C18 Analysis and numerics of multidimensional models for elastic phase transformations in shape-memory alloys

Alexander Mielke
Dorothee Knees, Adrien Petrov

DFG Research Center MATHEON
Mathematics for key technologies

Center Days, April 8, 2008
**Shape-memory alloys** are used because of their

- memory of shape after a cycle of heating and cooling,
- superelastic properties under mechanical loading,
- hysteretic behavior for damping of vibrations.

**Applications:**
biomedicine, MEMS, space applications...
Shape-memory alloys are used because of their

- memory of shape after a cycle of heating and cooling,
- superelastic properties under mechanical loading,
- hysteretic behavior for damping of vibrations.

Applications:
biomedicine, MEMS, space applications...

AIM: Find good mathematical models (analysis and numerics)
The functionality of SMAs have their origin in microstructures, which evolve under thermal or mechanical loading.

**NEED:** Model that describes evolution of phase mixtures

Pure phases can be measured experimentally:

\[ z \in \left\{ e_1, \ldots, e_K, \ldots, e_N \right\} \subset \mathbb{R}^N \]

- \( e_1 \): mart1
- \( e_K \): martK
- \( e_N \): aust

Energy functionals:

\[ W(E, e_j), j=1, \ldots, N \]
The functionality of SMAs have their origin in microstructures, which evolve under thermal or mechanical loading.

**NEED:** Model that describes evolution of phase mixtures

Pure phases can be measured experimentally: 

\[ z \in \{ e_1, \ldots, e_K, \ldots, e_N \} \subset \mathbb{R}^N \]

mixtures \( z \in Z := \text{conv}\{ e_1, \ldots, e_N \} \subset \mathbb{R}^N \)

Energy functionals 

\[ W(\mathbf{E}, e_j), \ j=1,\ldots,N \]

\[ W: \left\{ \mathbb{R}_\text{sym}^{d\times d} \times Z \to \mathbb{R} \right\} \]

mixture function (see also C13)
State variables
\( u : \Omega \rightarrow \mathbb{R}^d \) displacement
\( z : \Omega \rightarrow Z \) phase indicator

Applied fields
\( \ell_{\text{appl}} : [0, T] \rightarrow \mathcal{F}^* \) mechan. loading
\( \theta_{\text{appl}} : [0, T] \times \Omega \rightarrow \mathbb{R} \) temperature

Energy: \( \mathcal{E}(t, u, z) = \int_\Omega W(\nabla u, z, \nabla z, \theta_{\text{appl}}(t)) \, dx - \langle \ell_{\text{appl}}(t), u \rangle \)

Dissipation distance: \( \mathcal{D}(z_1, z_2) = \int_\Omega D(x, z_1(x), z_2(x)) \, dx \)
State variables
\( u : \Omega \to \mathbb{R}^d \) displacement
\( z : \Omega \to \mathbb{Z} \) phase indicator

Applied fields
\( \ell_{\text{appl}} : [0, T] \to \mathcal{F}^* \) mechan. loading
\( \theta_{\text{appl}} : [0, T] \times \Omega \to \mathbb{R} \) temperature

Energy: \( \mathcal{E}(t, u, z) = \int_\Omega W(\nabla u, z, \nabla z, \theta_{\text{appl}}(t)) \, dx - \langle \ell_{\text{appl}}(t), u \rangle \)
Dissipation distance: \( \mathcal{D}(z_1, z_2) = \int_\Omega D(x, z_1(x), z_2(x)) \, dx \)

\((u, z) : [0, T] \to \mathcal{F} \times \mathbb{Z}\) is called energetic solution, if
\((\mathcal{S}) ~ \mathcal{E}(t, u(t), z(t)) \leq \mathcal{E}(t, \tilde{u}, \tilde{z}) + \mathcal{D}(z(t), \tilde{z}) \) for all \((\tilde{u}, \tilde{z}) \in \mathcal{F} \times \mathbb{Z}\)
\((\mathcal{E}) ~ \mathcal{E}(t, u(t), z(t)) + \text{Diss}_\mathcal{D}(z; [0, t]) = \mathcal{E}(0, u_0, z_0) + \int_0^t \partial_s \mathcal{E}(\cdot, u, z) \, ds \)

