Variational based effective models for inelastic materials

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Mechanical systems with inelastic materials and given boundary conditions can be generally defined and solved. However, for large systems, this problem becomes non trivial and computationally costly, especially when microstructures occur. Therefore, multi-scale modeling is used to capture the behavior of the system.

In this study, we present a methodology to provide such models for inelastic materials starting from the variational scheme. Using the variational principle we define the material strain energy and dissipation potential at the coarse scale (macro scale) starting from their counterparts on the fine scale, through the homogenization scheme. Then we solve the material model at the macro level instead of solving the fine scale model or the whole combination of scales. This multi-scale model offers a reduced number of degrees of freedom and can generally provide the behavior of the system. Moreover, the macro scale model preserves the mathematical structure of the micro scale one. Nevertheless, for this effective model, special care needs to be given to the selection of the inelastic variables solved on the macro scale. This model is illustrated by the application to problems in classical plasticity.

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1 Variational framework

We will introduce a variational approach for the description of inelastic processes resting on thermodynamical extremum principles. For this purpose let us consider a physical system described by external state variables \( x \) and internal state variables \( z \), parametrized as

\[
x = x(\xi), \quad z = z(\xi), \quad \xi \in \Omega,
\]

where \( \Omega \) denotes a suitable parameter space.

Let this physical system be defined using only two scalar potentials: a free energy \( \Psi(\nabla x, x, z) \) and a dissipation potential \( \Delta(z, \dot{z}) \), where \( \nabla \) denotes the gradient with respect to \( \xi \).

The external state variable \( x \) will be given by minimization of system potential energy as in

\[
\inf_x \left\{ \int_{\Omega} \Psi(\nabla x, x, z) \, d\xi + f_{\text{ext}}(x) \mid x = x_0 \text{ on } \partial\Omega \right\}, \tag{2}
\]

where \( f_{\text{ext}}(x) \) is the potential of external driving forces. The evolution of the internal variables is described by the Biot-equation resulting from the minimization problem

\[
\inf_z \left\{ \Psi + \Delta \right\}, \quad \text{Biot-equation} \quad \frac{\partial \Psi}{\partial z} + \frac{\partial \Delta}{\partial \dot{z}} = 0. \tag{3}
\]

Our goal is to capture the behavior of the system described by Eqs. (2) and (3) using only a finite (small) number of parameters. Assume that our state variables are, as functions of \( \xi \), members of suitable function spaces: \( x \in X, z \in Z \). Let us moreover introduce linear projection operators to finite-dimensional spaces and the resulting essential parameters.

\[
P : X \to \mathbb{R}^M \quad Q : Z \to \mathbb{R}^N
\]

\[
X = X_{\text{ess}} \oplus \left\{ x \in X \mid Px = 0 \right\} \quad Z = Z_{\text{ess}} \oplus \left\{ x \in Z \mid Px = 0 \right\}
\]

We would like the kinetics of the system under consideration to be captured by the essential parameters as closely as possible. This occurs when the potentials \( \Psi \) and \( \Delta \) are invariant under variations within the marginal spaces. Hence,

\[
\frac{\partial \Psi}{\partial x} : \delta x = 0 \text{ for } \delta x \in X_{\text{mar}}, \quad \frac{\partial \Psi}{\partial z} : \delta z = 0 \text{ for } \delta z \in Z_{\text{mar}}, \quad \frac{\partial \Delta}{\partial x} : \delta x = 0 \text{ for } \delta x \in X_{\text{mar}}, \quad \frac{\partial \Delta}{\partial z} : \delta z = 0 \text{ for } \delta z \in Z_{\text{mar}}.
\]

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Then, the minimization problem in Eq. (3) is approximated by

\[
\inf_{z_{ess} \in \mathbb{R}^N} \left\{ \Psi_{macro} + \Delta_{macro} \right\}.
\]

(6)

Additionally assume that the potential of external loads in Eq. (2) can be expressed via the essential parameters, \( f_{ext}(x) = f_{ess}(x_{ess}) \), and that the boundary conditions may be expressed in terms of the essential parameters, too, by specifying a projection \( Bx_{ess} \). In this setting, we replace the minimization problem in Eq. (2) with the macroscopic form:

\[
\inf_{x_{ess} \in \mathbb{R}^N} \left\{ \int_{\Omega} \Psi_{macro}(x_{ess}, z_{ess}) \, d\xi + f_{ess}(x_{ess}) \right\} \quad | \quad Bx_{ess} = x_{ess0} \text{ on } \partial\Omega.
\]

(7)

In what follows, the two minimization problems in Eqs. (6) and (7) will be shown to capture the kinetics of the macroscopic system, thus approximating the behavior of the original system. Given \( f_{ess} \) and \( x_{ess0} \) as functions of time, they allow for the computation of \( x_{ess} \) and \( z_{ess} \) as functions of time.

