# ON RECENT PROGRESS IN THE THEORY AND NUMERICS OF MATERIAL FORCES

Ralf Denzer and Paul Steinmann
Chair of Applied Mechanics
University of Kaiserslautern
P.O. Box 3049, D-67653 Kaiserslautern, Germany
email: denzer@rhrk.uni-kl.de

ABSTRACT

Within the setting of analytical mechanics forces are regarded as a secondary concept, i.e. as being derived from a potential. In the spririt of virtual work we may call a force a quantity that is energetically conjugated to variations of kinematic quantities. If on the one hand these kinematic quantities are considered as the (standard) spatial deformation map in continuum mechanics of solids, i.e. relating the (initial) material placements to the (deformed) spatial coordinates, the corresponding forces are the standard once. In the slang of differential geometry, these forces live in the tangent space to the (deformed) spatial configuration. They are usually the given Neumann data for the solution of a boundary value problem. If on the other hand the (inverse) material deformation map, i.e. the map relating the spatial placement to the material coordinates, is considered, the forces conjugated to these kinematic quantities turn out to be (configurational) material forces. Material forces act in the tangent space to the (initial) material configuration. They are results of the computation of a boundary value problem and serve to assess the tendency of defects like cracks, dislocations, interfaces etc. to change their position with respect to the ambient material. Since material forces contribute to a balance equation of material momentum, more or less standard schemes can be invoked to a-posteriori compute discrete material forces for example within a FE-setting.

## 1 INTRODUCTION

In this work we discuss material forces by the example of a coupled problem (e.g. thermo–hyperelasticity) and continuously distributed heterogeneities (e.g. continuum damage) and the calculation of the $J$-integral for this class of problems. Our developments are essentially based on the exposition of the continuum mechanics of inhomogeneities as comprehensively outlined by Maugin [7, 8], Gurtin [4] and our own recent contributions by Steinmann [12], Steinmann et al. [14] and Denzer et al. [2]. Material (configurational) forces are concerned with the response to variations of material placements of 'physical particles' with respect to the ambient material.
Thereby the algorithmic representation of the material balance of momentum resulting in the notion of discrete material forces is proposed as the so called Material Force Method, see Steinmann [11, 14]. First numerical concepts of material forces within the FE-method

date back to Braun [1], who derived for the hyperelastic case node point forces from the discretized potential energy with respect to the material node point positions, that contain the material stress in the spirit of Eshelby [3]

In the case of continuum damage and thermo–hyperelasticity distributed material volume forces evolves due to damage or temperature gradients, which coincides with the evolution of continuous heterogeneities in the material. Thus the Galerkin discretization of the damage or temperature variable as an independent field becomes necessary in addition to the deformation field. The coupled problem will be solved using a monolithic solution strategy. The resulting material node point quantities, which we shall denote discrete material node point forces are demonstrated to be closely related to the classical $J$-integral in fracture mechanic problems. In particular we investigate the behavior of the Material Force Method in the case of cracked specimen while the damage zone or the temperature field evolves. Thereby e.g. a shielding effect of the distributed damage field w.r.t. the macroscopic crack is clearly demonstrated.

# 2 KINEMATICS AND KINETICS

In the material motion problem $\mathcal{B}_t$ denotes the spatial configuration occupied by the body of interest at time $t$. Then $\boldsymbol{\Phi}(\boldsymbol{x})$ denotes the non–linear deformation map assigning the spatial placements $\boldsymbol{x} \in \mathcal{B}_t$ of a 'physical particle' to the material placements $\boldsymbol{X} = \boldsymbol{\Phi}(\boldsymbol{x}) \in \mathcal{B}_0$ of the same 'physical particle'. Thus, the material placements are followed through the ambient material at fixed spatial position, i.e. the observer takes essentially the Eulerian viewpoint.

Next, the material motion linear tangent map is given by the deformation gradient $\boldsymbol{f} = \nabla_x \boldsymbol{\Phi}$ transforming line elements from the tangent space $T\mathcal{B}_t$ to line elements from the tangent space $T\mathcal{B}_0$. The spatial Jacobian, i.e. the determinant of $\boldsymbol{f}$ is denoted by $j = \det \boldsymbol{f}$ and relates volume elements $\mathrm{d}v \in \mathcal{B}_t$ to volume elements $\mathrm{d}V \in \mathcal{B}_0$.