If \( \mathcal{D}(z_1, z_2) = \mathcal{R}(z_2 - z_1) \) and \( \mathcal{E}(t, \cdot) : \mathcal{F} \times \mathbb{Z} \to \mathbb{R}_\infty \) convex, then
\((\mathcal{S})\&(\mathcal{E}) \iff \begin{cases} 0 \in \partial_u \mathcal{E}(t, u, z) & \text{elastic equilibrium} \\ 0 \in \partial \mathcal{R}(\dot{z}) + \partial_z \mathcal{E}(t, u, z) & \text{flow rule} \end{cases} \)
The results obtained since 2006 fall into four categories:

1. Modeling of Temperature-Induced Phase Transformations
2. Numerical Convergence of Space-Time Discretizations
3. Γ-Limits and Microstructures
4. Models Including Rate-Dependent Effects
The results obtained since 2006 fall into four categories:

1. Modeling of Temperature-Induced Phase Transformations
2. Numerical Convergence of Space-Time Discretizations
3. $\Gamma$-Limits and Microstructures
4. Models Including Rate-Dependent Effects

Today only 1. and 2.

For 3. and 4. see the report or the web page
www.wias-berlin.de/research-groups/pde/projects/matheonC18.html
**State variables**

\( u : \Omega \to \mathbb{R}^d \) displacement

\( z : \Omega \to \mathbb{R}^{d \times d}_{0, \text{sym}} \) mesoscopic transformation strain

**Applied fields**

\( \ell_{\text{appl}} \in C^1([0, T], \mathcal{F}^*) \) loading

\( \theta_{\text{appl}} \in C^1([0, T]; L^\infty(\Omega)) \) temp.

**Energy:** \( \mathcal{E}(t, u, z) = \int_\Omega W(E(u), z, \nabla z, \theta_{\text{appl}}(t)) \, dx - \langle \ell_{\text{appl}}(t), u \rangle \)

**Dissipation distance:** \( \mathcal{D}(z_1, z_2) = \mathcal{R}(z_2 - z_1) = \int_\Omega \rho |z_2 - z_1| \, dx \)

where \( W = \frac{1}{2}(E - z) : C(\theta) : (E - z) + H_{\text{SoAu}}(z, \theta) + \sigma |\nabla z|^2 \)
State variables \( u : \Omega \to \mathbb{R}^d \) displacement
\( z : \Omega \to \mathbb{R}^{d\times d}_{0,\text{sym}} \) mesoscopic transformation strain

Applied fields
\( \ell_{\text{appl}} \in C^1([0, T], \mathcal{F}^*) \) loading
\( \theta_{\text{appl}} \in C^1([0, T]; L^\infty(\Omega)) \) temp.

Energy: \( \mathcal{E}(t, u, z) = \int_\Omega W(E(u), z, \nabla z, \theta_{\text{appl}}(t)) \, dx - \langle \ell_{\text{appl}}(t), u \rangle \)

Dissipation distance: \( \mathcal{D}(z_1, z_2) = \mathcal{R}(z_2 - z_1) = \int_\Omega \rho |z_2 - z_1| \, dx \)
where \( W = \frac{1}{2} (E - z) : \mathcal{C}(\theta) : (E - z) + H_{\text{SoAu}}(z, \theta) + \sigma |\nabla z|^2 \)

\( \triangleright \ E(u) = \frac{1}{2} (\nabla u + \nabla u^T) \): infinitesimal strain

\( \triangleright \ H_{\text{SoAu}}(z, \theta) = c_1(\theta) |z| + \frac{c_2(\theta)}{2} |z|^2 + \chi_{\{|z| \leq c_3(\theta)\}}(z) \)
  \( \triangleright \ c_1(\theta) \): activation threshold
  \( \triangleright \ c_2(\theta) \): hardening in the martensitic regime
  \( \triangleright \ c_3(\theta) \): maximal transformation strain
**State variables**

\[ u : \Omega \rightarrow \mathbb{R}^d \text{ displacement} \]
\[ z : \Omega \rightarrow \mathbb{R}^{d \times d}_{0,\text{sym}} \text{ mesoscopic transformation strain} \]

