

Energy-Momentum-Entropy consistent numerical methods for thermomechanical solids based on the GENERIC formalism

Mark Schiebl, Peter Betsch

Institute of Mechanics, Karlsruhe Institute of Technology, Germany,
{mark.schiebl,peter.betsch}@kit.edu, www.ifm.kit.edu

Keywords: *Thermomechanical Problems, Thermoelasticity, Structure-Preserving Numerical Methods*

This work deals with the Energy-Momentum-Entropy (EME) consistent time integration of open thermoelastic systems. While energy-momentum preserving integrators are well-known for conservative mechanical systems, Romero introduced in [1] the class of thermodynamically consistent integrators for coupled thermomechanical systems, which further respect symmetries of the underlying coupled system and are therefore capable of conserving associated momentum maps.

As mathematical framework for the geometric structure of the non-equilibrium thermodynamics the GENERIC (**G**eneral **E**quation for **N**on-**E**quilibrium **R**eversible-**I**rreversible **C**oupling) formalism is used. The GENERIC formalism, originally proposed by Grmela and Öttinger for complex fluids [2], expresses the evolution equation as the sum of reversible and irreversible contribution via a Poisson and a dissipative bracket.

Since the GENERIC formalism does not depend of a specific choice of the thermodynamical state variables [3], we explore the structure of GENERIC formalism using the entropy density (see e.g. [4]), the absolute temperature (see e.g. [5]) and further the internal energy density as thermodynamical state variable from which the weak form of the initial boundary value problem can be gained. Applying the notion of a discrete gradient in the sense of Gonzalez [6] leads to an EME integrator.

As boundary conditions rely on the specific choice of the thermodynamical state variable we extend the GENERIC formalism to be suitable for open systems following the procedure in [7]. The presentation will indicate key differences and similarities between the alternative choices of thermodynamical state variables and will include several simulations with different boundary conditions using an energy-based termination criterion.

REFERENCES

- [1] Ignacio Romero. Thermodynamically consistent time-stepping algorithms for nonlinear thermomechanical systems. *International journal for numerical methods in engineering*, 79(6):706–732, 2009.
- [2] Miroslav Grmela and Hans Christian Öttinger. Dynamics and thermodynamics of complex fluids. i. development of a general formalism. *Physical Review E*, 56(6):6620, 1997.

- [3] Alexander Mielke. Formulation of thermoelastic dissipative material behavior using generic. *Continuum Mechanics and Thermodynamics*, 23(3):233–256, 2011.
- [4] Melanie Krüger, Michael Groß and Peter Betsch. An energy-entropy-consistent time stepping scheme for nonlinear thermo-viscoelastic continua. *ZAMM-Journal of Applied Mathematics and Mechanics/Zeitschrift für Angewandte Mathematik und Mechanik*, 96(2):141–178, 2016.
- [5] Markus Hütter and Bob Svendsen. Thermodynamic model formulation for viscoplastic solids as general equations for non-equilibrium reversible–irreversible coupling. *Continuum Mechanics and Thermodynamics*, 24(3):211–227, 2012.
- [6] Oscar Gonzalez. *Design and analysis of conserving integrators for nonlinear Hamiltonian systems with symmetry*. PhD thesis, Stanford University, 1996.
- [7] Hans Christian Öttinger. Nonequilibrium thermodynamics for open systems. *Physical Review E*, 73(3):036126, 2006.