On a 3D model for shape-memory alloys

Dedicated to the memory of M. Schatzman

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joint work with A. Mielke, L. Paoli and U. Stefanelli

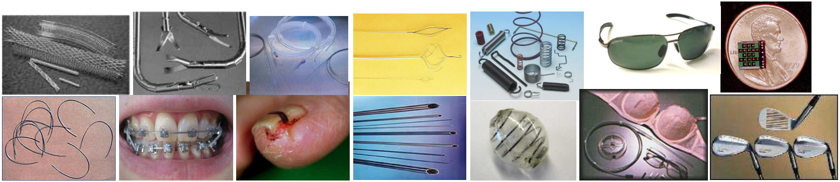
DFG Research Center MATHEON
Mathematics for key technologies

Weierstraß-Institut für Angewandte Analysis und Stochastik

Banff, 2nd September 2010

1. Background of SMAs
2. Background on the Energetic Formulation
3. The Souza-Auricchio model for SMAs
4. Error estimates for space-time discretizations
5. Numerics
6. Conclusion

Shape-Memory Alloys are used today in real life:



WHY?

[1]Souza, Mamiya, Zouain. *Europ. J. Mech., A/Solids*, 1998.

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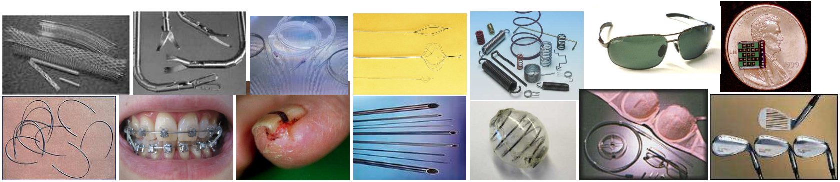

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- shape memory under heating and cooling
- superelastic properties under mechanical loading
- hysteretic behavior for damping of vibrations

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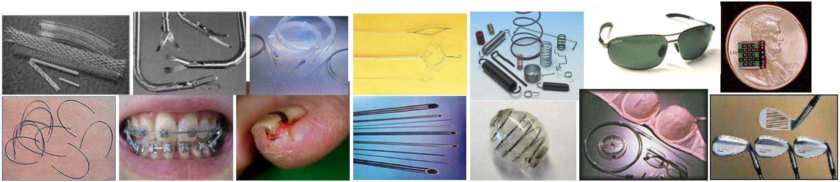

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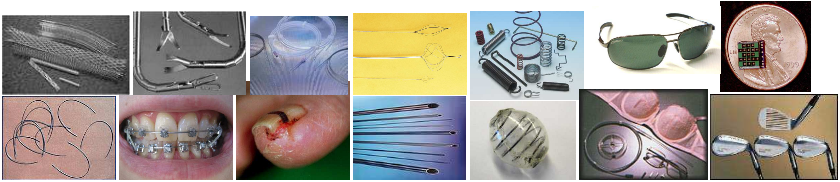

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$\Longrightarrow$ Souza-Auricchio model for shape-memory alloys[1]

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State variables

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

$z : \Omega \to Z$ phase indicator

Applied field

$\ell_{\mathrm{appl}} : [0, T] \to \mathcal{X}'$ mechanical loading

Energy functional: $\mathcal{E}(t, u, z) = \int_\Omega W(\nabla u, z, \nabla z)\,\mathrm{d}x - \langle \ell_{\mathrm{appl}}(t), u \rangle$

Dissipation functional: $\mathcal{D}(z_1, z_2) = \int_\Omega D(x, z_1(x), z_2(x))\,\mathrm{d}x$

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$(u, z) : [0, T] \to \mathcal{U} \times \mathcal{Z}$ is called **energetic solution**[2], if

(S) $\mathcal{E}(t, u(t), z(t)) \leq \mathcal{E}(t, \widetilde{u}, \widetilde{z}) + \mathcal{D}(z(t), \widetilde{z})$ for all $(\widetilde{u}, \widetilde{z}) \in \mathcal{U} \times \mathcal{Z}$

(E) $\mathcal{E}(t, u(t), z(t)) + \mathrm{Var}_{\mathcal{D}}(z; [0, t]) = \mathcal{E}(0, u_0, z_0) + \int_0^t \partial_s \mathcal{E}(\cdot, u, z)\,\mathrm{d}s$

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If $\mathcal{D}(z_1, z_2) = \Psi(z_2 - z_1)$ and $\mathcal{E}(t, \cdot) : \mathcal{U} \times \mathcal{Z} \to \mathbb{R}_\infty$ convex, then