For the material motion problem the quasi–static balance of momentum reads

$$-\mathrm{div}\boldsymbol{\pi}^t = \boldsymbol{B}_t \quad \longrightarrow \quad -\mathrm{Div}\boldsymbol{\Sigma}^t = \boldsymbol{B}_0 \tag{1}$$

It involves the momentum flux $\boldsymbol{\pi}^t$, a two–point tensor, and the momentum source $\boldsymbol{B}_t$, a vector in material description with spatial reference called the material motion volume force density.

The Piola transformation of $\boldsymbol{\pi}^t$ is called the Eshelby stress $\boldsymbol{\Sigma}^t = J\boldsymbol{\pi}^t \cdot \boldsymbol{f}^t$, alternatively the terminology energy-momentum tensor or configurational stress tensor is frequently adopted. The spatial motion volume force density with material reference is given by $\boldsymbol{B}_0 = J\boldsymbol{B}_t$.

# 3 CONSTITUTIVE EQUATION

For the material motion problem the free energy density $\psi_t = j\psi_0$ with spatial reference is expressed in terms of the material motion deformation gradient $\boldsymbol{f}$ (or its inverse $\boldsymbol{F}$) and additional internal variable $\alpha$ for a generic scalar or tensorial quantity, as $\psi_t = \psi_t(\boldsymbol{f}, \alpha, \boldsymbol{\Phi}(\boldsymbol{x}))$, where the explicit dependence on the material placement is captured by the field $\boldsymbol{X} = \boldsymbol{\Phi}(\boldsymbol{x})$ The conjugated counterpart to the internal variable $\alpha$ is given by $A_t = jA_0 = -d_\alpha \psi_t$. Then the familiar constitutive equations for the so-called Eshelby stress in $\mathcal{B}_0$ are given as $\boldsymbol{\Sigma}^t = j\boldsymbol{\pi}^t \cdot \boldsymbol{f}^t = \psi_0 \boldsymbol{I} - \boldsymbol{F}^t \cdot \boldsymbol{\Pi}^t$ with $\boldsymbol{\Pi}^t = \partial_F \Psi_0$. Note that the distributed volume forces now take the following particular format with respect to the additional internal variable $\alpha$

$$\boldsymbol{B}_t = A_t \, \nabla_X \alpha - \partial_{\boldsymbol{\Phi}} \psi_t + \boldsymbol{B}_t^{ext} \tag{2}$$

where the first part is related to material heterogeneities and the second to material inhomogeneities.

# 4 DISCRETIZATION AND $J$-INTEGRAL

By expanding the geometry $\boldsymbol{x}$ elementwise with shape functions $N_x^k$ in terms of the positions $\boldsymbol{x}_k$ of the node points and by using a Bubnov-Galerkin finite element method based on the iso–parametric concept, we end up with discrete algorithmic material node point (surface) forces at the global node point $K$ given by

$$\boldsymbol{\mathfrak{F}}_{sur,K}^h = \mathop{\mathbf{A}}_e \int_{\mathcal{B}_0^e} \boldsymbol{\Sigma}^t \cdot \nabla_X N^k - N_{\Phi}^k \boldsymbol{B}_0 \, \mathrm{d}V, \tag{3}$$

whereby we denote the material surface forces $\boldsymbol{\mathfrak{F}}_{sur,K}^h$ by 'SUR' in the diagrams later in the example section. Furthermore we separate them into an internal ('INT') and a volume part ('VOL')

$$\boldsymbol{\mathfrak{F}}_{int,K}^h = \mathop{\mathbf{A}}_e \int_{\mathcal{B}_0^e} \boldsymbol{\Sigma}^t \cdot \nabla_X N^k \, \mathrm{d}V \quad \text{and} \quad \boldsymbol{\mathfrak{F}}_{vol,K}^h = \mathop{\mathbf{A}}_e \int_{\mathcal{B}_0^e} N_{\Phi}^k \boldsymbol{B}_0 \, \mathrm{d}V \tag{4}$$