### 2 Inelastic homogenization in periodic microstructures

Let us consider now a material having a microstructure defined by periodically varying \( C(r) \) and \( \sigma_\varepsilon(r) \). Then \( \Omega \) may be chosen as a rectangular representative volume element. The average of a quantity \( f \) over \( \Omega \) is then given by

\[
\langle f \rangle = \frac{1}{|\Omega|} \int_{\Omega} f \, dr.
\]

(8)

The macroscopic material behavior may be determined by subjecting the representative volume element to a macroscopic strain \( e_M(t) = \langle \varepsilon \rangle \) and calculating the macroscopic stress \( \sigma_M(t) = \langle \sigma \rangle \). The imposed macroscopic strain may be realized by decomposing the displacement field as

\[
u = e_M \cdot r + u_{per},
\]

(9)

where \( u_{per} \) satisfies so-called periodic boundary conditions, i.e. it holds \( u_{per}(r_-) = u_{per}(r_+) \) on corresponding boundary points \( r_- \), \( r_+ \) on opposite sides of \( \Omega \).

#### 2.1 The macroscopic model and essential variables

The problem is in principle infinite-dimensional because the plastic strains \( \varepsilon_p(r, t) \) have to be known at all points of \( \Omega \) for all times. In order to devise a macroscopic model of the system under consideration let us subdivide our representative volume element into \( N_{sd} \) distinct sub-domains \( \Omega_i \) such that

\[
\Omega = \bigcup_{i=1}^{N_{sd}} \Omega_i, \quad \text{with the local averages } \langle f \rangle_i = \frac{1}{|\Omega_i|} \int_{\Omega_i} f \, dr.
\]

(10)

In every sub-domain we are only interested in mean values of the plastic strains. Which constitute the essential internal parameters and as essential external parameters, we will choose the macroscopic strain.

\[
z_{ess} = e_{pi} = \langle \varepsilon_p \rangle_i, \quad x_{ess} = e_M.
\]

(11)

With the definitions above the macroscopic free energy is given as

\[
\Psi_{macro}(e_M, e_p) = \inf_{u_{per}, e_p} \left\{ \left( \frac{1}{2} (\varepsilon - \varepsilon_p) : C : (\varepsilon - \varepsilon_p) \right) \right\} \quad | \quad u = e_M \cdot r + u_{per}, \quad e_{pi} = \langle \varepsilon_p \rangle_i.
\]

(12)

Introducing Lagrange-parameters \( \mu_i \) for the second constraint we obtain the Lagrangian for the minimization problem above as

\[
L = \left( \frac{1}{2} (\varepsilon - \varepsilon_p) : C : (\varepsilon - \varepsilon_p) \right) + \sum_{i=1}^{N_{sd}} \mu_i \left( e_{pi} - \langle \varepsilon_p \rangle_i \right).
\]

(13)

As stationarity conditions we obtain

\[
\nabla \cdot (C : (\varepsilon - \varepsilon_p)) = 0 \quad \text{in } \Omega, \quad C : (\varepsilon - \varepsilon_p) = \mu_i \quad \text{in } \Omega_i.
\]

(14)
From the second relation in Eq. (14) we see that the stress $\sigma = \mu i$ is constant in every sub-domain $\Omega_i$ and that the first condition in Eq. (14) is trivially satisfied. By Substitution we get

$$\Psi_{\text{macro}}(e_M, e_p) = \inf_{u_{\per}} \left\{ \frac{1}{N_{sd}} \sum_{i=1}^{N_{sd}} \frac{|\Omega_i|}{|\Omega|} \frac{1}{2} (e_i - e_{pi}) : C_{effi} : (e_i - e_{pi}) \mid u = e_M \cdot \mathbf{r} + u_{\per} \right\}. \quad (15)$$

It can be seen that $\Psi_{\text{macro}}(e_M, e_p)$ is a quadratic expression in $e_M$ and $e_p$.

