

Consider finite element spatial discretization of the position and density

$$\mathbf{x}(\boldsymbol{\xi}) = \sum_{a=1}^{n_{\text{en}}} N_a(\boldsymbol{\xi}) \mathbf{x}_a \quad (1)$$

$$\rho(\boldsymbol{\xi}) = \sum_{a=1}^{n_{\text{en}}} N_a(\boldsymbol{\xi}) \rho_a \quad (2)$$

Further, let us introduce a squared distance function as

$$d(\boldsymbol{\xi}) = \frac{1}{2} \|\mathbf{x}(\boldsymbol{\xi}) - \mathbf{x}_g\|^2 \quad (3)$$

The problem at hand can be formulated as

$$\begin{cases} \text{find} & \boldsymbol{\xi} = \arg \min d(\boldsymbol{\xi}) \\ \text{subjected to} & \rho(\boldsymbol{\xi}) = \rho_t \\ & \xi_i = \bar{\xi} \end{cases} \quad (4)$$

This constrained problem can be reformulated as an unconstrained one using the method of Lagrange multipliers. To this end, let us introduce the Lagrangian as

$$\mathcal{L}(\boldsymbol{\xi}, \boldsymbol{\lambda}) = d(\boldsymbol{\xi}) + \lambda_1 (\rho(\boldsymbol{\xi}) - \rho_t) + \lambda_2 (\xi_i - \bar{\xi}) \quad (5)$$

Its extremal point $(\boldsymbol{\xi}, \boldsymbol{\lambda})$ have to satisfy

$$\frac{\partial \mathcal{L}(\boldsymbol{\xi}, \boldsymbol{\lambda})}{\partial \boldsymbol{\xi}} = \frac{\partial d(\boldsymbol{\xi})}{\partial \boldsymbol{\xi}} + \frac{\partial \rho(\boldsymbol{\xi})}{\partial \boldsymbol{\xi}} \lambda_1 + \frac{\partial \xi_i}{\partial \boldsymbol{\xi}} \lambda_2 = 0 \quad (6)$$

$$\frac{\partial \mathcal{L}(\boldsymbol{\xi}, \boldsymbol{\lambda})}{\partial \lambda_1} = \rho(\boldsymbol{\xi}) - \rho_t = 0 \quad (7)$$

$$\frac{\partial \mathcal{L}(\boldsymbol{\xi}, \boldsymbol{\lambda})}{\partial \lambda_2} = \xi_i - \bar{\xi} = 0 \quad (8)$$

This is a system of non-linear algebraic equation which can be resolved for instance by the Newton-Raphson method. To this end one must perform the Taylor expansion around point $(\boldsymbol{\xi}_k, \boldsymbol{\lambda}_k)$ up to first order

$$\frac{\partial \mathcal{L}(\boldsymbol{\xi}_k, \boldsymbol{\lambda}_k)}{\partial \boldsymbol{\xi}} + \frac{\partial^2 \mathcal{L}(\boldsymbol{\xi}_k, \boldsymbol{\lambda}_k)}{\partial \boldsymbol{\xi}^2} \Delta \boldsymbol{\xi} + \frac{\partial^2 \mathcal{L}(\boldsymbol{\xi}_k, \boldsymbol{\lambda}_k)}{\partial \boldsymbol{\xi} \partial \lambda_1} \Delta \lambda_1 + \frac{\partial^2 \mathcal{L}(\boldsymbol{\xi}_k, \boldsymbol{\lambda}_k)}{\partial \boldsymbol{\xi} \partial \lambda_2} \Delta \lambda_2 = 0 \quad (9)$$

$$\frac{\partial \mathcal{L}(\boldsymbol{\xi}_k, \boldsymbol{\lambda}_k)}{\partial \lambda_1} + \frac{\partial^2 \mathcal{L}(\boldsymbol{\xi}_k, \boldsymbol{\lambda}_k)}{\partial \lambda_1 \partial \boldsymbol{\xi}} \Delta \boldsymbol{\xi} + \frac{\partial^2 \mathcal{L}(\boldsymbol{\xi}_k, \boldsymbol{\lambda}_k)}{\partial \lambda_1^2} \Delta \lambda_1 + \frac{\partial^2 \mathcal{L}(\boldsymbol{\xi}_k, \boldsymbol{\lambda}_k)}{\partial \lambda_1 \partial \lambda_2} \Delta \lambda_2 = 0 \quad (10)$$