**Applied fields**

\[ \ell_{\text{appl}} \in C^1([0, T], \mathcal{F}^*) \text{ loading} \]
\[ \theta_{\text{appl}} \in C^1([0, T]; L^\infty(\Omega)) \text{ temp.} \]

**Energy:**

\[ \mathcal{E}(t, u, z) = \int_\Omega W(E(u), z, \nabla z, \theta_{\text{appl}}(t)) \, dx - \langle \ell_{\text{appl}}(t), u \rangle \]

**Dissipation distance:**

\[ \mathcal{D}(z_1, z_2) = R(z_2 - z_1) = \int_\Omega \rho |z_2 - z_1| \, dx \]

where

\[ W = \frac{1}{2}(E - z) : C(\theta) : (E - z) + H_{\text{SoAu}}(z, \theta) + \sigma |\nabla z|^2 \]

Regularized version of \( H_{\text{SoAu}} \):

\[ H_\delta(z, \theta) = c_1(\theta) \sqrt{\delta^2 + |z|^2} + \frac{c_2(\theta)}{2} |z|^2 + \frac{1}{\delta} (|z| - c_3((\theta))^+)^3 \]

**Theorem (Existence and uniqueness)**

*For all \( \delta \geq 0 \) there exists a solution of \((S)\&(E)\).*

*For \( \delta > 0 \) the solutions are unique since \( \mathcal{E} \in C^3([0, T] \times H^1(\Omega)) \).*
Finite-element spaces $\mathcal{F}_h \subset \mathcal{F}$ and $\mathcal{Z}_h \subset \mathcal{Z}$, time step $\tau > 0$

**Space-Time Discretization for general systems**

$$\text{(IMP)}^{h,\tau} \quad (u^{h,\tau}_k, z^{h,\tau}_k) \in \text{Argmin} \quad \left( \mathcal{E}(k\tau, u, z) + \mathcal{D}(z^{h,\tau}_{k-1}, z) \right)_{(u,z) \in \mathcal{F}_h \times \mathcal{Z}_h}$$

Piecewise constant interpolants $(\overline{u}^{h,\tau}, \overline{z}^{h,\tau}) : [0, T] \rightarrow \mathcal{F}_h \times \mathcal{Z}_h$
Finite-element spaces $\mathcal{F}_h \subset \mathcal{F}$ and $\mathcal{Z}_h \subset \mathcal{Z}$, time step $\tau > 0$

**Space-Time Discretization for general systems**

$$(\text{IMP})^{h,\tau} \quad (u^{h,\tau}_k, z^{h,\tau}_k) \in \text{Argmin}_{(u,z) \in \mathcal{F}_h \times \mathcal{Z}_h} \left( \mathcal{E}(k \tau, u, z) + \mathcal{D}(z^{h,\tau}_{k-1}, z) \right)$$

Piecewise constant interpolants $(\bar{u}^{h,\tau}, \bar{z}^{h,\tau}) : [0, T] \rightarrow \mathcal{F}_h \times \mathcal{Z}_h$

**Theorem (Convergence of the space-time discretization)**

*There exists a subsequence $(\bar{u}^{h_n,\tau_n}, \bar{z}^{h_n,\tau_n})$ such that this subsequence converges to a solution $(u, z)$ of $(S)\&(E)$.*

- Problem: solutions of $(S)\&(E)$ are not unique.
- uniform a priori estimates $\rightsquigarrow$ numerical stability
- accumulation points are solutions $\rightsquigarrow$ consistency (no ghost s/lns.)
For the regularized **Souza-Auricchio model** \((\delta > 0)\) we have

- **uniqueness of solutions** and
- **higher spatial regularity**

\[(u, z) \in L^\infty([0, T], H^2(\Omega)) \times W^{1,\infty}([0, T], H^1(\Omega))\]

by studying the elliptic problem

\[
\begin{cases}
-\text{div} \left( C(\theta_{\text{appl}}(t)):(E(u) - z) \right) = \ell_{\text{appl}}(t) \text{ in } \Omega \text{ & bdy. cond.} \\
C(\theta_{\text{appl}}(t)):(z - E(u)) + D_z H_\delta(z, \theta_{\text{appl}}(t)) - \sigma \Delta z + \partial R(\dot{z}) \ni 0
\end{cases}
\]