Thus we have in summary the obvious result $\boldsymbol{\mathfrak{F}}_{sur,K}^h = \boldsymbol{\mathfrak{F}}_{int,K}^h - \boldsymbol{\mathfrak{F}}_{vol,K}^h$.
Based on these results we advocate the Material Force Method with the notion of global discrete material node point (surface) forces, that (in the sense of Eshelby) are generated by variations relative to the ambient material at fixed spatial positions. Such forces corresponding to the material motion problem are trivially computable once the spatial motion problem has been solved.
Consider the resulting discrete material node point (surface) force $\boldsymbol{\mathfrak{F}}_{sur,s}^h$ acting on a crack tip. The exact value $\boldsymbol{\mathfrak{F}}_{sur,s}$ can be approximated by the discrete regular surface part $\boldsymbol{\mathfrak{F}}_{sur,r}^h$ and the discrete volume part $\boldsymbol{\mathfrak{F}}_{vol}^h$ of the discrete material node point (surface) forces $\boldsymbol{\mathfrak{F}}_{sur,s} \approx -\boldsymbol{\mathfrak{F}}_{sur,r}^h - \boldsymbol{\mathfrak{F}}_{vol}^h$. These in turn are balanced by discrete singular material surface forces $\boldsymbol{\mathfrak{F}}_{sur,s}^h$ and (spurious) discrete internal material surface forces $\boldsymbol{\mathfrak{F}}_{sur,i}^h$, which stem from an insufficient discretization accuracy as $-\boldsymbol{\mathfrak{F}}_{sur,r}^h - \boldsymbol{\mathfrak{F}}_{vol}^h = \boldsymbol{\mathfrak{F}}_{sur,s}^h + \boldsymbol{\mathfrak{F}}_{sur,i}^h$. Note thus, that the sum of all discrete algorithmic material node point surface forces $\boldsymbol{\mathfrak{F}}_{sur,K}^h$ corresponds according to Eq. 3 to the resulting value

$$\boldsymbol{\mathfrak{F}}_{sur,s} \approx \sum_{K \in \mathcal{V}_0^h \setminus \partial \mathcal{V}_0^{r,h}} \boldsymbol{\mathfrak{F}}_{sur,K}^h = \boldsymbol{\mathfrak{F}}_{sur,s}^h + \boldsymbol{\mathfrak{F}}_{sur,i}^h \tag{5}$$

Thus an improved value for $\boldsymbol{\mathfrak{F}}_{sur,s}$ is obtained by summing up all discrete material node point surface forces in the vicinity of the crack tip, see also Denzer et al. [2].

# 5 NUMERICAL EXAMPLES

As a first example we look at a hyperelastic material coupled to isotropic damage. Thereby isotropic damage is characterized by a degradation measure in terms of a scalar damage

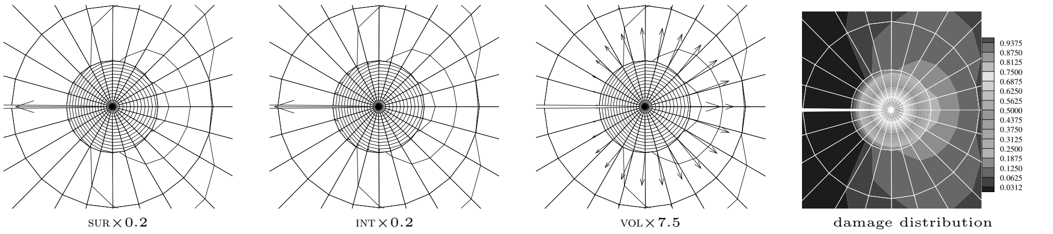


Figure 1: Damage distribution at crack tip

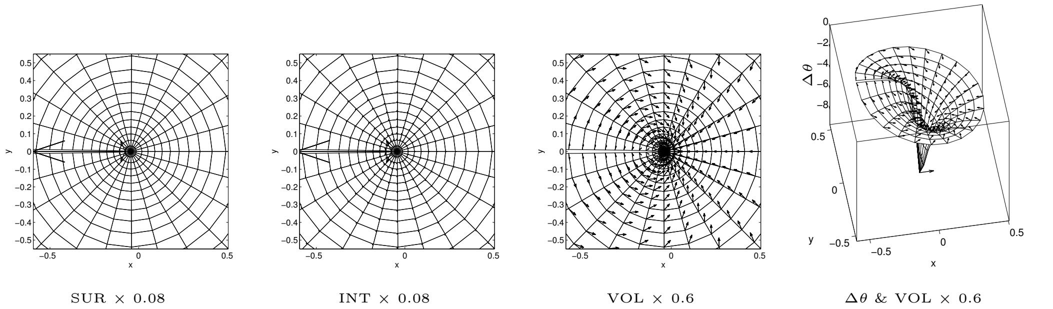


Figure 2: Discrete material node point surface, internal and volume forces and temperature distribution in the vicinity of the crack tip

