



**THE FINITE ELEMENT METHOD  
FOR THREE-DIMENSIONAL  
THERMOMECHANICAL APPLICATIONS**

GUIDO DHONDT



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# **The Finite Element Method for Three-dimensional Thermomechanical Applications**

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**Guido Dhondt**

*Munich, Germany*



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*To my wife Barbara and my children Jakob and Lea*

# Contents

<b>Preface</b>	<b>xiii</b>
<b>Nomenclature</b>	<b>xv</b>
<b>1 Displacements, Strain, Stress and Energy</b>	<b>1</b>
1.1 The Reference State . . . . .	1
1.2 The Spatial State . . . . .	4
1.3 Strain Measures . . . . .	9
1.4 Principal Strains . . . . .	13
1.5 Velocity . . . . .	19
1.6 Objective Tensors . . . . .	22
1.7 Balance Laws . . . . .	25
1.7.1 Conservation of mass . . . . .	25
1.7.2 Conservation of momentum . . . . .	25
1.7.3 Conservation of angular momentum . . . . .	26
1.7.4 Conservation of energy . . . . .	26
1.7.5 Entropy inequality . . . . .	27
1.7.6 Closure . . . . .	28
1.8 Localization of the Balance Laws . . . . .	28
1.8.1 Conservation of mass . . . . .	28
1.8.2 Conservation of momentum . . . . .	29
1.8.3 Conservation of angular momentum . . . . .	31
1.8.4 Conservation of energy . . . . .	31
1.8.5 Entropy inequality . . . . .	31
1.9 The Stress Tensor . . . . .	31
1.10 The Balance Laws in Material Coordinates . . . . .	34
1.10.1 Conservation of mass . . . . .	35
1.10.2 Conservation of momentum . . . . .	35
1.10.3 Conservation of angular momentum . . . . .	37
1.10.4 Conservation of energy . . . . .	37
1.10.5 Entropy inequality . . . . .	37
1.11 The Weak Form of the Balance of Momentum . . . . .	38
1.11.1 Formulation of the boundary conditions (material coordinates) . . . . .	38
1.11.2 Deriving the weak form from the strong form (material coordinates) . . . . .	39
1.11.3 Deriving the strong form from the weak form (material coordinates) . . . . .	41
1.11.4 The weak form in spatial coordinates . . . . .	41
1.12 The Weak Form of the Energy Balance . . . . .	42
1.13 Constitutive Equations . . . . .	43

1.13.1	Summary of the balance equations . . . . .	43
1.13.2	Development of the constitutive theory . . . . .	44
1.14	Elastic Materials . . . . .	47
1.14.1	General form . . . . .	47
1.14.2	Linear elastic materials . . . . .	49
1.14.3	Isotropic linear elastic materials . . . . .	52
1.14.4	Linearizing the strains . . . . .	54
1.14.5	Isotropic elastic materials . . . . .	58
1.15	Fluids . . . . .	59
<b>2</b>	<b>Linear Mechanical Applications</b>	<b>63</b>
2.1	General Equations . . . . .	63
2.2	The Shape Functions . . . . .	67
2.2.1	The 8-node brick element . . . . .	68
2.2.2	The 20-node brick element . . . . .	69
2.2.3	The 4-node tetrahedral element . . . . .	71
2.2.4	The 10-node tetrahedral element . . . . .	72
2.2.5	The 6-node wedge element . . . . .	73
2.2.6	The 15-node wedge element . . . . .	73
2.3	Numerical Integration . . . . .	75
2.3.1	Hexahedral elements . . . . .	76
2.3.2	Tetrahedral elements . . . . .	78
2.3.3	Wedge elements . . . . .	78
2.3.4	Integration over a surface in three-dimensional space . . . . .	81
2.4	Extrapolation of Integration Point Values to the Nodes . . . . .	82
2.4.1	The 8-node hexahedral element . . . . .	83
2.4.2	The 20-node hexahedral element . . . . .	84
2.4.3	The tetrahedral elements . . . . .	86
2.4.4	The wedge elements . . . . .	86
2.5	Problematic Element Behavior . . . . .	86
2.5.1	Shear locking . . . . .	87
2.5.2	Volumetric locking . . . . .	87
2.5.3	Hourglassing . . . . .	90
2.6	Linear Constraints . . . . .	91
2.6.1	Inclusion in the global system of equations . . . . .	91
2.6.2	Forces induced by linear constraints . . . . .	96
2.7	Transformations . . . . .	97
2.8	Loading . . . . .	103
2.8.1	Centrifugal loading . . . . .	103
2.8.2	Temperature loading . . . . .	104
2.9	Modal Analysis . . . . .	106
2.9.1	Frequency calculation . . . . .	106
2.9.2	Linear dynamic analysis . . . . .	108
2.9.3	Buckling . . . . .	112
2.10	Cyclic Symmetry . . . . .	114
2.11	Dynamics: The $\alpha$ -Method . . . . .	120