(S)&(E) $\iff \begin{cases} 0 \in \partial_u \mathcal{E}(t, u, z) & \text{elastic equilibrium} \\ 0 \in \partial \Psi(\dot{z}) + \partial_z \mathcal{E}(t, u, z) & \text{flow rule} \end{cases}$

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

$z : \Omega \to \mathbb{R}^{d\times d}_{0,\mathrm{sym}}$ mesoscopic transformation strain

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$\ell_{\mathrm{appl}} \in \mathrm{C}^3([0,T],\mathcal{X}')$ mechanical load

Energy functional: $\mathcal{E}(t,u,z) = \int_\Omega W(\mathbf{e}(u),z,\nabla z)\,\mathrm{d}x - \langle \ell_{\mathrm{appl}}(t), u\rangle$

where $W = \frac{1}{2}\mathbb{C}(\mathbf{e}(u)-z):(\mathbf{e}(u)-z) + H_{\mathrm{SoAu}}(z) + \sigma|\nabla z|^2$

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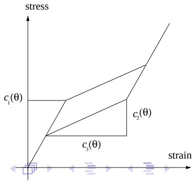
- $\mathcal{U} \overset{\mathrm{def}}{=} \{\, u \in \mathrm{H}^1(\Omega;\mathbb{R}^d) : u = 0 \text{ on } \Gamma_{\mathrm{Dir}} \,\}$, $\mathcal{Z} \overset{\mathrm{def}}{=} \mathrm{H}^1(\Omega;\mathbb{R}^{d\times d}_{0,\mathrm{sym}})$, $\mathcal{Q} \overset{\mathrm{def}}{=} \mathcal{U}\times\mathcal{Z}$
- $\mathcal{X}$: Banach space s.t. $\mathcal{Q} \subset \mathcal{X} \subset \mathcal{Q}'$
- $\mathbf{e}(u) = \frac{1}{2}(\nabla u{+}\nabla u^{\mathsf{T}})$: infinitesimal strain

$\mathbb{C}$: elasticity tensor

- $H_{\mathrm{SoAu}}(z) = c_1|z| + \frac{c_2}{2}|z|^2 + \chi_{\{|z|\le c_3\}}(z)$
  - c_1: activation threshold
  - c_2: hardening in the martensitic regime
  - c_3: maximal transformation strain



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For the regularized version of H_{SoAu}:

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

Theorem (Existence and uniqueness[a])

For all $\delta \geq 0$ there exists a solution of **(S)&(E)**.
For $\delta > 0$ the solutions are unique since $\mathcal{E} \in \mathrm{C}^3([0,T];\mathrm{H}^1(\Omega))$.

[a] Mielke, P. *Adv. Math. Sci. Appl.*, 2007.

Since $\mathcal{E}(t,\cdot) : \mathcal{U} \times \mathcal{Z} \to \mathbb{R}_\infty$ convex, then

(S)&(E) $\Longleftrightarrow \begin{cases} 0 \in \partial_u \mathcal{E}(t,u,z) & \text{elastic equilibrium} \\ 0 \in \partial\Psi(\dot{z}) + \partial_z \mathcal{E}(t,u,z) & \text{flow rule} \end{cases}$

- $\partial_u \mathcal{E}(t,u,z) = -\mathrm{div}\,(\mathbb{C}(\mathbf{e}(u) - z)) - \ell_{\mathrm{appl}}(t)$
- $\partial_z \mathcal{E}(t,u,z) = -\mathbb{C}(\mathbf{e}(u) - z) + \partial_z H_{\mathsf{SoAu}}(z) - \sigma \Delta z$

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Then our problem can be rewritten as follows

(DI) $\qquad 0 \in \partial\Psi(\dot{q}) + \mathbf{A}q + \mathrm{D}_q \mathcal{H}_{\mathsf{SoAu}}(q) - \mathbf{L}(t)$ a.e. in $[0,T]$

