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Variational constitutive updates based on hyper-dual numbers - theory of gradient enhanced thermoplasticity

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Micro Abstract
We present a generic framework for thermomechanically coupled gradient-enhanced plasticity theory based on variational constitutive updates, i.e., all relevant equations are fulfilled by minimizing an incremental potential. Within the numerical implementation, the exact derivatives of this potential are computed by means of hyper-dual numbers. By doing so, the laborious task of implementation is highly reduced.

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Introduction

In almost every field of engineering and beyond, there exists a vast amount of processes exhibiting significant thermomechanical interactions. Particularly in metals, a strong coupling between thermal and mechanical behavior can be observed. To run sufficiently accurate simulations of these processes, a well-founded theory has to be formulated on the basis of which efficient numerical schemes can be developed. State-of-the-art implementations of thermomechanically coupled theories are usually based on staggered or monolithic algorithms in order to solve balance of linear momentum and the problem associated with heat conduction. The heat increase due to dissipative plastic deformation is frequently computed using an empirical model often referred to as the Taylor and Quinney-Factor. Consequently, the first law of thermodynamics is ignored. By way of contrast, Yang, Stainier and Ortiz used the first law of thermodynamics in [4] for the thermomechanical coupling. Furthermore, by using a Hu-Washizu principle and an integrating factor, they proved that the coupled theory shows a variational structure.
The general variational framework in [4] is suitable for the development of different thermomechanically coupled material models. In the present work, the time necessary for the implementation of models within this framework is reduced by means of numerical differentiation based on so-called hyper-dual numbers. According to [2], hyper-dual numbers allow to compute the first as well as the second derivative of a function exactly – in sharp contrast to other numerical differentiation schemes.
An isotropic finite strain von Mises plasticity model is implemented to showcase the performance of the aforementioned framework. To capture length scale effects, a gradient enhancement is embedded into the model, cf. [1]. Simulations of necking in a bar show the ability of the model to predict the experimentally observed thermomechanical response.

1 Gradient enhanced thermoplasticity

1.1 Gradient enhancement

Within nowadays established local (finite strain) plasticity theory, a higher gradient is incorporated in line with [1]. Denoting the Helmholtz energy of the local models by $\psi^{\text{loc}} = \psi^{\text{loc}}(\bullet, \alpha)$

which depends – among other variables – on the equivalent plastic strain α, energy of the extended model reads

$$\psi^{\text{nonloc}}(\bullet, \alpha, \varphi_{\text{p}}) = \psi^{\text{loc}}(\bullet, \alpha) + \underbrace{\frac{1}{2}\, c\, [\varphi_{\text{p}} - \alpha]^2}_{=:\psi^{\text{intr}}} + \underbrace{\frac{1}{2}\, \mu\, l_{\text{e}}^2\, \|\, \text{GRAD}\, \varphi_{\text{p}} \|^2}_{=:\psi^{\text{global}}}$$

The underlying idea is to introduce a new global field φ_{p}, additionally to the placement $\boldsymbol{\varphi}$, which is coupled to the equivalent plastic strain α, using the penalty term ψ^{intr} with penalization factor c. Based on this new field, a higher-order gradient term is embedded into the model by means of the energy ψ^{global}. This energy depends on the gradient of φ_{p} and thus captures a length scale l_{e} while μ denotes the shear modulus. This way, the local constitutive model is unaffected. In particular no inequality condition resulting from the Karush-Kuhn-Tucker conditions has to be solved on global level.
The proposed method has been shown to effectively regularize pathological mesh-dependencies in the softening regime (see [1]). Additionally, non-local plastic behavior is achieved, which extends the model to describe non-local phenomena like e.g. the well-known Hall-Petch effect.