2.11.1	Implicit formulation . . . . .	120
2.11.2	Extension to nonlinear applications . . . . .	123
2.11.3	Consistency and accuracy of the implicit formulation . . . . .	126
2.11.4	Stability of the implicit scheme . . . . .	130
2.11.5	Explicit formulation . . . . .	136
2.11.6	The consistent mass matrix . . . . .	138
2.11.7	Lumped mass matrix . . . . .	140
2.11.8	Spherical shell subject to a suddenly applied uniform pressure . . .	141
<b>3</b>	<b>Geometric Nonlinear Effects</b>	<b>143</b>
3.1	General Equations . . . . .	143
3.2	Application to a Snapping-through Plate . . . . .	148
3.3	Solution-dependent Loading . . . . .	150
3.3.1	Centrifugal forces . . . . .	150
3.3.2	Traction forces . . . . .	151
3.3.3	Example: a beam subject to hydrostatic pressure . . . . .	154
3.4	Nonlinear Multiple Point Constraints . . . . .	154
3.5	Rigid Body Motion . . . . .	155
3.5.1	Large rotations . . . . .	155
3.5.2	Rigid body formulation . . . . .	159
3.5.3	Beam and shell elements . . . . .	162
3.6	Mean Rotation . . . . .	167
3.7	Kinematic Constraints . . . . .	171
3.7.1	Points on a straight line . . . . .	171
3.7.2	Points in a plane . . . . .	173
3.8	Incompressibility Constraint . . . . .	174
<b>4</b>	<b>Hyperelastic Materials</b>	<b>177</b>
4.1	Polyconvexity of the Stored-energy Function . . . . .	177
4.1.1	Physical requirements . . . . .	177
4.1.2	Convexity . . . . .	180
4.1.3	Polyconvexity . . . . .	184
4.1.4	Suitable stored-energy functions . . . . .	189
4.2	Isotropic Hyperelastic Materials . . . . .	190
4.2.1	Polynomial form . . . . .	191
4.2.2	Arruda–Boyce form . . . . .	193
4.2.3	The Ogden form . . . . .	194
4.2.4	Elastomeric foam behavior . . . . .	195
4.3	Nonhomogeneous Shear Experiment . . . . .	196
4.4	Derivatives of Invariants and Principal Stretches . . . . .	199
4.4.1	Derivatives of the invariants . . . . .	199
4.4.2	Derivatives of the principal stretches . . . . .	200
4.4.3	Expressions for the stress and stiffness for three equal eigenvalues .	206
4.5	Tangent Stiffness Matrix at Zero Deformation . . . . .	209
4.5.1	Polynomial form . . . . .	210
4.5.2	Arruda–Boyce form . . . . .	211



