THE FINITE ELEMENT METHOD FOR THREE-DIMENSIONAL THERMOMECHANICAL APPLICATIONS

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To my wife Barbara and my children Jakob and Lea

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Preface

In 1998, in times of ever increasing computer power, I had the unusual idea of writing my own finite element program, with just 20-node brick elements for elastic fracture-mechanics calculations. Especially with the program FEAP as a guide, it proved exceedingly simple to get a program with these minimal requirements to run. However, time has shown that this was only the beginning of a long and arduous journey. I was soon joined by my colleague Klaus Wittig, who had written a fast postprocessor for visualizing the results of several other finite element programs and who thought of expanding his program with preprocessing capabilities. He also brought along quite a few ideas for the solver. Coming from a modal-analysis department, he suggested including frequency and linear dynamic calculations. Furthermore, since he was interested in running real-size engine models, he required the code to be not only correct but also fast. This really meant that the code was to be competitive with the major commercial finite element codes. In terms of speed, the mathematical linear equation solver plays a dominant role. In this respect, we were very lucky to come across SPOOLES for static problems and ARPACK for eigenvalue problems, both excellent packages that are freely available on the Internet. I think it was at that time that we decided that our code should be free. The term "free" here primarily means freedom of thought as proclaimed by the GNU General Public License. We had profited enormously from the free equation solvers; why would not others profit from our code?

The demands on the code, but, primarily, also our eagerness to include new features, grew quickly. New element types were introduced. Geometric nonlinearity was implemented, hyperelastic constitutive relations and viscoplasticity followed. We selected the name CalculiX®, and in December 2000 we put the code on the web. Major contributions since then include nonlinear dynamics, cyclic symmetry conditions, anisotropic viscoplasticity and heat transfer. The comments and enthusiasm from users all over the world encourage us to proceed. But above all, the conviction that one cannot master a theory without having gone through the agony of implementing it ever anew drives me to go on.

This book contains the theory that was used to implement CalculiX®. This implies that the topics treated are ready to be coded, and, with a few exceptions, their practical implementation can be found in the CalculiX® code (www.calculix.de). One of the criteria for including a subject in CalculiX® or not is its industrial relevance. Therefore, topics such as cyclic symmetry or multiple point constraints, which are rarely treated in textbooks, are covered in detail. As a matter of fact, multiple point constraints constitute a very versatile workhorse in any industrial finite element application. Conditions such as rigid body motion, the application of a mean rotation, or the requirement that a node has to stay in a plane defined by three other moving nodes are readily formulated as nonlinear multiple point constraints. Clearly, new theories have to face several barriers before being accepted in an industrial environment. This especially applies to material models because of the enormous cost of the parameter identification through testing. Nevertheless, a couple of newer models in the area of anisotropic hyperelasticity and single-crystal viscoplasticity are covered, since they are the prototypes of new constitutive developments and because of the analytical insight they produce.

Although the applications are very practical, the theory cannot be developed without a profound knowledge of continuum mechanics. Therefore, a lot of emphasis is placed on the introduction of kinematic variables, the formulation of the balance laws and the derivation of the constitutive theory. The kinematic framework of a theory is its foundation. Among the kinematic tensors, the deformation gradient plays a special role, as amply demonstrated by the multiplicative decomposition used in viscoplastic theories. The balance equations in their weak form are the governing equations of the finite element method. Finally, the constitutive theory tells us what kind of conditions must be fulfilled by a material law to make sense physically. The knowledge of these rules is a prerequisite for the skillful description of new kinds of materials. This is clearly shown in the treatment of hyperelastic and viscoplastic materials, both in their isotropic and anisotropic form.

The only prerequisite for reading this book is a profound mathematical background in tensor analysis, matrix algebra and vector calculus. The book is largely self-contained, and all other knowledge is introduced within the text. It is oriented toward

1. graduate students working in the finite element field, enabling them to acquire a profound background,
2. researchers in the field, as a reference work,
3. practicing engineers who want to add special features to existing finite element programs and who have to familiarize themselves with the underlying theory.