- ▷ $q \stackrel{\mathrm{def}}{=} (u,z)^{\mathsf{T}}, \quad \mathbf{L}(t) \stackrel{\mathrm{def}}{=} (\ell(t), 0)^{\mathsf{T}}$
- ▷ $\partial\Psi(\dot{q}) \stackrel{\mathrm{def}}{=} (0, \partial\Psi(\dot{z}))^{\mathsf{T}}, \quad \mathcal{H}_{\mathsf{SoAu}}(q) \stackrel{\mathrm{def}}{=} (0, H_{\mathsf{SoAu}}(z) - \frac{c_2}{2}|z|^2)^{\mathsf{T}}$
- ▷ $\mathbf{A} \stackrel{\mathrm{def}}{=} \begin{pmatrix} -\mathrm{div}(\mathbb{C}\mathbf{e}(\cdot)) & \mathrm{div}\,(\mathbb{C}(\cdot)) \\ -\mathbb{C}(\mathbf{e}(\cdot)) & \mathbb{C}(\cdot) - \sigma\Delta(\cdot) + \frac{c_2}{2}\mathbf{I} \end{pmatrix} \in \mathrm{Lin}(\mathcal{Q}, \mathcal{Q}')$

Since $\mathcal{E}(t,\cdot):\mathcal{U}\times\mathcal{Z}\to\mathbb{R}_\infty$ convex, then

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(DI) $\quad 0\in\partial\Psi(\dot{q}(t)) + \mathrm{D}_q\mathcal{E}(t,q(t))$ a.e. in $[0,T]$

Here **(DI)** is equivalent to the *variational inequality*

(VI) $\quad \forall v\in\mathcal{Q}:\ \langle \mathrm{D}_q\mathcal{E}(t,q(t)), v-\dot{q}(t)\rangle_{\mathcal{Q}} + \Psi(v) - \Psi(\dot{q}(t)) \geq 0$

Finite-element spaces: $\mathcal{U}_h \subset \mathcal{U}$ and $\mathcal{Z}_h \subset \mathcal{Z}$ with $\mathcal{Q}_h = \mathcal{U}_h \times \mathcal{Z}_h$
Time step: $\tau > 0$

Space-Time Discretization: $q^k_{\tau,h} = (u^k_{\tau,h}, z^k_{\tau,h})$ and $\widehat{q}_h = (\widehat{u}_h, \widehat{z}_h)$

(IP)$_{\tau,h}$ $$q^k_{\tau,h} \in \arg\min_{\widehat{q}_h \in \mathcal{Q}_h} \Big(\mathcal{E}(t^k_\tau, \widehat{q}_h) + \psi(\widehat{z}_h - z^{k-1}_{\tau,h})\Big)$$

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- $\mathcal{E} : [0, T] \times \mathcal{Q} \to \mathbb{R}$: the energy functional
  - **(E1)** $\mathcal{E} \in \mathrm{C}^3([0, T]; \mathcal{Q})$
  - **(E2)** $\mathcal{E}(t, \cdot)$ is κ-uniformly convex
  - **(E3)** $\exists c, C > 0 \ : \ \forall \widehat{q} \in \mathcal{Q} \ \ c\|\widehat{q}\|^2_{\mathcal{Q}} - C \leq \mathcal{E}(t, \widehat{q}) \leq C\|\widehat{q}\|^2_{\mathcal{Q}} + C$
- $\Psi : \mathcal{Q} \to [0, \infty)$: the dissipation functional
  - **(D1)** $\forall \gamma \geq 0, q \in \mathcal{Q} : \Psi(\gamma q) = \gamma \Psi(q)$
  - **(D2)** $\forall q_1, q_2 \in \mathcal{Q} : \ \Psi(q_1 + q_2) \leq \Psi(q_1) + \Psi(q_2)$
  - **(D3)** $\exists C_\Psi > 0 \ \forall \widehat{q} \in \mathcal{Q} : \ \Psi(\widehat{q}) \leq C_\Psi \|\widehat{q}\|_{\mathcal{Q}}$

Finite-element spaces: $\mathcal{U}_h \subset \mathcal{U}$ and $\mathcal{Z}_h \subset \mathcal{Z}$ with $\mathcal{Q}_h = \mathcal{U}_h \times \mathcal{Z}_h$
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Space-Time Discretization: $q^k_{\tau,h} = (u^k_{\tau,h}, z^k_{\tau,h})$ and $\widehat{q}_h = (\widehat{u}_h, \widehat{z}_h)$

$$(\mathrm{IP})_{\tau,h} \qquad q^k_{\tau,h} \in \underset{\widehat{q}_h \in \mathcal{Q}_h}{\arg\min} \big(\mathcal{E}(t^k_\tau, \widehat{q}_h) + \psi(\widehat{z}_h - z^{k-1}_{\tau,h})\big)$$

Theorem

For all $h \geq 0$*, there exists a unique solution* $q_h : [0,T] \to \mathcal{Q}_h$ *to* **(DI)** *and there exists* $R > 0$ *such that* $\|q_h(t)\|_{\mathcal{Q}} \leq R$ *for all* $t \in [0,T]$ *and* $\|\dot{q}_h(t)\|_{\mathcal{Q}} \leq C(R,\kappa)$ *for a.e.* $t \in [0,T]$*.*

Idea of the proof: Use Mielke&Theil'04.

