Energy barrier

Tom de Geus

December 3, 2020

The protocol is as follows.

- 1. An element is selected for triggering (in the example below chosen in the center of the system). Its location is denoted by \vec{r}'
- 2. A perturbation around a stress and strain free configuration is computed. To this end first the selected element (only) is subjected to an eigen stress σ' . The corresponding equilibrium configuration then constitutes to the perturbation that will be used.
- 3. Two types of perturbation are considered:
 - Simple shear: $\sigma' = \sigma'_s = \vec{e}_x \vec{e}_y + \vec{e}_x \vec{e}_y$.
 - Pure shear: $\sigma' = \sigma'_n = \vec{e}_x \vec{e}_x \vec{e}_y \vec{e}_y$.

This leads to two purburtive displacement fields $\vec{u}_s^*(\vec{r})$ and $\vec{u}_p^*(\vec{r})$ with accompanying stress fields $(\sigma_s^*(\vec{r}) \text{ and } \sigma_p^*(\vec{r}))$ and strain fields $(\varepsilon_s^*(\vec{r}) \text{ and } \varepsilon_p^*(\vec{r}))$.

4. The two perturbative modes are scaled such that the energy increase to a perturbubation with $\delta \vec{u}(\vec{r}) = s\vec{u}_s(\vec{r}) + p\vec{u}_p(\vec{r})$ is isotropic in the (s,p)-space. In particular, prefactors η_s and η_p are used to obtain

$$\vec{u}_i = \eta_i \vec{u}_i^*, \qquad \boldsymbol{\sigma}_i = \eta_i \boldsymbol{\sigma}_i^*, \qquad \boldsymbol{\varepsilon}_i = \eta_i \boldsymbol{\varepsilon}_i^*, \qquad \text{for } i \in (s, p)$$
 (1)

whereby

- Simple shear: $\eta_s = 1/[(\sigma_{xy})_s^*(\vec{r}')(\varepsilon_{xy})_s^*(\vec{r}')]$
- Simple shear: $\eta_p = 1/[(\sigma_{yy})_p^*(\vec{r}')(\varepsilon_{yy})_p^*(\vec{r}')]$

(i.e. in both cases based on the triggered element at \vec{r}').

The resulting perturbative (rescaled) displacement and stress modes are shown in Fig. 1.

5. A perturbation with $\delta \vec{u}(\vec{r}) = s\vec{u}_s(\vec{r}) + p\vec{u}_p(\vec{r})$ now results in an energy increase in the system that is isotropic in the (s,p) domain, see Fig. 2. In contrast the increase in equivalent stress and strain are an ellipse in the (s,p) domain, see Fig. 3.

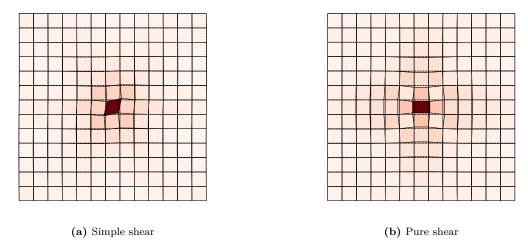


Figure 1. Perturbation modes. The shown colour is the equivalent stress resulting from the perturbation.

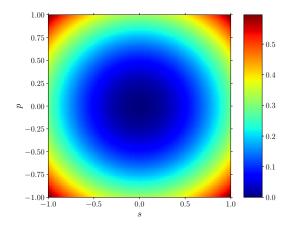


Figure 2. Energetic cost of a perturbation with a linear combination of the two perturbation modes: $\sigma^* = p\sigma_p^* + s\sigma_s^*$.

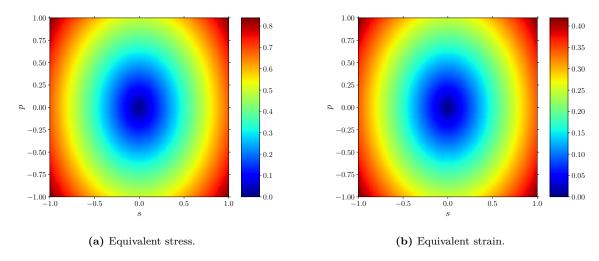


Figure 3. Resulting (a) equivalent stress and (b) equivalent strain for a perturbation with a linear combination of the two perturbation modes: $\sigma^* = p\sigma_p^* + s\sigma_s^*$.