This book would not have been possible without the help of several people. First, I would like to thank two teachers of mine: Lic. Antoine Van de Velde, for introducing me to the fascinating world of calculus, and Professor A. Cemal Eringen, for acquainting me with continuum mechanics. Readers of his numerous publications will doubtless recognize his stamp on my thinking. Further, I am very indebted to my colleague and friend Klaus Wittig; together we have developed the CalculiX® code in a rare symbiosis. His encouragement and the ever new demands on the code were instrumental in the growth of CalculiX®. I would also like to thank all the colleagues who read portions of the text and gave valuable comments: Dr Bernard Fedelich (Bundesanstalt für Materialforschung), Dr Hans-Peter Hackenberg (MTU Aero Engines), Dr Stefan Hartmann (University of Kassel), Dr Manfred Köhl (MTU Aero Engines), Dr Joop Nagtegaal (ABAQUS®), Dr Erhard Reile (MTU Aero Engines), Dr Harald Schönenborn (MTU Aero Engines) and others. Last but not least, I am very grateful to my wife Barbara and my children Jakob and Lea, who bravely endured my mental absence of the last few months.

Nomenclature

$\boldsymbol{A}$, A^{KL}	kinematic internal variable in material coordinates
$\boldsymbol{A}$, A_{MN}	thermal strain tensor per unit temperature
$\boldsymbol{A}$, $\boldsymbol{a}$, A^K, a^k	acceleration vector
A	deformed area of the body
A_0	undeformed area of the body
$A = \sigma\epsilon$	radiation coefficient
$\{A\}$	global acceleration vector
$\boldsymbol{b}$, b^{kl}	left Cauchy–Green tensor
$\boldsymbol{b}^{\mathrm{e}-1}$	inverse left elastic Cauchy–Green tensor or elastic Finger tensor
$\boldsymbol{C}^{\mathrm{p}}$, C^{p}_{KL}	right plastic Cauchy–Green tensor
$\mathrm{Cof}\boldsymbol{E}$	cofactor matrix of a second rank tensor E
cofactor E_{KL}	cofactor of tensor component E_{KL}
$[C]$	global capacity matrix
c	specific heat
c_0	speed of light in vacuum
c_{p}	specific heat at constant pressure
c_{v}	specific heat at constant volume
$\boldsymbol{d}$, d_{kl}	deformation rate tensor
$\mathrm{d}\boldsymbol{A}$, $\mathrm{d}A_K$	infinitesimal area one-form in material coordinates
$\mathrm{d}\boldsymbol{a}$, $\mathrm{d}a_k$	infinitesimal area one-form in spatial coordinates
$\det \boldsymbol{E}$	determinant of a second rank tensor E

dev $\boldsymbol{\sigma}$	deviatoric tensor of a second rank tensor $\boldsymbol{\sigma}$
dS	infinitesimal length in material coordinates
ds	infinitesimal length in spatial coordinates
dV	infinitesimal volume in material coordinates
dv	infinitesimal volume in spatial coordinates
d$\boldsymbol{X}$, dX^K	infinitesimal length vector in material coordinates
d$\boldsymbol{x}$, dx^k	infinitesimal length vector in spatial coordinates
dΣ	infinitesimal length in the intermediate configuration
dω	infinitesimal spatial angle
$\tilde{\boldsymbol{E}}$, $\tilde{E}_{KL}$	infinitesimal strain tensor in material coordinates
$\mathcal{E}$	total internal energy in the body
$\boldsymbol{E}$, E_{KL}	Lagrange strain tensor
E	Young's modulus
E	total emissive power
E_b	total emissive power of a blackbody
E_λ	spectral, hemispherical emissive power
$\tilde{\boldsymbol{e}}$, $\tilde{e}_{kl}$	infinitesimal strain tensor in spatial coordinates
$\boldsymbol{e}$, e_{kl}	Euler strain tensor
e_{LMP}, e^{LMP}	alternating symbols
$\boldsymbol{F}$, $F^k{}_K$	deformation gradient
F_{ij}	viewfactor: fraction of the radiation power leaving surface i that is intercepted by surface j
$\{F\}$	global force vector
$\{F\}_\mathrm{e}$	element force vector
$\boldsymbol{f}$, f^k, f^K	force per unit mass
$\boldsymbol{G}$, $\boldsymbol{G}^\flat$, G_{KL}	covariant metric tensor in the reference system
$\boldsymbol{G}$, $\boldsymbol{G}^\sharp$, G^{KL}	contravariant metric tensor in the reference system