AIM: evaluate $\|q_{\tau,h}(t) - q(t)\|_{\mathcal{Q}}$ by some polynomial function of τ and h

Let $\mathbf{P}_h : \mathcal{Q} \to \mathcal{Q}_h$ s.t. $\forall p_h \in \mathcal{Q}_h$: $\langle \mathbf{A}\mathbf{P}_h q, p_h \rangle_{\mathcal{Q}} = \langle \mathbf{A} q, p_h \rangle_{\mathcal{Q}}$
There exist $\alpha \in (0,1]$ $C_{\mathbf{P}} > 0$ s.t. $\forall h > 0$ $\forall q \in \mathcal{Q}$: $\|(\mathbf{P}_h - \mathbf{I})q\|_{\mathcal{X}} \leq C_{\mathbf{P}} h^{\alpha} \|q\|_{\mathcal{Q}}$

(CC)
$$\exists C > 0\ \forall h > 0\ \forall (t, \bar{q}_h) \in [0,T] \times \mathcal{Q}_h\ \forall w \in \mathcal{Q}\ \exists v_h \in \mathcal{Q}_h :$$
$$\langle \mathrm{D}_q \mathcal{E}(t, \bar{q}_h), v_h - w \rangle_{\mathcal{Q}} + \Psi(v_h - w) \leq C h^{\alpha} \|w\|_{\mathcal{Q}}$$

Theorem

There exist $C > 0$ and $\alpha \in (0,1]$ s.t. for all $h \in [0, h_0]$ and all $q_h(0) \in \mathcal{S}_h(0)$,
$\forall t \in [0,T]$ $\forall \tau \in (0,T]$: $\|q_{\tau,h}(t) - q(t)\|_{\mathcal{Q}} \leq C\left(h^{\alpha/2} + \sqrt{\tau} + \|q_h(0) - q(0)\|_{\mathcal{Q}}\right)$

$\mathcal{S}_h(t) \stackrel{\text{def}}{=} \left\{ q_h \in \mathcal{Q}_h \,\middle|\, \forall \widehat{q}_h \in \mathcal{Q}_h : \mathcal{E}(t, q_h) \leq \mathcal{E}(t, \widehat{q}_h) + \Psi(\widehat{q}_h - q_h) \right\}$: the stable states

Sketch of proof: Let us remark that

$$\|q_{\tau,h}(t) - q(t)\|_{\mathcal{Q}} \leq \underbrace{\|q_{\tau,h}(t) - q_h(t)\|_{\mathcal{Q}}}_{\leq C\sqrt{\tau}\ \text{(cf. Mielke\&Theil'04)}} + \underbrace{\|q_h(t) - q(t)\|_{\mathcal{Q}}}_{\leq C(h^{\alpha/2} + \|q_h(0) - q(0)\|_{\mathcal{Q}})}$$

Define now

(G1) $$\gamma(t) \overset{\text{def}}{=} \langle \mathrm{D}_q\mathcal{E}(t, q_h) - \mathrm{D}_q\mathcal{E}(t, q), q_h - q\rangle_{\mathcal{Q}} \geq \kappa\|q - q_h\|^2_{\mathcal{Q}}$$

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$\mathcal{E}(t,\cdot)$ is κ-unif. convex $\underset{\text{Ciarlet'82}}{\Longrightarrow}$ $\mathcal{E}(t,\widehat{q}) \geq \mathcal{E}(t,q) + \langle \mathrm{D}_q\mathcal{E}(t,q), \widehat{q} - q\rangle_{\mathcal{Q}} + \frac{\kappa}{2}\|q - \widehat{q}\|^2_{\mathcal{Q}}$