variable $0 \leq d \leq 1$ that acts as a reduction factor of the local stored energy density of the virgin material $W_0 = JW_t$ per unit volume in $\mathcal{B}_0$ (or $W_t = jW_0$ per unit volume in $\mathcal{B}_t$, respectively), which is supposed to be an objective and isotropic function in $\boldsymbol{F}$ (or $\boldsymbol{f}$, respectively), see Liebe et al. [6]. The free energy density then reads $\psi_t = \psi_t(d, \boldsymbol{f}, \boldsymbol{\Phi}(\boldsymbol{x})) = [1-d]W_t(\boldsymbol{f}, \boldsymbol{\Phi}(\boldsymbol{x}))$ and $Y_0 = -\partial_d \psi_0 = W_0$. In this case the distributed volume forces take the particular format $\boldsymbol{B}_0 = Y_0 \nabla_X d - \partial_{\boldsymbol{X}} \psi_0 - \boldsymbol{F}^t \cdot \boldsymbol{b}_0^{ext}$.
The second example consists of thermo-hyperelastic material with the free energy function $\psi_0 = \psi_0(\boldsymbol{F}, \theta; \boldsymbol{X})$ depending on the absolute temperature $\theta$ with the entropy density given as $S_0 = -D_\theta \psi_0$. Here the distributed volume forces results in $\boldsymbol{B}_0 = S_0 \nabla_X \theta - \partial_{\boldsymbol{X}} \psi_0 - \boldsymbol{F}^t \cdot \boldsymbol{b}_0^{ext}$, see Kuhl et al. [5].
For a cracked specimen under mode I loading the discrete material forces and the distribution of the damage variable and the temperature variable are depict in Fig. 1 and Fig. 2, respectivily.

# 6 Conclusion

The objective of this work was to exploit the notion of material forces within the framework of isotropic geometrically non-linear continuum damage and thermo–hyperelasticity. Thereby the Material Force Method, see e.g. Steinmann et al. [14] was combined with an internal variable formulation of computational continuum damage mechanics and thermo–hyperelasticity. This particularly leads to the notion of distributed material volume forces that are conjugated to the damage or the temperature gradient, respectively. To this end, it was necessary to set up a two field formulation, i.e. the additional discretization of the damage variable or the temperature as an independent field next to the deformation field. With regard to fracture mechanics it could be shown that the evolving damage zone shields the crack tip. Hence the driving material surface force at the crack tip is significantly less than the applied external material load. This is the crucial difference with the hyperelastic case, where both are equal.

# References


[1] M. Braun, *Configurational forces induced by finite-element discretization*, Proc. Estonian Acad. Sci. Phys. Math., **46** (1997), pp. 24–31.

[2] R. Denzer, F.J. Barth, and P. Steinmann, *Studies in elastic fracture mechanics based on the material force method*, Int. J. Num. Meth. Eng., in press (2003).

[3] J.D. Eshelby, *The force on an elastic singularity*, Philosophical transactions of the Royal Society of London A, 244 (1951), pp. 87–112.

[4] M.E. Gurtin, *Configurational Forces as Basic Concepts of Continuum Physics*, (Springer, 1999).

[5] E. Kuhl, R. Denzer, F.J. Barth and P. Steinmann *Application of the material force method to thermo–hyperelasticity*, Comp. Meth. Appl. Mech. Eng. accepted (2003).

[6] T. Liebe, R. Denzer and P. Steinmann *Application of the material force method to isotropic continuum damage*, Computational Mechanics, **30** (2003), pp. 171–184.

[7] G.A. Maugin, *Material Inhomogeneities in Elasticity*, (Chapman & Hall, London, 1st ed., 1993).

[8] G.A. Maugin, *Material forces: Concepts and applications*, Appl. Mech. Rev., **48** (1995), pp. 213–245.

[9] G.A. Maugin, *Canonical momentum and energy in elastic systems with additional state variables*, C. R. Acad. Sci. Paris, **323IIb** (1996), pp. 407–412.

[10] G.A. Maugin, *On the universality of the thermomechanics of forces driving singular sets*, Arch. Appl. Mech., **70** (2000), pp. 31–45.

[11] P. Steinmann, *Application of material forces to hyperelastostatic fracture mechanics. Part I: continuum mechanical setting*, Int. J. Solids Struct., **37** (2000), pp. 7371–7391.

[12] P. Steinmann, *On spatial and material settings of hyperelastodynamics*, Acta Mechanica, **156** (2002), pp. 193–218.

[13] P. Steinmann, *On spatial and material settings of thermo-hyperelastodynamics*, J. Elasticity, **66** (2002), pp. 109–157.

[14] P. Steinmann, D. Ackermann, and F.J. Barth, *Application of material forces to hyperelastostatic fracture mechanics. Part II: computational setting*, Int. J. Solids Struct., **38** (2001), pp. 5509–5526.