname{div} \left( \frac{\partial}{\partial t} \left( \frac{d\mathbf{D}}{dp} \right) \right) d\Omega dt \quad (11)$$

$$= \int_0^T \int_{\Omega} \operatorname{grad}(w) \cdot \frac{\partial}{\partial t} \left( \frac{d\mathbf{D}}{dp} \right) d\Omega dt - \int_0^T \oint_{\partial\Omega} w \frac{\partial}{\partial t} \left( \frac{d\mathbf{D}}{dp} \right) \cdot d\mathbf{S} dt. \quad (12)$$

Integration by parts in time removes the time derivative from  $\frac{d\mathbf{D}}{dp}$ , i.e.,

$$\begin{aligned} \textcircled{3} &= \int_{\Omega} \operatorname{grad}(w) \cdot \frac{d\mathbf{D}}{dp} d\Omega \Big|_{t=T} - \int_{\Omega} \operatorname{grad}(w) \cdot \frac{d\mathbf{D}}{dp} d\Omega \Big|_{t=0} \\ &\quad - \int_0^T \int_{\Omega} \frac{\partial}{\partial t} (\operatorname{grad}(w)) \cdot \frac{d\mathbf{D}}{dp} d\Omega dt - \int_0^T \oint_{\partial\Omega} w \frac{\partial}{\partial t} \left( \frac{d\mathbf{D}}{dp} \right) \cdot d\mathbf{S} dt, \end{aligned} \quad (13)$$

where the integral evaluated at  $t = 0$  is given through the sensitivity of the initial condition (4g). Since the goal is to factor out  $\frac{d\phi}{dp}$  and  $\frac{d\mathbf{D}}{dp}$  implicitly contains  $\frac{d\phi}{dp}$ , the third integral of (13) is unravelled further. Inserting (4c) and integrating by parts yields

$$- \int_0^T \int_{\Omega} \frac{\partial}{\partial t} (\operatorname{grad}(w)) \cdot \frac{d\mathbf{D}}{dp} d\Omega dt \quad (14)$$

$$= - \int_0^T \int_{\Omega} \frac{\partial}{\partial t} (\operatorname{grad}(w)) \left( \frac{\partial\varepsilon}{\partial p} \mathbf{E} - \varepsilon_d \operatorname{grad} \left( \frac{d\phi}{dp} \right) \right) d\Omega dt \quad (15)$$

$$= - \int_0^T \int_{\Omega} \frac{\partial}{\partial t} (\operatorname{grad}(w)) \cdot \frac{\partial\varepsilon}{\partial p} \mathbf{E} + \operatorname{div} \left( \varepsilon_d \frac{\partial}{\partial t} (\operatorname{grad}(w)) \right) \frac{d\phi}{dp} d\Omega dt \quad (16)$$

$$+ \int_0^T \oint_{\partial\Omega} \varepsilon_d \frac{\partial}{\partial t} (\operatorname{grad}(w)) \frac{d\phi}{dp} \cdot d\mathbf{S} dt.$$

The boundary integrals occurring in ② and ③ can be simplified using (4e) and (4f), i.e.

$$- \int_0^T \oint_{\partial\Omega} \boldsymbol{\sigma}_d \operatorname{grad}(w) \frac{d\phi}{dp} \cdot d\mathbf{S} dt \stackrel{(4e)}{=} - \int_0^T \int_{\Gamma_m} \boldsymbol{\sigma}_d \operatorname{grad}(w) \frac{d\phi}{dp} \cdot d\mathbf{S} dt; \quad (17)$$

$$\int_0^T \oint_{\partial\Omega} \varepsilon_d \frac{\partial}{\partial t} (\operatorname{grad}(w)) \frac{d\phi}{dp} \cdot d\mathbf{S} dt \stackrel{(4e)}{=} \int_0^T \int_{\Gamma_m} \varepsilon_d \frac{\partial}{\partial t} (\operatorname{grad}(w)) \frac{d\phi}{dp} \cdot d\mathbf{S} dt; \quad (18)$$

