On the error estimates for space-time discretizations of rate-independent processes

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Mathematics for key technologies

Weierstraß-Institut für Angewandte Analysis und Stochastik

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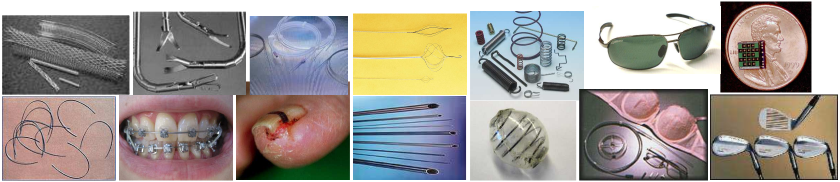
Shape-Memory Alloys (SMA) are used today in real life:



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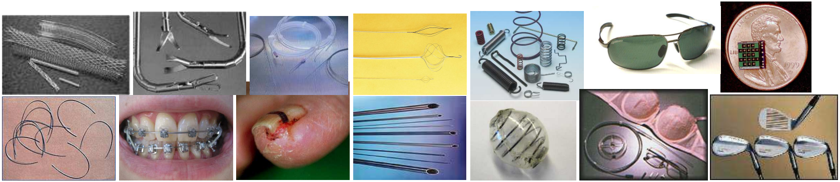

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- shape memory under heating and cooling
- superelastic properties under mechanical loading
- hysteretic behavior for damping of vibrations

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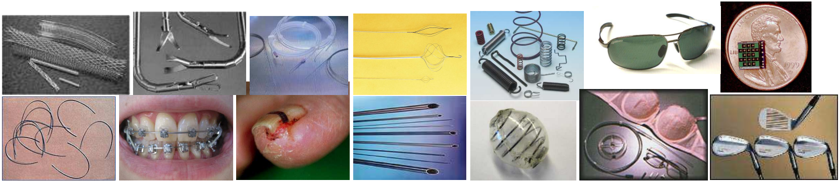

WHY? Because their have the following properties:

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AIM: Find good mathematical models (analysis and numerics)

- **Energy functional:** $\mathcal{E}(t,q) \stackrel{\text{def}}{=} \frac{1}{2}\langle \mathbf{A}q, q\rangle_{\mathcal{Q}} + \underbrace{\mathcal{H}(q)}_{\text{hardening funct.}} - \langle \underbrace{\mathbf{l}(t)}_{\text{load. funct.}}, q\rangle$

(E1) $\mathbf{A} \in \mathrm{Lin}(\mathcal{Q}, \mathcal{Q}')$ is a symmetric operator and there exists $\kappa > 0$: $\langle \mathbf{A}\widehat{q}, \widehat{q}\rangle_{\mathcal{Q}} \geq \kappa \|\widehat{q}\|_{\mathcal{Q}}$ for all $\widehat{q} \in \mathcal{Q}$

(E2) $\mathcal{H} \in \mathrm{C}^3(\mathcal{Q}, \mathbb{R})$ is convex and $\mathrm{D}_q\mathcal{H} \in \mathrm{C}^0(\mathcal{Q}; \mathcal{X}')$

(E3) $\mathbf{l} \in \mathrm{C}^3([0,T]; \mathcal{X}')$

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▷ **Dissipation functional:** $\Psi : \mathcal{Q} \to [0, \infty)$

(D1) $\Psi(\gamma q) = \gamma\Psi(q)$ for all $\gamma \geq 0, q \in \mathcal{Q}$

(D2) $\Psi(q_1 + q_2) \leq \Psi(q_1) + \Psi(q_2)$ for all $q_1, q_2 \in \mathcal{Q}$

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Notations:

- $\mathcal{X}$: the Banach space such that $\mathcal{Q} \subset \mathcal{X} \subset \mathcal{Q}'$
- $\mathcal{S}(t) \stackrel{\text{def}}{=} \{ q \in \mathcal{Q} \,|\, \mathcal{E}(t,q) \leq \mathcal{E}(t,\widehat{q}) + \Psi(\widehat{q} - q)$ for all $\widehat{q} \in \mathcal{Q}\}$: the stable set

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We consider the *doubly nonlinear evolution equation*

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(DI) is also equivalent to the *energetic formulation* (cf. Mielke&Theil'04)

(S)	$\mathcal{E}(t,q(t)) \leq \mathcal{E}(t,\widetilde{q}) + \Psi(\widetilde{q}-q(t))$ for all $\widetilde{q} \in \mathcal{Q}$
(E)	$\mathcal{E}(t,q(t)) + \int_0^t \Psi(\dot{q}(s))\,\mathrm{d}s = \mathcal{E}(0,q(0)) + \int_0^t \partial_s\mathcal{E}(s,q(s))\,\mathrm{d}s$

- Finite-element spaces $\mathcal{Q}_h \subset \mathcal{Q}$
- Time step $\tau > 0$

Space-Time Discretization

$$(\mathrm{IP})^{\tau,h} \qquad q_k^{\tau,h} \in \underset{\widehat{q}^h \in \mathcal{Q}_h}{\mathrm{Argmin}} \Big(\mathcal{E}(t_k^\tau, \widehat{q}^h) + \psi(\widehat{q}^h - q_{k-1}^{\tau,h}) \Big)$$

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Theorem (Mielke&Theil'04)

Assume that **(E1)-(E3)** *and* **(D1)-(D3)** *hold. Then for all* $h \geq 0$, *there exists a unique solution* $q_h : [0, T] \to \mathcal{Q}_h$ *to* **(DI)** *and there exists* $R > 0$ *s.t.* $\|q_h(t)\|_{\mathcal{Q}} \leq R$ *for all* $t \in [0, T]$ *and* $\|\dot{q}_h(t)\|_{\mathcal{Q}} \leq C(R, \kappa)$ *for a.e.* $t \in [0, T]$.