$\boldsymbol{G}^K$	contravariant curvilinear basis vectors in the reference system
$\boldsymbol{G}_K$	covariant curvilinear basis vectors in the reference system
G	hemispherical irradiation power
$\boldsymbol{g}, \boldsymbol{g}^\flat, g_{kl}$	covariant metric tensor in the spatial system
$\boldsymbol{g}, \boldsymbol{g}^\sharp, g^{kl}$	contravariant metric tensor in the spatial system
$g^{Kk}, g^K{}_k, g^k{}_K$	shifters
$\boldsymbol{g}^k$	contravariant curvilinear basis vectors in the spatial system
$\boldsymbol{g}_k$	covariant curvilinear basis vectors in the spatial system
h	Planck constant
h	convection coefficient
h	heat generation per unit mass
$\mathbb{I}_A$	unit tensor of rank four where the unit tensor $\boldsymbol{I}$ is replaced by the tensor $\boldsymbol{A}$
$\mathbb{I}_I$	unit tensor of rank four
$\boldsymbol{I}, I_{KL}, I^{KL}, \delta^K{}_L$	metric tensor in rectangular coordinates in the reference system
$\boldsymbol{I}^K, \boldsymbol{I}_K$	rectangular basis vectors in the reference system
I_E	spectral, directional radiation intensity
$I_{E,\mathrm{b}}$	spectral intensity of blackbody radiation
I_I	spectral, directional irradiation intensity
I_{kd}	kth invariant of the deformation rate tensor
I_{kE}	kth invariant of the Lagrangian strain tensor
$\overline{I}_k, I_{k\overline{C}}$	kth invariant of the reduced Cauchy−Green tensor
I_k, I_{kC}	kth invariant of the Cauchy−Green tensor
$I_{k\sigma}$	kth invariant of the Cauchy tensor
$\boldsymbol{i}, i_{kl}, i^{kl}, \delta^k{}_l$	metric tensor in rectangular coordinates in the spatial system
$\boldsymbol{i}^k, \boldsymbol{i}_k$	rectangular basis vectors in the spatial system
$\boldsymbol{J}, J^K$	Jacobian vector

J	Jacobian determinant of the deformation
J	radiosity
J^*	Jacobian of the global–local transformation
J_k, J_{kC}	kth invariant of the Cauchy–Green tensor of the form tr$\boldsymbol{C}^k$
$\mathcal{K}$	total kinetic energy in the body
K	bulk modulus
$[K]$	global stiffness matrix
$[K]_\mathrm{e}$	element stiffness matrix
k	Boltzmann constant
$[L]_\mathrm{e}$	element localization matrix
$\boldsymbol{l}$, l_{kl}	velocity gradient
$\boldsymbol{M}_i = \boldsymbol{N}_i \otimes \boldsymbol{N}_i$, M_i^{KL}	contravariant structural tensors in material coordinates
$\boldsymbol{M}^i = \boldsymbol{N}^i \otimes \boldsymbol{N}^i$, M^i_{KL}	covariant structural tensors in material coordinates
$[M]$	global mass matrix
$[M]_\mathrm{e}$	element mass matrix
$\dot{m}_{ij}$	absolute value of the mass flow between node i and node j
$\boldsymbol{N}_i$, N_i^K	ith normalized eigenvector in material coordinates
$\boldsymbol{N}^i$, N^i_K	ith normalized eigen-one-form in material coordinates
$\boldsymbol{N}$, N_K	normalized area one-form in material coordinates
$\boldsymbol{n}_i$, n_i^k	ith normalized eigenvector in spatial coordinates
$\boldsymbol{n}^i$, n^i_k	ith normalized eigen-one-form in spatial coordinates
$\boldsymbol{n}$, n_k	normalized area one-form in spatial coordinates
$\boldsymbol{P}$, P^{Kk}	first Piola–Kirchhoff stress tensor
P	radiation power
p	pressure
$\boldsymbol{Q}$	internal dynamic variable in material coordinates