$$\frac{\partial \mathcal{L}(\boldsymbol{\xi}_k, \boldsymbol{\lambda}_k)}{\partial \lambda_2} + \frac{\partial^2 \mathcal{L}(\boldsymbol{\xi}_k, \boldsymbol{\lambda}_k)}{\partial \lambda_2 \partial \boldsymbol{\xi}} \Delta \boldsymbol{\xi} + \frac{\partial^2 \mathcal{L}(\boldsymbol{\xi}_k, \boldsymbol{\lambda}_k)}{\partial \lambda_2 \partial \lambda_1} \Delta \lambda_1 + \frac{\partial^2 \mathcal{L}(\boldsymbol{\xi}_k, \boldsymbol{\lambda}_k)}{\partial \lambda_2^2} \Delta \lambda_2 = 0 \quad (11)$$

which can be written in matrix notation as

$$\begin{bmatrix} \frac{\partial^2 \mathcal{L}_k}{\partial \xi^2} & \frac{\partial^2 \mathcal{L}_k}{\partial \xi \partial \lambda_1} & \frac{\partial^2 \mathcal{L}_k}{\partial \xi \partial \lambda_2} \\ \frac{\partial^2 \mathcal{L}_k}{\partial \lambda_1 \partial \xi} & \mathbf{0} & \mathbf{0} \\ \frac{\partial^2 \mathcal{L}_k}{\partial \lambda_2 \partial \xi} & \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{Bmatrix} \Delta \xi \\ \Delta \lambda_1 \\ \Delta \lambda_2 \end{Bmatrix} = - \begin{Bmatrix} \frac{\partial \mathcal{L}_k}{\partial \xi} \\ \frac{\partial \mathcal{L}_k}{\partial \lambda_1} \\ \frac{\partial \mathcal{L}_k}{\partial \lambda_2} \end{Bmatrix} \quad (12)$$

In the sequel, all required derivatives will be derived

$$\frac{\partial^2 \mathcal{L}(\xi_k, \lambda_k)}{\partial \lambda_1^2} = \frac{\partial^2 \mathcal{L}(\xi_k, \lambda_k)}{\partial \lambda_2^2} = \frac{\partial^2 \mathcal{L}(\xi_k, \lambda_k)}{\partial \lambda_1 \partial \lambda_2} = 0 \quad (13)$$

$$\frac{\partial^2 \mathcal{L}(\xi, \lambda)}{\partial \lambda_1 \partial \xi} = \frac{\partial \rho(\xi)}{\partial \xi} \quad (14)$$

$$\frac{\partial^2 \mathcal{L}(\xi, \lambda)}{\partial \lambda_2 \partial \xi} = \frac{\partial \xi_i}{\partial \xi} \quad (15)$$

$$\frac{\partial^2 \mathcal{L}_k}{\partial \xi^2} = \frac{\partial}{\partial \xi} \left(\frac{\partial d(\xi)}{\partial \xi} + \frac{\partial \rho(\xi)}{\partial \xi} \lambda_1 + \frac{\partial \rho_i}{\partial \xi} \lambda_2 \right) \quad (16)$$

$$= \frac{\partial^2 d(\xi)}{\partial \xi^2} + \frac{\partial^2 \rho(\xi)}{\partial \xi^2} \lambda_1 \quad (17)$$

where

$$\frac{\partial d(\xi)}{\partial \xi} = \frac{\partial}{\partial \xi} \left(\frac{1}{2} \|x(\xi) - x_g\|^2 \right) \quad (18)$$

$$= \frac{\partial}{\partial \xi} \left(\frac{1}{2} \{x(\xi) - x_g\} \cdot \{x(\xi) - x_g\} \right) \quad (19)$$

$$= \frac{\partial x(\xi)}{\partial \xi} \cdot \{x(\xi) - x_g\} \quad (20)$$

and

$$\frac{\partial^2 d(\xi)}{\partial \xi^2} = \frac{\partial}{\partial \xi} \left(\frac{\partial x(\xi)}{\partial \xi} \cdot \{x(\xi) - x_g\} \right) \quad (21)$$

$$= \frac{\partial^2 x(\xi)}{\partial \xi^2} \cdot \{x(\xi) - x_g\} + \frac{\partial x(\xi)}{\partial \xi} \cdot \frac{\partial x(\xi)}{\partial \xi} \quad (22)$$