$$- \int_0^T \oint_{\partial\Omega} w \left( \frac{d\mathbf{J}}{dp} + \frac{\partial}{\partial t} \left( \frac{d\mathbf{D}}{dp} \right) \right) \cdot d\mathbf{S} dt \stackrel{(4f)}{=} - \int_0^T \int_{\Gamma_e} w \left( \frac{d\mathbf{J}}{dp} + \frac{\partial}{\partial t} \left( \frac{d\mathbf{D}}{dp} \right) \right) \cdot d\mathbf{S} dt. \quad (19)$$

The sensitivity can now be written as

$$\begin{aligned}
\frac{dG}{dp} &= \int_0^T \int_{\Omega} \frac{\partial g}{\partial p} + \text{grad}(w) \cdot \frac{\partial \sigma}{\partial p} \mathbf{E} - \frac{\partial}{\partial t} (\text{grad}(w)) \cdot \frac{\partial \varepsilon}{\partial p} \mathbf{E} d\Omega dt \\
&+ \int_0^T \int_{\Omega} \left( \frac{\partial g}{\partial \phi} + \text{div}(\boldsymbol{\sigma}_d \text{grad}(w)) - \text{div} \left( \varepsilon_d \frac{\partial}{\partial t} (\text{grad}(w)) \right) \right) \frac{d\phi}{dp} d\Omega dt \\
&- \int_0^T \int_{\Gamma_e} w \left( \frac{d\mathbf{J}}{dp} + \frac{\partial}{\partial t} \left( \frac{d\mathbf{D}}{dp} \right) \right) \cdot d\mathbf{S} dt \\
&- \int_0^T \int_{\Gamma_m} \left( \boldsymbol{\sigma}_d \text{grad}(w) - \varepsilon_d \frac{\partial}{\partial t} (\text{grad}(w)) \right) \frac{d\phi}{dp} \cdot d\mathbf{S} dt \\
&+ \int_{\Omega} \text{grad}(w) \cdot \frac{d\mathbf{D}}{dp} d\Omega \Big|_{t=T} - \int_{\Omega} \text{grad}(w) \cdot \frac{d\mathbf{D}}{dp} d\Omega \Big|_{t=0},
\end{aligned} \tag{20}$$

where all unknown terms are highlighted in red. These terms vanish, if the test function is chosen as the solution of the adjoint problem,

$$-\text{div}(\boldsymbol{\sigma}_d \text{grad}(w)) + \text{div} \left( \varepsilon_d \frac{\partial}{\partial t} (\text{grad}(w)) \right) = \frac{dg}{d\phi}, \quad t \in [0, T], \quad \mathbf{r} \in \Omega; \tag{21a}$$

$$w = 0, \quad t \in [0, T], \quad \mathbf{r} \in \Gamma_e; \tag{21b}$$

$$-(\boldsymbol{\sigma}_d \text{grad}(w) - \varepsilon_d \frac{\partial}{\partial t} (\text{grad}(w)) \cdot \mathbf{n} = 0, \quad t \in [0, T], \quad \mathbf{r} \in \Gamma_m; \tag{21c}$$

$$w = 0, \quad t = T, \quad \mathbf{r} \in \Omega. \tag{21d}$$

Finally, the sensitivity reduces to

$$\begin{aligned}
\frac{dG}{dp}(p_0) &= \int_0^T \int_{\Omega} \frac{\partial g}{\partial p} + \text{grad}(w) \cdot \frac{\partial \sigma}{\partial p} \mathbf{E} - \frac{\partial}{\partial t} (\text{grad}(w)) \cdot \frac{\partial \varepsilon}{\partial p} \mathbf{E} d\Omega dt \\
&- \int_{\Omega} \text{grad}(w) \cdot \frac{d\mathbf{D}}{dp} d\Omega \Big|_{t=0}.
\end{aligned} \tag{22}$$

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