$\boldsymbol{Q}$, $Q^{K'}_{\ L}$	orthogonal transformation matrix
$\boldsymbol{Q}$, Q^K, $\boldsymbol{Q}^\theta$	heat vector in material coordinates
$\{Q\}$	global heat flux vector
$\{Q\}_e$	element heat flux vector
$\boldsymbol{q}$, $\boldsymbol{q}^i$	internal dynamic variable in spatial coordinates
$\boldsymbol{q}$, q^k, $\boldsymbol{q}^\theta$	heat vector in spatial coordinates
$\tilde{\boldsymbol{R}}$, $\tilde{R}_{KL}$	infinitesimal rotation tensor in material coordinates
$\boldsymbol{R}$, $R^k_{\ L}$	rotation tensor
R	specific gas constant
$\boldsymbol{S}$, S^K	entropy vector in material coordinates
$\boldsymbol{S}$, S^{KL}	second Piola–Kirchhoff stress tensor
$\boldsymbol{s}$, s^k	entropy vector in spatial coordinates
$\boldsymbol{T}^K$	traction vector on a surface with normal parallel to $\boldsymbol{G}^K$
$\boldsymbol{T}_{(\boldsymbol{N})}$, $T^K_{(\boldsymbol{N})}$	traction vector on a surface with normal $\boldsymbol{N}$ in material coordinates
T	relative temperature
$\{T\}$	global temperature vector
$\{T\}_\mathrm{e}$	element temperature vector
$\boldsymbol{t}^k$	traction vector on a surface with normal parallel to $\boldsymbol{g}^k$
$\boldsymbol{t}_{(\boldsymbol{n})}$, $t^k_{(\boldsymbol{n})}$	traction vector on a surface with normal $\boldsymbol{n}$ in spatial coordinates
$\mathrm{tr}\boldsymbol{E}$	trace of a second rank tensor E
$\boldsymbol{U}$, $U^K_{\ L}$	right stretch tensor
$\boldsymbol{U}$, $\boldsymbol{u}$, U^K, u^k	displacement vector
U	volumetric free energy potential
$\{U\}$	global displacement vector
$\{U\}_e$	element displacement vector
$\boldsymbol{V}$, $V^k_{\ l}$	left stretch tensor
$\boldsymbol{V}$, $\boldsymbol{v}$, V^K, v^k	velocity vector

V	deformed volume of the body
V_0	undeformed volume of the body
V_{0e}	undeformed volume of a finite element
$\{V\}$	global velocity vector
$\mathcal{W}$	total rate of work in the body
$\boldsymbol{w}, w_{kl}$	spin tensor
$\boldsymbol{X}, X^K$	position vector in material coordinates
$\boldsymbol{x}, x^k$	position vector in spatial coordinates
$\boldsymbol{\alpha}, \alpha^{kl}$	kinematic internal variable in spatial coordinates
α	total, hemispherical absorptivity
$\boldsymbol{\beta}, \beta^{KL}$	thermal stress tensor per unit temperature
$\boldsymbol{\gamma}, \gamma^{KL}$	residual stress tensor
$\boldsymbol{\gamma}(\xi, \eta, \zeta)$	vector of local coordinates
$\dot{\gamma}$	consistency parameter
$\delta^K{}_L$	mixed-variant metric tensor in the reference system
$\delta^k{}_l$	mixed-variant metric tensor in the spatial system
δT	temperature perturbation
$\delta \boldsymbol{U}, \delta U_K$	displacement perturbation
$\boldsymbol{\epsilon}, \epsilon_{kl}$	infinitesimal strain tensor in spatial coordinates
$\boldsymbol{\epsilon}^{\mathrm{e}}, \epsilon^e_{kl}$	infinitesimal elastic strain tensor in spatial coordinates
$\boldsymbol{\epsilon}^{\mathrm{p}}, \epsilon^p_{kl}$	infinitesimal plastic strain tensor in spatial coordinates
ϵ	emissivity
$\epsilon_{\lambda,\omega}$	spectral, directional emissivity
ε	energy density
ζ	local coordinate
η	entropy per unit mass
η	local coordinate

θ	absolute temperature
θ_e	absolute environmental temperature
θ_{ref}	reference temperature
$\kappa, \kappa^K, \kappa^{KL}, \kappa^{KLM}$	conduction coefficients
Λ_{iE}	ith eigenvalue of the Lagrangian strain tensor
Λ_{iS}	ith eigenvalue of the second Piola–Kirchhoff stress tensor
Λ_i, Λ_{iC}	ith eigenvalue of the Cauchy–Green tensor
λ	Lamé constant
λ_i	principal stretches, eigenvalues of $\boldsymbol{F}$
$\lambda_{i\sigma}$	ith eigenvalue of the Cauchy stress tensor
λ_v	fluid constant
μ	Lamé constant
μ_v	fluid constant
ν	Poisson coefficient
$\boldsymbol{\Xi}, \Xi^{KL}$	relative stress tensor in material coordinates
ξ	local coordinate
ρ	mass density in the spatial configuration
ρ	total, hemispherical reflectivity
ρ_0	mass density in the material configuration
$\Sigma_0, \Sigma^{KL}, \Sigma^{KLMN}$	free energy coefficients
$\Sigma = \rho_0\psi$	free energy per unit volume in the reference configuration
$\boldsymbol{\sigma}, \sigma^{kl}$	Cauchy stress tensor
σ	Stefan–Boltzmann constant
τ	total, hemispherical transmissivity
$\varphi_i(\xi, \eta, \zeta)$	shape functions
ψ	free energy per unit mass
ω	circular frequency
∇	spatial gradient
∇_0	material gradient