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M. Sc. Dipl.-Ing. (FH) Patrick Erbts,
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Partitioned solution strategies for electro-thermo-mechanical problems applied to the field-assisted sintering technology

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Dedicated to engineers and scientists in the field of coupled problems and computational mechanics, this thesis addresses partitioned solution strategies for electro-thermo-mechanically coupled problems applied to the field-assisted sintering technology (FAST). By simultaneously applying uniaxial pressure and an electric current to generate high heating rates, the FAST process offers short production cycles for sintering materials. To approach the process conditions at high temperatures in a realistic and holistic way radiative heat transfer is numerically treated as an additional field. Finally, a fully coupled four-field problem is composed where for the electric, thermal and mechanical fields the finite element method is applied while solving the radiation field using computational fluid dynamic (CFD) solvers. The numerical results are compared to experiments. Moreover, an in-depth study of coupling algorithms is carried out to improve the convergence of the partitioned solution procedure.

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Vorwort

Die vorliegende Arbeit wurde von mir während meiner Zeit als wissenschaftlicher Mitarbeiter am Institut für Konstruktion und Festigkeit von Schiffen in der Arbeitsgruppe *Numerische Strukturanalyse mit Anwendungen in der Schiffstechnik* der Technischen Universität Hamburg von April 2011 bis Mai 2015 angefertigt. Sie entstand im Rahmen des von der Deutschen Forschungsgemeinschaft (DFG) geförderten Projektes *Electro-thermo-mechanical modeling of the field-assisted sintering technology using high-order finite elemenst validated by experiments*. Während dieser Zeit habe ich viel Unterstützung erfahren, wofür ich mich im folgenden besonders bedanken möchte.

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Patrick Erbts — Hamburg, im April 2016

Für Joscha

Contents

Nomenclature

A distinction is made in scalars, vectors, tensors, and matrices and the following notation is introduced: scalars are written in italic letters A, vectors in the Euclidean space are indicated by arrows $\vec{a}$, second-order tensors are written with an under-tilde $\underset{\sim}{S}$. This holds also for Greek letters. For high-order tensors calligraphic letters with an under-tilde $\underset{\sim}{\mathcal{C}}$ are used. Matrices are written in bold letters. The combination of an italic and bold letter indicates local finite element matrices $\boldsymbol{A}$, whereas standard bold letters $\mathbf{A}$ refer to global matrices. In addition, lowercase letters $\mathbf{a}$ or $\boldsymbol{a}$ are used for column matrices. This notation is used throughout this thesis except where it is explicitly mentioned in the text.

Some frequently used tensor operations are also summarized in the following. Further reading on tensor-algebra and tensor-analysis for continuum mechanics is provided in [84, 13] for instance.

Tensors

A	Scalar value
$\vec{a} = a_i \, \vec{g}_i$	First-order tensor (vector)
$\underset{\sim}{S} = S_{ij} \, \vec{g}_i \otimes \vec{g}_j$	Second-order tensor
$\underset{\sim}{\mathcal{C}} = \mathcal{C}_{i_1 \ldots i_n} \, \vec{g}_{i_1} \otimes \vec{g}_{i_2} \otimes \ldots \otimes \vec{g}_{i_n}$	Tensors of higher order

Matrices / column matrices

$\mathbf{a}$	Global column matrix
$\mathbf{A}$	Global matrix
$\boldsymbol{a}$	Local finite element column matrix
$\boldsymbol{A}$	Local finite element matrix

Mathematical operators

$\vec{u} \otimes \vec{v} = u_i\, v_j\, \vec{g}_i \otimes \vec{g}_j$	Dyadic product
$\underset{\approx}{S} \cdot \underset{\approx}{F} = S_{ij}\, F_{ij}$	Inner, scalar or dot product
$\underset{\approx}{S}\, \underset{\approx}{F} = S_{ij}\, F_{jk}\, \vec{g}_i \otimes \vec{g}_k$	Tensor product
$\underset{\approx}{S}^T = S_{ij}\, \vec{g}_j \otimes \vec{g}_i$	Transposed tensor
$\underset{\approx}{S}^{-1}$	Inverse of a tensor
$\mathrm{tr}\, \underset{\approx}{S} = S_{ii}$	Trace of a tensor (first invariant I_S)
$\det \underset{\approx}{S}$	Determinant of a tensor (third invariant III_S)
div, Div	Divergence operator
grad, Grad	Gradient operator
∇	Nabla operator

List of symbols

A list of the main symbols is given in the following. Subordinate variables of minor importance – typically appearing only once in the text – are not listed and are explicitly mentioned. Due to the multitude of different variables, a double seizure of some symbols cannot be avoided. This is also mentioned in the text.