From Eq. (15) we obtain immediately the conjugate driving forces to the essential internal parameters as

$$q_i = -\frac{\partial \Psi_{\text{macro}}}{\partial e_{pi}} = \frac{|\Omega_i|}{|\Omega|} \sigma_i, \quad \text{where} \quad \sigma_i = C_{effi} : (e_i - e_{pi}) \quad (16)$$

denotes the constant stress in every sub-domain. The macroscopic dissipation potential is defined as

$$\Delta_{\text{macro}}(e_p) = \sqrt{2/3} \frac{1}{|\Omega|} \sum_{i=1}^{N_{sd}} |\Omega_i| \sigma_{yi} \|\varepsilon_{pi}\|.$$ \quad (17)

assuming that $\sigma_y = \sigma_{yi}$ is constant in every sub-domain. The yield conditions in each sub-domain is of the form

$$\|\text{dev} \sigma_i\| \leq \sqrt{2/3} \sigma_{yi}. \quad (18)$$

2.2 Polyhedral sub-domains

Let us consider now microstructures consisting of polyhedral sub-domains bounded by facets $F_i$. Of course, any microstructure may be approximated in this way with arbitrary accuracy by choosing the facets small enough. Suppose the facets posses outward normal vectors $\mathbf{n}_i$. Then the average strains in every sub-domain can be calculated according to

$$e_i = e_M + \frac{1}{|\Omega_i|} \sum_{F_i \subset \partial \Omega_i} \text{sym} \mathbf{a}_j \otimes \mathbf{n}_j, \quad \text{where} \quad \mathbf{a}_i = \int_{F_i} u_{\per} \mathrm{d}S. \quad (19)$$

Note that because of the periodic boundary conditions some of the $\mathbf{a}_j$ are dependent if $F_j \subset \partial \Omega$. Let the number of independent amplitude vectors be $N_a$. The macroscopic free energy can now be written as

$$\Psi_{\text{macro}}(e_M, e_p) = \inf \left\{ \psi_{\text{rve}}(e_M, e_p, a_1, \ldots, a_{N_a}) \mid a_1, \ldots, a_{N_a} \right\}. \quad (20)$$

where

$$\psi_{\text{rve}}(e_M, e_p, a_1, \ldots, a_{N_a}) = \frac{1}{N_{sd}} \sum_{i=1}^{N_{sd}} \frac{|\Omega_i|}{|\Omega|} \frac{1}{2} (e_i - e_{pi}) : C_{effi} : (e_i - e_{pi}). \quad (21)$$

The stationarity conditions corresponding to minimization are

$$\frac{\partial \psi_{\text{rve}}}{\partial a_i} = 0, \quad i = 1, \ldots, N_a. \quad (22)$$

The macroscopic energy will be quadratic of the form

$$\Psi_{\text{macro}} = \frac{1}{2} e_M : C_{eff} : e_M - \sum_{i=1}^{N_{sd}} e_{pi} : G_{effi} : e_M + \sum_{i,j=1}^{N_{sd}} \frac{1}{2} e_{pi} : G_{effij} : e_{pj}. \quad (23)$$

The conjugate driving forces follow as

$$q_i = -\frac{\partial \Psi_{\text{macro}}}{\partial e_{pi}} = \frac{|\Omega_i|}{|\Omega|} \sigma_i = F_{effi} : e_M - \sum_{j=1}^{N_{sd}} G_{effij} : e_{pj}. \quad (24)$$

2.3 Non-symmetric RVE with octagon center inclusion

In this example, we examine a non-uniform matrix with 9 different sub-domains. 20 different amplitude vectors are to be computed. Fig. 1 shows the different sub-domains with the corresponding amplitude vectors, in addition to the three different elastoplastic materials, assigned to the sub-domains. The problem is then compared to the results from the finite element method, in which a very fine mesh (40x40) elements/domain was used to capture the micro scale. The implementation was performed considering the averaged strains as an input, and the averaged macroscopic stresses as an output applying the Hill-Mandel homogenization scheme.

The stress per time step and stress-strain response averaged over the whole composite in comparison to the FE computations can be inferred from Fig. 2. We can observe a very good compliance with the FE output, where the behavior is captured qualitatively and quantitatively. Nevertheless, a deviation from the exact stiffness is observed in which the model is reflecting Reuss effective stiffness.
Fig. 1: A representative volume element with octagon center inclusion and 20 amplitude vectors describing the different facets. $Mat_1$ is assigned to the center inclusion, $Mat_2$ is assigned to sub-domain $\Omega_2$, and $Mat_3$ is assigned elsewhere.

Fig. 2: Output comparison from the reduced model and the finite element method for the RVE with octagon center inclusion. The graphs above show the macroscopic stresses per time step and the ones below show the macroscopic response in loading directions.

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