\([\in L^\infty(\Omega)]\)
For the regularized Souza-Auricchio model ($\delta > 0$) we have

- uniqueness of solutions and
- higher spatial regularity

$$(u, z) \in L^\infty([0, T], H^2(\Omega)) \times W^{1,\infty}([0, T], H^1(\Omega))$$

by studying the elliptic problem

$$\begin{cases}
-\text{div}(\mathbb{C}(\theta_{\text{appl}}(t))(\mathbf{E}(u) - z)) = \ell_{\text{appl}}(t) \text{ in } \Omega \& \text{ bdy. cond.} \\
\mathbb{C}(\theta_{\text{appl}}(t))(z - \mathbf{E}(u)) + D_z H_\delta(z, \theta_{\text{appl}}(t)) - \sigma \Delta z + \partial \mathcal{R}(\dot{z}) \geq 0
\end{cases}$$

\text{for } t \in [0, T]

\text{and } \delta > 0.

\text{Theorem (Explicit convergence rates for SoAu model)}

forall $\delta > 0 \exists C, \gamma > 0$ : $\|(u(t_k), z(t_k)) - (u_{k}^{\tau, h}, z_{k}^{\tau, h})\|_{H^1} \leq C(\tau^{1/2} + h^{\gamma/2})$

where $h > 0$ is the mesh size of a finite-element discretization.
Cooperations within Application Area C

- **C13**: study of incremental minimization problems
  - relaxation of non-quasiconvex problems
  - analysis of accumulated errors in many timesteps

- **C17** (just starting): efficient solution of nonsmooth minimization problems via semi-smooth Newton methods

Cooperations with ICM Warszawa
M. Danielewski, M. Gokieli, P. Rybka

External Cooperations

- **Mathematics**: G. Francfort (Paris), A. Garroni (Roma), L. Paoli (St. Etienne), T. Roubíček (Praha), U. Stefanelli (Pavia), C. Zanini (Trieste),

- **Engineering**: F. Auricchio (Pavia), S. Govindjee (Zürich), K. Hackl (Bochum), P.M. Mariano (Firenze), J.A.C. Martins (Lisboa), Ch. Miehe (Stuttgart), J. Zeman (Praha).
Outlook:

- improve the convergence rates $O(\tau^\alpha + h^\gamma)$
- find efficient solvers for $(\text{IMP})^{h,\tau}$
  ∸ collaboration with C13 and C17
- study polycrystalline and grain-boundary effects
  ∸ collaboration with M. Gokieli (ICM)
- understand the limit when $\sigma \rightarrow 0$ (formation of microstructure)
  ∸ collaboration with L. Paoli
- include rate-dependent effects like a heat equation
  ∸ collaboration with T. Roubíček
- develop the theory to include other multifunctional materials
  (ferroelectric materials, magnetostrictive materials)
- develop a FE simulation tool (2D and 3D)
Thank you for your attention

... more infos are under

www.wias-berlin.de/research-groups/pde/projects/matheonC18.html
Refereed Publications 09/2006-03/2008: 9
Submitted Articles: 5
Book Chapters and Books: 1+1

Plenary Lectures: 3
Invited Talks: 7

Offers (Prof. and similar): 0
A. Mielke:
*Regularizations and relaxations of time-continuous problems in plasticity*
Project within the **DFG Research Unit FOR 797**
“Analysis and computation of microstructure in finite plasticity”.
(one PostDoc for 3 years, plus 3 years possible).

D. Knees (with Ch. Kraus):
*Modellierung von Schädigungsprozessen*
Project in **Wettbewerb der Leibniz-Gemeinschaft**
(two PreDocs and one PostDoc for 2009-2011)
External cooperations with partners from Application Area C

... with engineering groups as indicated above

Industry projects associated with project

___

Patents

___