4.5.3	Ogden form . . . . .	211
4.5.4	Elastomeric foam behavior . . . . .	211
4.5.5	Closure . . . . .	212
4.6	Inflation of a Balloon . . . . .	212
4.7	Anisotropic Hyperelasticity . . . . .	216
4.7.1	Transversely isotropic materials . . . . .	217
4.7.2	Fiber-reinforced material . . . . .	219
<b>5</b>	<b>Infinitesimal Strain Plasticity</b>	<b>225</b>
5.1	Introduction . . . . .	225
5.2	The General Framework of Plasticity . . . . .	225
5.2.1	Theoretical derivation . . . . .	225
5.2.2	Numerical implementation . . . . .	232
5.3	Three-dimensional Single Surface Viscoplasticity . . . . .	235
5.3.1	Theoretical derivation . . . . .	235
5.3.2	Numerical procedure . . . . .	239
5.3.3	Determination of the consistent elastoplastic tangent matrix . . . . .	242
5.4	Three-dimensional Multisurface Viscoplasticity: the Cailletaud Single Crystal Model . . . . .	244
5.4.1	Theoretical considerations . . . . .	244
5.4.2	Numerical aspects . . . . .	248
5.4.3	Stress update algorithm . . . . .	249
5.4.4	Determination of the consistent elastoplastic tangent matrix . . . . .	259
5.4.5	Tensile test on an anisotropic material . . . . .	260
5.5	Anisotropic Elasticity with a von Mises–type Yield Surface . . . . .	262
5.5.1	Basic equations . . . . .	262
5.5.2	Numerical procedure . . . . .	263
5.5.3	Special case: isotropic elasticity . . . . .	270
<b>6</b>	<b>Finite Strain Elastoplasticity</b>	<b>273</b>
6.1	Multiplicative Decomposition of the Deformation Gradient . . . . .	273
6.2	Deriving the Flow Rule . . . . .	275
6.2.1	Arguments of the free-energy function and yield condition . . . . .	275
6.2.2	Principle of maximum plastic dissipation . . . . .	276
6.2.3	Uncoupled volumetric/deviatoric response . . . . .	278
6.3	Isotropic Hyperelasticity with a von Mises–type Yield Surface . . . . .	279
6.3.1	Uncoupled isotropic hyperelastic model . . . . .	279
6.3.2	Yield surface and derivation of the flow rule . . . . .	280
6.4	Extensions . . . . .	284
6.4.1	Kinematic hardening . . . . .	284
6.4.2	Viscoplastic behavior . . . . .	285
6.5	Summary of the Equations . . . . .	287
6.6	Stress Update Algorithm . . . . .	287
6.6.1	Derivation . . . . .	287
6.6.2	Summary . . . . .	291
6.6.3	Expansion of a thick-walled cylinder . . . . .	293

CONTENTS	xi
6.7 Derivation of Consistent Elastoplastic Moduli . . . . .	294
6.7.1 The volumetric stress . . . . .	295
6.7.2 Trial stress . . . . .	295
6.7.3 Plastic correction . . . . .	296
6.8 Isochoric Plastic Deformation . . . . .	300
6.9 Burst Calculation of a Compressor . . . . .	302
<b>7 Heat Transfer</b>	<b>305</b>
7.1 Introduction . . . . .	305
7.2 The Governing Equations . . . . .	305
7.3 Weak Form of the Energy Equation . . . . .	307
7.4 Finite Element Procedure . . . . .	309
7.5 Time Discretization and Linearization of the Governing Equation . . . . .	310
7.6 Forced Fluid Convection . . . . .	312
7.7 Cavity Radiation . . . . .	317
7.7.1 Governing equations . . . . .	317
7.7.2 Numerical aspects . . . . .	324
<b>References</b>	<b>329</b>
<b>Index</b>	<b>335</b>

# 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 SPOLES 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<sup>®</sup>, 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<sup>®</sup>. 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<sup>®</sup> code ([www.calculix.de](http://www.calculix.de)). One of the criteria for including a subject in CalculiX<sup>®</sup> 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<sup>®</sup> code in a rare symbiosis. His encouragement and the ever new demands on the code were instrumental in the growth of CalculiX<sup>®</sup>. 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<sup>®</sup>), 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

$A, A^{KL}$	kinematic internal variable in material coordinates
$A, A_{MN}$	thermal strain tensor per unit temperature
$A, \mathbf{a}, A^K, a^k$	acceleration vector
$A$	deformed area of the body
$A_0$	undeformed area of the body
$A = \sigma \epsilon$	radiation coefficient
$\{A\}$	global acceleration vector
$\mathbf{b}, b^{kl}$	left Cauchy–Green tensor
$\mathbf{b}^{e-1}$	inverse left elastic Cauchy–Green tensor or elastic Finger tensor
$C^p, C_{KL}^p$	right plastic Cauchy–Green tensor
$\text{Cof} \mathbf{E}$	cofactor matrix of a second rank tensor $\mathbf{E}$
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
$\mathbf{d}, d_{kl}$	deformation rate tensor
$dA, dA_K$	infinitesimal area one-form in material coordinates
$da, da_k$	infinitesimal area one-form in spatial coordinates
$\det \mathbf{E}$	determinant of a second rank tensor $\mathbf{E}$