1.2 Variational formulation of thermoplasticity

Usually, thermomechanically coupled problems do not show a variational structure – in sharp contrast to the isothermal case, where variational principles like the *postulate of minimum potential energy* are widely applied. However, as shown in [4], an extended variational principle can also be derived for thermomechanically coupled problems. Without going too much into detail, the proposed time-continuous functional is given by

$$\mathcal{L} := \int_{t_0}^{t} \left[\int_{\Omega} \left[\dot{E} - \Theta\, \dot{N} + f\, \mathcal{D}_{\text{int}} + \chi \right] \text{d}V - \mathcal{P}_{\dot{\boldsymbol{\varphi}}} + \mathcal{P}_{\Theta} \right] \text{d}t$$

depending on integrating factor $f := \Theta/\partial_N E$, temperature Θ, entropy N, internal energy E, internal dissipation $\mathcal{D}_{\text{int}}$, dissipation potential $\chi(\Theta)$ describing the Fourier-type heat-flux and external mechanical as well as thermal powers $\mathcal{P}_{\dot{\boldsymbol{\varphi}}}$ and $\mathcal{P}_{\Theta}$. Balance of linear momentum as well as the first law of thermodynamics follow naturally by means of the stationary conditions of this functional. To be more precise,

$$\left\{ \dot{\boldsymbol{\varphi}}, \dot{\varphi}_{\text{p}}, \Theta, \dot{N}, \dot{\alpha} \right\} = \underset{\{\dot{\boldsymbol{\varphi}}, \dot{\varphi}_{\text{p}}, \Theta, \dot{N}, \dot{\alpha}\}}{\text{stat}} \mathcal{L}\,.$$

This elegant formulation yields many advantages, including a symmetric albeit indefinite tangent, which gives the possibility of applying highly efficient and robust solution schemes.

2 Implementation using automatic differentiation based on Hyper-Dual Numbers

In order to solve the saddle-point problem discussed before, the first and the second derivative of the underlying (time discretized) potential have to be computed if a Newton-type algorithm is to be implemented. While a symbolical differentiation is regarded as the most accurate and fastest method (w.r.t. program runtime), it is usually very time consuming and error-prone within derivation and implementation. Here, a numerical differentiation scheme proposed in [2] is applied, which computes the first as well as the second derivative in an exact manner. The algebra utilized within this scheme is similar to the ordinary complex numbers and is called the algebra of *hyper-dual numbers*. These numbers have non-real components ϵ_i with properties

$$\epsilon_i\, \epsilon_j = \epsilon_j\, \epsilon_i \qquad\qquad \epsilon_i^2 = 0\,.$$

In [2], the authors have shown by expansion of the Taylor series that first and second derivatives of a real function $f(x)$ can be obtained by simultaneous perturbation in two dual directions, e.g.

$$\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x_0} = \frac{\mathfrak{D}_1\, f(x^*)}{a} \qquad\qquad \left.\frac{\mathrm{d}^2 f}{\mathrm{d}x^2}\right|_{x_0} = \frac{\mathfrak{D}_{12}\, f(x^*)}{a\, b}$$

with $x^* = x_0 + a\,\epsilon_1 + b\,\epsilon_2 + 0\,\epsilon_1\,\epsilon_2$. $\mathfrak{D}_1 \bullet$ and $\mathfrak{D}_{12} \bullet$ represent the coefficients of the first dual and of the mixed dual component, respectively. In contrast to widely applied schemes like finite differences, the magnitude of perturbation here does not influence the precision of the scheme and thus, for the sake of simplicity, can be chosen as $a = b = 1$.
In [3] this framework was successfully applied to isothermal plasticity models.

3 Numerical example

A prototype implementation of a thermomechanically coupled gradient-enhanced elasto-plasticity model with a von Mises yield criterion is considered here. Based on this model, a cyclically loaded plate with a hole is analyzed, see Fig. 2 (due to symmetry of the problem, only the first quadrant is depicted).

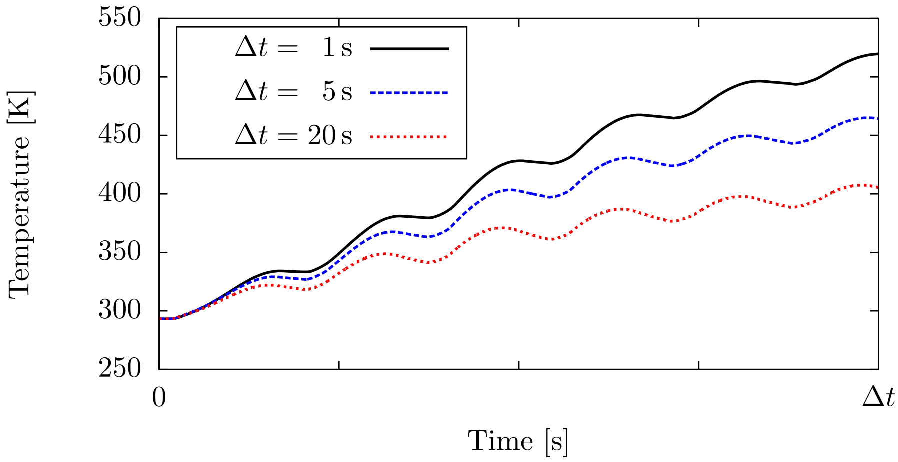

Figure 1. Temperature evolution for different loading velocities – the point with the highest temperature increase is considered.

