Numerical implementation of incremental minimization principle for materials with multiple rate-independent dissipative mechanisms

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1. Introduction

New experimental techniques allow for a more comprehensive examination of the mechanical response of materials, providing the opportunity for the development of more detailed material models. The incremental energy minimization approach is a compact variational formulation of the evolutionary boundary value problem for constitutive models of materials with a rate-independent response, see e.g. [3]. Although it can be easily applied to many conventional models, its main advantages arise when applied to models with multiple strongly coupled dissipation mechanisms, where the direct construction of the coupled yield conditions and flow rules may be challenging. However, the approach usually requires a more complex numerical treatment of the resulting sequence of time-incremental boundary value problems resolved via the finite element method.

2. Incremental minimization principle

In what follows, we focus on a quasi-static evolutionary boundary value problem under isothermal conditions. Let us introduce a partition of the time interval from time 0 to $\mathcal{T}$ in the form $0 = t_0 \leq t_1 \leq \cdots \leq t_N = \mathcal{T}$, $N \in \mathbb{N}$. In this time-discrete setting, the mechanical response of the system at time $t_{n+1}, n \in \{0, \ldots, N-1\}$ can then be determined by solving the incremental minimization problem

$$\inf_{\boldsymbol{\chi}} L^\tau(\boldsymbol{\chi}, \boldsymbol{\chi_n}), \tag{1}$$

where $\boldsymbol{\chi}$ represents the set of all thermodynamic descriptors of the system. The superscript τ denotes the time-discretized counterparts of time-continuous functionals of the corresponding weak formulation, and the subscript n denotes the values of the previous time step. Let us note that the minimization can be subject to some additional (kinematic and physically-based) internal constraints, see [3] for details.

The (Lagrangian) functional L^τ usually combines the incremental energy functional, E^τ, the incremental dissipation functional, D^τ, and the incremental external work functional P^τ. For many engineering-relevant solid materials, the objective function of the minimization from (1) takes the the following form:

$$L^\tau(u, \boldsymbol{\alpha}, \boldsymbol{\alpha}_n) := E^\tau(u, \boldsymbol{\alpha}, \boldsymbol{\alpha}_n) + D^\tau(\boldsymbol{\alpha}, \boldsymbol{\alpha}_n) - P^\tau(u, \boldsymbol{\alpha}, \boldsymbol{\alpha}_n). \tag{2}$$

Here, u denotes the displacement and $\boldsymbol{\alpha}$ encompasses thermodynamic descriptors of the microstructure, which can be further constrained to an admissible set $\mathcal{A}^\tau$. The most common examples include (hyper)elastic materials, where $\boldsymbol{\alpha}$ and D^τ disappear, or perfectly plastic material with $\boldsymbol{\alpha}$ being the plastic strain and D^τ being a one-homogeneous function of the difference $\boldsymbol{\alpha} - \boldsymbol{\alpha}_n$ with an imposed constraint $\operatorname{tr} \boldsymbol{\alpha} = 0$.

3. Numerical solution strategies

At least two distinct methods can be utilised to solve the rate-independent problem stated in (2). In the first case, frequently used in finite element software, the minimisation problem is split into a nested form, where a sequence of "structural" nonlinear minimization problems and "material" nonlinear minimization problems is resolved. The second approach benefits from the clear variational structure of (1) and directly applies minimization.

To illustrate these approaches, let us consider the following form of incremental functionals for a material body:

$$E_{n+1}^\tau(u, \boldsymbol{\alpha}; u_n, \boldsymbol{\alpha}_n) \;=\; \int_\Omega f_{n+1}(u, \boldsymbol{\alpha}) - f_n(u_n, \boldsymbol{\alpha}_n)\, \mathrm{d}V, \tag{3}$$

$$D_{n+1}^\tau(\boldsymbol{\alpha}; \boldsymbol{\alpha}_n) \;=\; \int_\Omega (t_{n+1} - t_n)\, \delta_{n+1}(\boldsymbol{\alpha}; \boldsymbol{\alpha}_n; t_{n+1} - t_n)\, \mathrm{d}V, \tag{4}$$

$$P_{n+1}^\tau(u; u_n) \;=\; \int_\Omega F_{n+1}^{\mathrm{vol}} \cdot (u - u_n)\, \mathrm{d}V + \int_{\Gamma_\mathrm{N}} F_{n+1}^{\mathrm{surf}} \cdot (u - u_n)\, \mathrm{d}S, \tag{5}$$

where f_i and δ_i stand for the *discretized* density of the thermodynamical (free energy) potential and dissipation (pseudo)potential, respectively. Moreover, the set $\Omega \subset \mathbb{R}^3$ is the geometric representation of the physical body in the space with (assumed Lipschitz) boundary $\partial\Omega$, and $\Gamma_\mathrm{N} \subset \partial\Omega$ represents its subset where the Neumann boundary condition is applied. The terms F_{vol}^i and F_{surf}^i represent the corresponding time discretizations of the prescribed volumetric and surface forces, respectively. Let us further assume that all necessary information on the system at $t_0 = 0$ (including $u_0, \boldsymbol{\alpha}_0$) is known and well defined. We can disregard the terms in (3)–(5), which are constant with respect to the minimization, and make profit from one-homogeneity of the dissipation (pseudo)potential to the eliminate the time increment in (4).