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

$\mathbf{G}^K$	contravariant curvilinear basis vectors in the reference system
$\mathbf{G}_K$	covariant curvilinear basis vectors in the reference system
$G$	hemispherical irradiation power
$\mathbf{g}, \mathbf{g}^b, g_{kl}$	covariant metric tensor in the spatial system
$\mathbf{g}, \mathbf{g}^\sharp, g^{kl}$	contravariant metric tensor in the spatial system
$g^{Kk}, g^K_k, g^k_K$	shifters
$\mathbf{g}^k$	contravariant curvilinear basis vectors in the spatial system
$\mathbf{g}_k$	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 $\mathbf{I}$ is replaced by the tensor $\mathbf{A}$
$\mathbb{I}_I$	unit tensor of rank four
$\mathbf{I}, I_{KL}, I^{KL}, \delta^K_L$	metric tensor in rectangular coordinates in the reference system
$\mathbf{I}^K, \mathbf{I}_K$	rectangular basis vectors in the reference system
$I_E$	spectral, directional radiation intensity
$I_{E,b}$	spectral intensity of blackbody radiation
$I_I$	spectral, directional irradiation intensity
$I_{kd}$	$k$ th invariant of the deformation rate tensor
$I_{kE}$	$k$ th invariant of the Lagrangian strain tensor
$\bar{I}_k, I_{k\bar{C}}$	$k$ th invariant of the reduced Cauchy–Green tensor
$I_k, I_{kC}$	$k$ th invariant of the Cauchy–Green tensor
$I_{k\sigma}$	$k$ th invariant of the Cauchy tensor
$\mathbf{i}, i_{kl}, i^{kl}, \delta^k_l$	metric tensor in rectangular coordinates in the spatial system
$\mathbf{i}^k, \mathbf{i}_k$	rectangular basis vectors in the spatial system
$\mathbf{J}, J^K$	Jacobian vector

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



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

xx

$V$	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
$\alpha$	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
$\delta T$	temperature perturbation
$\delta \boldsymbol{U}, \delta U_K$	displacement perturbation
$\boldsymbol{\epsilon}, \epsilon_{kl}$	infinitesimal strain tensor in spatial coordinates
$\boldsymbol{\epsilon}^e, \epsilon^e_{kl}$	infinitesimal elastic strain tensor in spatial coordinates
$\boldsymbol{\epsilon}^p, \epsilon^p_{kl}$	infinitesimal plastic strain tensor in spatial coordinates
$\epsilon$	emissivity
$\epsilon_{\lambda, \omega}$	spectral, directional emissivity
$\epsilon$	energy density
$\zeta$	local coordinate
$\eta$	entropy per unit mass
$\eta$	local coordinate

$\theta$	absolute temperature
$\theta_e$	absolute environmental temperature
$\theta_{\text{ref}}$	reference temperature
$\kappa, \kappa^K, \kappa^{KL}, \kappa^{KLM}$	conduction coefficients
$\Lambda_{iE}$	$i$ th eigenvalue of the Lagrangian strain tensor
$\Lambda_{iS}$	$i$ th eigenvalue of the second Piola–Kirchhoff stress tensor
$\Lambda_i, \Lambda_{iC}$	$i$ th eigenvalue of the Cauchy–Green tensor
$\lambda$	Lamé constant
$\lambda_i$	principal stretches, eigenvalues of $\mathbf{F}$
$\lambda_{i\sigma}$	$i$ th eigenvalue of the Cauchy stress tensor
$\lambda_v$	fluid constant
$\mu$	Lamé constant
$\mu_v$	fluid constant
$\nu$	Poisson coefficient
$\Xi, \Xi^{KL}$	relative stress tensor in material coordinates
$\xi$	local coordinate
$\rho$	mass density in the spatial configuration
$\rho$	total, hemispherical reflectivity
$\rho_0$	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
$\sigma, \sigma^{kl}$	Cauchy stress tensor
$\sigma$	Stefan–Boltzmann constant
$\tau$	total, hemispherical transmissivity
$\varphi_i(\xi, \eta, \zeta)$	shape functions
$\psi$	free energy per unit mass
$\omega$	circular frequency
$\nabla$	spatial gradient
$\nabla_0$	material gradient