Scalars

α	Absorptance
α_Θ	Thermal expansion coefficient
α_φ	Linear temperature coefficient
β	Extinction coefficient
γ	Thermo-elastic coupling term
ϵ	Tolerance
ε	Emissivity or emittance
η	Wave-number
ϑ	Thermal stretch-ratio
θ	Angle of colatitude
Θ	Temperature
κ	Absorption coefficient
$\varkappa$	Wave-length
Λ	Iteration residual
λ	First Lamé constant
λ_Θ	Heat conduction coefficient
λ_φ	Electric conduction coefficient
μ	Second Lamé constant / Shear modulus
ν	Viscosity
ξ	Entropy per unit volume
ϖ	Number of solver calls
ρ	Mass density
ρ_{c}	Charge density
ϱ	Reflectance
ς	Coupling iterations per time-step
σ_{sb}	Stefan-Boltzmann constant
σ_{S}	Scatter coefficient
Σ	Entropy

τ	Transmittance
υ	Wave-frequency
Υ	Solid angle
φ	Electric potential
ϕ	Angle of latitude
Φ	Scatter phase function
ψ	Angle of longitude
Ψ	Helmholtz free-energy
ω	Relaxation coefficient
Ω	Domain / Configuration
Ω_e	Element volume
a, A	Area
c_0	Speed of light in vacuum
c_p	Heat capacity / specific heat
d, D	Dissipation
e	Specific internal energy
E	Emissive power
f	(Angular) Frequency
F	View factor
G	Incident radiation
h	Electric charge
H	Irradiation
I	Radiative intensity
J	Determinant of the deformation gradient
K	Bulk modulus
l, L	Length
m, M	Mass
N	Shape function
p	(Polynomial) Order
p_f	Fluid pressure
P	Point
q, Q	Heat flux
r, R	Heat source
s	Path
S	Distance
t	Time
T	Time interval
U	Volumetric part of the strain-energy density function
v, V	Volume
w	Weights / weight function
$\bar{w}$	Isochoric part of strain-energy density function
W	Strain-energy density function
x, X	Coordinates
Y	Surface radiosity
$\mathcal{E}$	Internal energy

$\mathcal{K}$	Kinetic energy
$\mathcal{Q}$	Thermal work
$\mathcal{W}$	Mechanical work

Vectors

$\vec{\eta}$	Test function
$\vec{\chi}$	Mapping function
$\vec{a}, \vec{A}$	Surface element vector
$\vec{b}$	Body force density vector per unit mass
$\vec{d}$	Domain displacement vector / boundary displacements
$\vec{e}$, $\vec{E}$	Electric field intensity
$\vec{f}$, $\vec{F}$	Force vector
$\vec{g}$	Basis vector in current configuration
$\vec{G}$	Basis vector in reference configuration
$\vec{h}$	Rotational or angular momentum vector
$\vec{j}$, $\vec{J}$	Electric current density vector
$\vec{k}$	Gravitation vector
$\vec{l}$	Linear or translational momentum vector
$\vec{m}$	Moment vector
$\vec{n}$, $\vec{N}$	Normal vector
$\vec{q}$, $\vec{Q}$	Heat flux vector
$\vec{q}_r$, $\vec{Q}_r$	Radiative heat flux vector
$\vec{r}$	Location or distance vector
$\vec{s}$	Direction vector
$\vec{t}, \vec{T}$	Traction vector
$\vec{u}$, $\vec{U}$	Displacement vector
$\vec{v}$	Velocity vector
$\vec{x}$, $\vec{X}$	Coordinate vector

Tensors

$\underset{\sim}{\varepsilon}$	Linear strain tensor
$\underset{\sim}{\lambda}_\Theta$, $\underset{\sim}{\Lambda}_\Theta$	Heat conductivity tensor
$\underset{\sim}{\lambda}_\varphi$, $\underset{\sim}{\Lambda}_\varphi$	Electric conductivity tensor
$\underset{\sim}{\sigma}$	Cauchy stress tensor
$\underset{\sim}{\mathrm{b}}$	Left Cauchy-Green tensor
$\underset{\sim}{\mathrm{C}}$	Right Cauchy-Green tensor
$\underset{\sim}{\mathrm{d}}$	Rate of deformation tensor
$\underset{\sim}{\mathrm{e}}$	Euler-Almansi strain tensor
$\underset{\sim}{\mathrm{E}}$	Green-Lagrange strain tensor
$\underset{\sim}{\mathrm{F}}$	Deformation gradient tensor
$\underset{\sim}{\mathrm{H}}$	Displacement gradient tensor
$\underset{\sim}{\mathrm{I}}$	Unit tensor
$\underset{\sim}{\mathrm{l}}$	Velocity gradient tensor