The point showing the highest temperature increase due to plastic deformation is monitored in Fig. 1. Accordingly, the distribution of the plastic strains is almost independent of the loading velocity (rate-independent model). By way of contrast, the temperatures are higher for higher loading velocities (smaller Δt). This is in line with the physical problem governing heat conduction.

Conclusion

The presented work proposes an elegant and efficient framework for the implementation and development of gradient-enhanced, thermomechanically coupled plasticity models. The variational formulation yields, besides many other advantages, the possibility to apply an exact numerical differentiation scheme based on the algebra of hyper-dual numbers. A prototype model showed the features as well as the advantages of the resulting framework.

References

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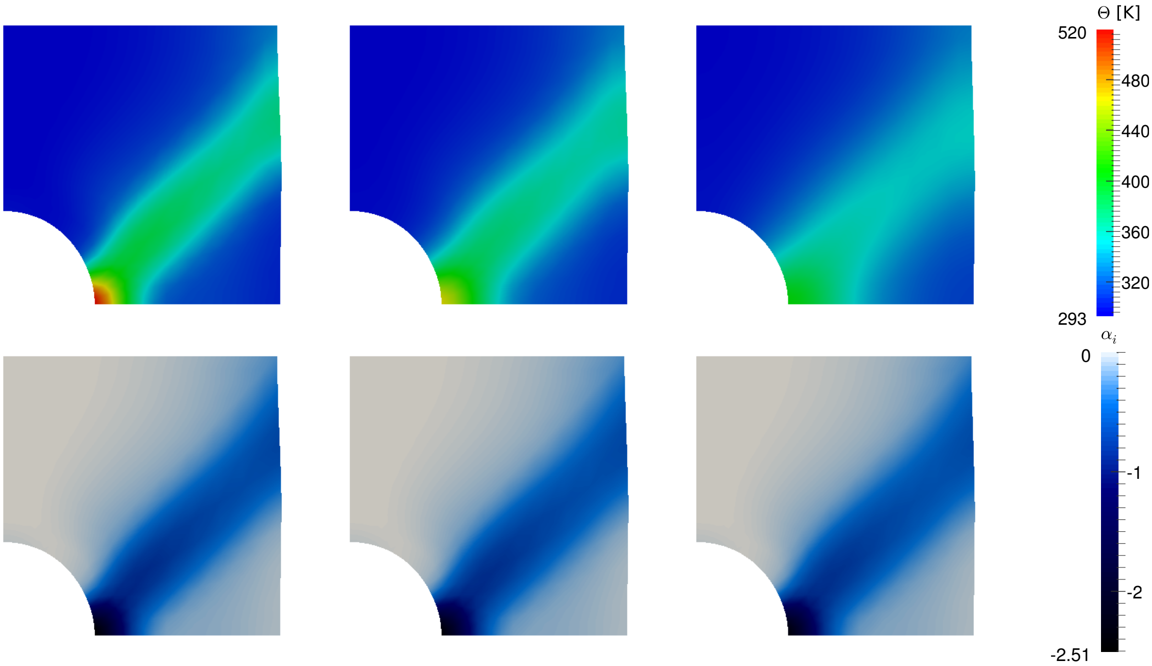

Figure 2. Distribution of temperature Θ (upper row) and equivalent plastic strain α (lower row) for different loading velocities (duration Δt of a cyclic loading is varied). (Left column) $\Delta t = 1\,\mathrm{s}$; (middle column) $\Delta t = 5\,\mathrm{s}$; (right column) $\Delta t = 20\,\mathrm{s}$. Higher loading velocities (smaller Δt) lead to higher temperatures. The limiting case $\Delta t \to 0$ characterizes adiabatic conditions.

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