The nested form of the boundary problem at a time instant t_{n+1} then reads as

$$u_{n+1,p+1} \;=\; \underset{u \in \mathcal{U}_{n+1}^\tau}{\operatorname{argmin}} \left\{ E_{n+1}^\tau(u, \boldsymbol{\alpha}_{n+1,p}; \boldsymbol{\alpha}_n) - P_{n+1}^\tau(u) \right\}, \tag{6}$$

$$\boldsymbol{\alpha}_{n+1,p+1} \;=\; \underset{\boldsymbol{\alpha} \in \mathcal{A}_{n+1}^\tau}{\operatorname{argmin}} \left\{ E_{n+1}^\tau(u_{n+1,p+1}, \boldsymbol{\alpha}; \boldsymbol{\alpha}_n) + D_{n+1}^\tau(\boldsymbol{\alpha}; \boldsymbol{\alpha}_n) - P_{n+1}^\tau(u_{n+1,p+1}) \right\}. \tag{7}$$

Whereas the first subscript denotes the time incrementation introduced above, the second one denotes the iteration $p+1$ ($p \in \mathbb{N} \cup 0$) within the resolution process at time t_{n+1}, where the the subproblems (6), (7) are solved consecutively and repeatedly until suitable convergence criteria are met, i.e. so-called alternating minimization; $\boldsymbol{\alpha}_{n+1,0} = \boldsymbol{\alpha}_n$. After a discretization in space, the first, "structural" subproblem formally corresponds to the principle of minimum potential energy. Its solution procedure is analogous to resolving an elastic body problem, which is a rather standard problem for finite element method. The second, "material" subproblem corresponds to minimization only with respect to internal variables, i.e. finding the local thermodynamical balance, and represents the constitutive response of a material point with fixed displacement. This is usually tackled via numerical procedures specific to the particular constitutive law or with some universal tool of mathematical programming, cf. [1]. A link between the two solution procedures is provided by the material tangent stiffness operator, which must

be derived from the constitutive law as well.

In the alternative approach, the problem is tackled via "complete" minimization, i.e., minimizing all control variables at once,

$$(u_{n+1}, \boldsymbol{\alpha}_{n+1}) = \underset{u \in \mathcal{U}_{n+1}^{\tau}, \boldsymbol{\alpha} \in \mathcal{A}_{n+1}^{\tau}}{\operatorname{argmin}} \{ E_{n+1}^{\tau}(u_{n+1}, \boldsymbol{\alpha}; \boldsymbol{\alpha}_n) + D_{n+1}^{\tau}(\boldsymbol{\alpha}; \boldsymbol{\alpha}_n) - P_{n+1}^{\tau}(u_{n+1}) \}. \quad (8)$$

This monolithic approach may be especially advantageous for material models with multiple, strongly coupled rate-independent dissipative processes. In such a situation, the evolution of individual thermodynamic descriptor cannot be addressed independently, benefiting from conventional active set search strategies. Solely a single "global yield function" driving the evolution can be derived, which may render the conventional numerical treatment elaborate and dependent on the model's particular mathematical structure. In contrast, resolving directly (8) allows to avoid transferring the results from one subproblem to the other, involving the construction of the material Jacobian matrix (material tangent modulus) and its incorporation into the structural Jacobian matrix. On the other hand, it requires to cope with with a non-smooth minimization problem with non-linear constraints, which provides a complex computational challenge.

4. Conclusion

Recently, a vectorized MATLAB tool for minimization of nonlinear (mathematically well-behaved) functionals discretized by the finite element method was developed [4]. The current work builds on it and investigates both the nested and monolithic approaches for a constitutive model with two strongly coupled dissipation process occurring in shape memory alloys, cf. [2].

The principal benefits of the monolithic approach stated above are counterbalanced by some drawbacks. One is related to the limits of the variational framework: some models might require some adaptation of the sketched treat or they even might not fit to (1) at all. Second, the dimension of the "complete" minimization problem is naturally higher than in the case when the problem is split in the nested formulation, which poses a challenge for computational resources. Third, applying universal minimization methods is often less efficient than employing customized algorithms and may lead to prohibitive computational time consumption for more complex evolutionary boundary problems. However, the advance of new optimization methods and increased computational power complemented with parallelization might provide some remedies in the future.

Acknowledgements

References

[1] Frost, M., Benešová, B., Sedlák, P., A microscopically motivated constitutive model for shape memory alloys: Formulation, analysis and computations, Mathematics and Mechanics of Solids 21 (3) (2016) 358-382.

[2] Frost, M., Valdman, J., Vectorized MATLAB implementation of the incremental minimization principle for rate-independent dissipative solids using FEM: A constitutive model of shape memory alloys, Mathematics 10 (2022) No. 4412.

[3] Miehe, C. J., A multi-field incremental variational framework for gradient-extended standard dissipative solids, Journal of the Mechanics and Physics of Solids 59 (4) (2011) 898-923.

[4] Moskovka, A., Valdman, J., Fast MATLAB evaluation of nonlinear energies using FEM in 2D and 3D: Nodal elements, Applied Mathematics and Computation 424 (2022) No. 127048.