$\underset{\sim}{\mathrm{P}}$	Piola-Kirchhoff stress tensor
$\underset{\sim}{\mathrm{R}}$	Rotation tensor
$\underset{\sim}{\mathrm{S}}$	2^{nd} Piola-Kirchhoff stress tensor
$\underset{\sim}{\mathrm{U}}$	Right stretch tensor
$\underset{\sim}{\mathrm{V}}$	Left stretch tensor
$\underset{\sim}{\mathrm{w}}$	Spin tensor
$\underset{\approx}{\mathcal{C}}$	Elasticity tensor
$\underset{\approx}{\mathcal{I}}$	First fundamental tensor

Global matrices / column matrices

$\boldsymbol{\alpha}$	Vector of interpolation coefficients
$\boldsymbol{\Theta}$	Discrete temperature vector
$\boldsymbol{\chi}$	Global coordinates vectors
$\boldsymbol{\Phi}$	Basis function matrix
$\boldsymbol{\varphi}$	Discrete electric potential vector
$\mathbf{A}$	System matrix
$\mathbf{B}$	Broyden's matrix
$\mathbf{d}$	Data transfer vector
$\mathbf{D}$	View factor matrix
$\mathbf{e}_{\mathrm{b}}$	Discrete black body emissive power
$\mathbf{G}$	System of nonlinear equations
$\mathbf{G}_{\mathrm{M}}$	System of nonlinear equations of the mechanical field
$\mathbf{G}_{\Theta}$	System of nonlinear equations of the thermal field
$\mathbf{G}_{\varphi}$	System of equations of the electric field
$\mathbf{H}$	Inverse of Broyden's matrix
$\mathbf{J}$	Jacobian matrix
$\mathbf{K}_{\mathrm{T,M}}$	Global tangential stiffness matrix of the mechanical field
$\mathbf{K}_{\mathrm{S}}$	Geometric part of $\mathbf{K}_{\mathrm{T,M}}$
$\mathbf{K}_{\mathrm{C}}$	Constitutive part of $\mathbf{K}_{\mathrm{T,M}}$
$\mathbf{K}_{\mathrm{T},\Theta}$	Global tangential stiffness matrix of the thermal field
$\mathbf{K}_{\varphi}$	Global stiffness matrix of the electric field
$\mathbf{M}$	Mass or system matrix
$\mathbf{n}$	Nearest neighbors vector
$\mathbf{p}$	Vector of polynomials
$\mathbf{P}$	Matrix of polynomial vectors
$\mathbf{p}_{\mathrm{M}}$	Load vector of the mechanical field
$\mathbf{p}_{\Theta}$	Load vector of the thermal field
$\mathbf{p}_{\varphi}$	Load vector of the electric field
$\mathbf{q}$	Discrete heat flux vector
$\mathbf{r}$, $\mathbf{R}$	Discrete (iteration) residual
$\mathbf{u}$	Global displacement vector
$\mathbf{v}$	Vector of a transformed sequence
$\mathbf{x}$	Coordinate vector
$\mathbf{y}$	Solution / sequence vector
$\mathbf{Y}$	Matrix of discrete solution vectors

$\mathbf{z}$	Solution / sequence vector
$\mathbf{Z}$	Matrix of discrete solution vectors

Local finite element matrices / column matrices

$\boldsymbol{\Theta}_e$	Element temperature vector
$\boldsymbol{\Lambda}_\Theta^e$	Heat conductivity matrix
$\boldsymbol{\Lambda}_\varphi^e$	Electric conductivity matrix
$\boldsymbol{\varphi}_e$	Element electric potential vector
$\boldsymbol{\xi}$	Local coordinate vector
$\boldsymbol{B}$	Matrix of shape function derivatives
$\boldsymbol{B}_\mathrm{L}$	Strain-displacement matrix
$\boldsymbol{b}_e$	Element body force vector
$\boldsymbol{C}_e$	Material matrix
$\boldsymbol{E}_e$	Green-Lagrange strains in Voigt notation
$\boldsymbol{F}_e$	Element deformation gradient
$\boldsymbol{J}_e$	Element Jacobian matrix
$\boldsymbol{K}_{\mathrm{T,M}}^e$	Tangential element stiffness matrix
$\boldsymbol{K}_\Theta^e$	Thermal element stiffness matrix
$\boldsymbol{K}_\varphi^e$	Electric element stiffness matrix
$\boldsymbol{N}$	Shape function matrix
$\boldsymbol{p}_\mathrm{M}^e$	Mechanical element load vector
$\boldsymbol{p}_\Theta^e$	Thermal element load vector
$\boldsymbol{p}_\varphi^e$	Electric element load vector
$\boldsymbol{Q}_e$	Mapping function
$\boldsymbol{S}_e$	Stress tensor in Voigt notation
$\bar{\boldsymbol{t}}_e$	Element traction vector
$\boldsymbol{u}_e$	Element displacement vector
$\boldsymbol{x}_e,\ \boldsymbol{X}_e$	Element coordinate vector