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By differentiation, we get

$$\begin{aligned}
\dot\gamma(t) = {} & \langle \partial_t \mathrm{D}_q\mathcal{E}(t,q_h) - \partial_t \mathrm{D}_q\mathcal{E}(t,q), q_h - q\rangle_{\mathcal{Q}} \\
& + \langle \mathrm{D}_q\mathcal{E}(t,q) - \mathrm{D}_q\mathcal{E}(t,q_h) + \mathrm{D}^2_q\mathcal{E}(t,q_h)[q_h - q], \dot q_h\rangle_{\mathcal{Q}} \\
& + \langle \mathrm{D}_q\mathcal{E}(t,q_h) - \mathrm{D}_q\mathcal{E}(t,q) + \mathrm{D}^2_q\mathcal{E}(t,q)[q - q_h], \dot q\rangle_{\mathcal{Q}} \\
& + 2 \underbrace{\langle \mathrm{D}_q\mathcal{E}(t,q_h) - \mathrm{D}_q\mathcal{E}(t,q), \dot q_h - \dot q\rangle_{\mathcal{Q}}}_{\overset{\text{(VI)}}{\leq} \langle \mathrm{D}_q\mathcal{E}(t,q_h), v_h - \dot q\rangle_{\mathcal{Q}} + \Psi(v_h - \dot q) \overset{\text{(CC)}}{\leq} Ch^\alpha \|\dot q\|_{\mathcal{Q}}}
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By differentiation, we get

$$\dot\gamma(t) \overset{\textbf{(E1)-(E3)}}{\leq} Ch^\alpha\|\dot q\|_{\mathcal{Q}} + C\big(1 + \|\dot q\|_{\mathcal{Q}} + \|\dot q_h\|_{\mathcal{Q}}\big)\|q - q_h\|_{\mathcal{Q}}^2 \overset{\text{Thm. M\&T'04}}{\leq} C\Big(h^\alpha + \frac{\gamma(t)}{\kappa}\Big)$$

$\Downarrow$ Int. + Grönwall

$$\gamma(t) \leq \big(\mathrm{e}^{Ct/\kappa} - 1\big)\kappa h^\alpha + \mathrm{e}^{Ct/\kappa}\underbrace{\gamma(0)}_{\leq C\|q(0) - q_h(0)\|_{\mathcal{Q}}^2}$$

$\Downarrow$ (G1)

$$\|q(t) - q_h(t)\|_{\mathcal{Q}}^2 \leq \big(\mathrm{e}^{Ct/\kappa} - 1\big)h^\alpha + \frac{C\mathrm{e}^{Ct/\kappa}}{\kappa}\|q(0) - q_h(0)\|_{\mathcal{Q}}^2$$

Lemma

There exists $C > 0$ *such that for all* $h \in (0, h_0]$*, we have* $q_h(0) \in \mathcal{S}_h(0)$ *and*

$$\|q_h(0) - q(0)\|_{\mathcal{Q}} \leq C h^{\alpha/2}$$

Idea of the proof: Since we have $\mathrm{D}_q\mathcal{E}(0, q(0)) \in \mathrm{Lin}(\mathcal{Q}, \mathcal{X}')$ and $\|\mathrm{D}_q\mathcal{E}(0, q(0))\|_{\mathrm{Lin}(\mathcal{Q},\mathcal{X}')} \leq C_\Psi$ which implies the lemma.

[3] Mielke, Paoli, P., Stefanelli. *SINUM*, 2010.

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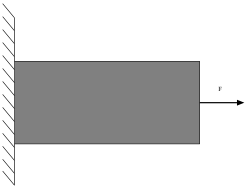
Theorem (Error estimates for space-time discretizations[3])

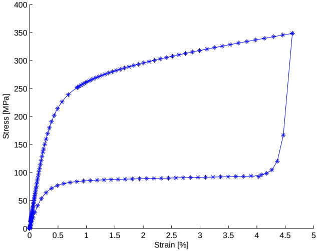
There exists $C > 0$ *such that* $q(0) \in \mathcal{S}(0)$*, we have*

$$\forall h \in [0, h_0]\ \exists q_h(0) \in \mathcal{S}_h(0)\ \forall t \in [0, T]\ \forall \tau \in (0, T] :$$
$$\|q_{\tau,h}(t) - q(t)\|_{\mathcal{Q}} \le C\left(h^{\alpha/2} + \sqrt{\tau}\right)$$

[3] Mielke, Paoli, P., Stefanelli. *SINUM*, 2010.

We have developed a 2D FE simulation tools based on some ideas of Carstensen et al.[4]





[4] Carstensen, Klose. *J. Numer. Math.*, 2002.

- include rate-dependent effects like a heat equation (work in progress with A. Mielke and L. Paoli)
- develop the theory to include other multifunctional materials (ferroelectric materials, magnetostrictive materials)

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Thank you for your attention !

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