Functionals, operators and spaces

$\mathcal{A}$	System operator
$\mathcal{B}$	Continuum body
$\mathcal{F}$	Solution operator in fixed-point iteration
$\mathcal{G}$	Solution operator in fixed-point iteration
$\mathcal{G}_\mathrm{M}$	Functional of the mechanical field
$\mathcal{G}_\Theta$	Functional of the thermal field
$\mathcal{G}_\varphi$	Functional of the electric field
$\mathcal{R}$	Residual operator
$\mathcal{S}$	Sequence of vectors
$\mathcal{T}$	Transformed sequence of vectors
$\mathcal{V}$	Test space

Frequently used sub- and superscripts

$(\,\cdot\,)_0$	Reference / initial value

$(\cdot)_b$	Black-body value
$(\cdot)^e$	Finite element quantity (e-th element)
$(\cdot)^i$	i-th iteration, i-th sequence
$(\cdot)^k$	k-th coupling iteration
$(\cdot)_n$	n-th time-step
$(\cdot)_{\mathrm{M}}$	Mechanical part of $(\cdot)$
$(\cdot)_{\Theta}$	Thermal part of $(\cdot)$
$(\cdot)_{\varphi}$	Electric part of $(\cdot)$
$(\cdot)^*$	Extra- or interpolated value

Abbreviations and acronyms

Acronym	Description	Page
BC	Boundary Conditions	124
BR	Broyden Method	91
CFD	Computational Fluid Dynamics	59
CV	Control-Volume	59
DAE	Differential-Algebraic Equation	59
DAR	Dynamic Aitken Relaxation	81
DSR	Dynamic Secant Relaxation	82
EXP	Explicit	115
FAST	Field Assisted Sintering Technology	1
FEM	Finite Element Method	6, 41
FSI	Fluid-Structure Interaction	4, 37
FVM	Finite Volume Method	59
GJ	Gauss-Jacobi	109
GMRES	Generalized Minimal Residual Method	4, 94
GS	Gauss-Seidel	109
IMP	Implicit	115
IQN	Interface Quasi-Newton	89
LE	Line Extrapolation	86
MLNA	Multi-Level Newton Algorithm	59
MP	Mechanical Predictor	132
MPI	Message Passing Interface	112
QN	Quasi-Newton (Method)	89
fvDOM	finite volume Discrete Ordinate Method	66
RTE	Radiative Transfer Equation	7, 35
SIMPLE	Semi Implicit Method for Pressure Linked Equations	63
SOR	Successive Over Relaxation	82
SUR	Successive Under Relaxation	82
TP	Thermal Predictor	119
VFM	View Factor Method	64

Abstract

With increasing computational capacity, simulations of multi-physically coupled problems become of more interest in many industrial applications. The numerical treatment of multi-field interactions calls for flexible and robust solution strategies. A partitioned coupling strategy has the advantage of high flexibility and allows for combinations of different software and specialized solvers for the physical fields involved. It divides the coupled system into iterations of subproblems with repetitive data exchange.

As a multi-field example, the electro-thermo-mechanical process of the *field assisted sintering technology* (FAST) is taken under consideration. FAST is an innovative technique for the compaction of powder materials. It offers short production cycles by simultaneously applying a uniaxial pressure and an electric current in order to generate high heating rates and hot temperatures by means of Joule heating. During processing, the temperature development is an important feature to obtain optimal process conditions. For high temperatures, the most prominent mechanism to transfer thermal energy is thermal radiation, which is why a comprehensive simulation of FAST should comprise the effects of radiating surfaces. This can be accomplished by treating the environment of the FAST machine tools as an additional individual field, denoted as the radiation field. It is coupled to the temperature and allows to model intricate interactions such as reflection or irradiation with other surfaces. This finally leads to a numerically challenging four-field problem that describes the FAST process. The electric, thermal and mechanical subproblems are solved using the finite element method (FEM) while the finite volume method is applied for the radiation field. Different numerical models are discussed to approximate the radiative transfer in vacuum and also in participating media.

Regarding the partitioned coupling strategy, the flexibility attribute comes at the expense of algorithmic stability. It is known that particularly strongly coupled problems can be unstable even if an implicit time stepping method is chosen for the subproblems. Here, external stabilization methods serve to increase the chances of stability. Typically, methods like this are known from the field of fluid-structure interaction (FSI), and they can be applied in connection with black-box solvers. Further, they can be used to improve the convergence and to reduce the computation time, as they accelerate the coupling iterations. In this thesis, several stabilization procedures are discussed. Based on sequential solver calls, a concept to design partitioned solution strategies for an arbitrary number of physical fields is proposed and applied to several numerical examples.