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

Let $\mathbf{P}_h : \mathcal{Q} \to \mathcal{Q}_h$ be a linear operator such that there exist $C_i^{\mathbf{P}} > 0$ and α_i, $i = 1, 2, 3$, such that for all $v \in \mathcal{Q}$ and $v_h \in \mathcal{Q}_h$, we have

(P1) $$\|(\mathbf{P}_h - \mathbf{Id})v\|_{\mathcal{X}} \leq C_1^{\mathbf{P}} h^{\alpha_1} \|v\|_{\mathcal{Q}}$$

(P2) $$\|(\mathbf{P}_h^* \mathbf{A} - \mathbf{A}\mathbf{P}_h)v\|_{\mathcal{Q}'} \leq C_2^{\mathbf{P}} h^{\alpha_2} \|v\|_{\mathcal{Q}}$$

(P3) $$\|(\mathbf{P}_h - \mathbf{Id})v_h\|_{\mathcal{Q}} \leq C_3^{\mathbf{P}} h^{\alpha_3} \|v_h\|_{\mathcal{Q}}$$

Theorem

Assume that **(E1)-(E3)**, **(D1)-(D3)** *hold. Then there exists* $C > 0$ *such that for all* $h \in [0, h_0]$ *and all* $q_h(0) \in \mathcal{S}_h(0)$,

$$\|q_{\tau,h}(t) - q(t)\|_{\mathcal{Q}} \leq C\left(h^{\alpha/2} + \sqrt{\tau} + \|q_h(0) - q(0)\|_{\mathcal{Q}}\right)$$

for all $t \in [0, T]$ *and* $\tau \in (0, T]$.

Sketch of proof: Let us remark that

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

Lemma

Assume that **(E1)-(E3)**, **(D1)-(D3)** *hold. Then we have*

$|\langle \mathbf{B}_h q, q\rangle_{\mathcal{Q}}| \le C^{\mathbf{B}} h^\alpha$ *with* $\mathbf{B}_h \overset{def}{=} -(\mathbf{A}(\mathbf{P}_h - \mathbf{Id}) + (\mathbf{A}(\mathbf{P}_h - \mathbf{Id}))^*)$

$\langle \mathrm{D}_q\mathcal{E}(t, q_h), v_h - w\rangle_{\mathcal{Q}} + \Psi(v_h - w) \le C\left(h^\alpha + \|q_h - q\|^2_{\mathcal{Q}}\right)\|w\|_{\mathcal{Q}} + \langle \mathbf{B}_h q, w\rangle_{\mathcal{Q}}$

with $\alpha = \min\{\alpha_1, 2\alpha_2, \alpha_3\}$.

Proof: Notice that

$$\begin{aligned}
&\langle \mathrm{D}_q\mathcal{E}(t, q_h), v_h - w\rangle_{\mathcal{Q}} + \Psi(v_h - w)\\
&= \langle \mathbf{A}q_h + \mathrm{D}_q\mathcal{H}(q_h) - \mathbf{l}(t), v_h - w\rangle_{\mathcal{Q}} + \Psi(v_h - w)\\
&\le \langle \mathbf{A}(q_h - q), v_h - w\rangle_{\mathcal{Q}} + CC_1^{\mathbf{P}} h^{\alpha_1}\|w\|_{\mathcal{Q}}
\end{aligned}$$

Taking $v_h = \mathbf{P}_h w$, we have

$$\langle \mathbf{A}(q_h - q), v_h - w\rangle_{\mathcal{Q}} = \underbrace{\langle \mathbf{A}(q_h - q), (\mathbf{P}_h - \mathbf{Id})w\rangle_{\mathcal{Q}}}$$

$$= \langle (\mathbf{P}_h^* \mathbf{A} - \mathbf{A}\mathbf{P}_h)(q_h - q), w\rangle_{\mathcal{Q}} + \langle \mathbf{A}(\mathbf{P}_h - \mathbf{Id})q_h, w\rangle_{\mathcal{Q}} + \langle \mathbf{A}q, (\mathbf{P}_h - \mathbf{Id})w\rangle_{\mathcal{Q}} + \langle \mathbf{B}_h q, w\rangle_{\mathcal{Q}}$$

$$\le C\left(C_2^{\mathbf{P}} h^{\alpha_2}\|q_h - q\|_{\mathcal{Q}} + C_3^{\mathbf{P}} h^{\alpha_3}\|q_h\|_{\mathcal{Q}} + C_1^{\mathbf{P}} h^{\alpha_1}\right)\|w\|_{\mathcal{Q}} + \langle \mathbf{B}_h q, w\rangle_{\mathcal{Q}}$$

Define now

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

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

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By differentiation, we get

$$\begin{aligned}
\dot{\gamma} = &\langle \partial_t\mathrm{D}_q\mathcal{E}(t,q_h) - \partial_t\mathrm{D}_q\mathcal{E}(t,q), q_h - q\rangle_{\mathcal{Q}} \\
&+\langle \mathrm{D}_q\mathcal{E}(t,q) - \mathrm{D}_q\mathcal{E}(t,q_h) + \mathrm{D}_q^2\mathcal{E}(t,q_h)[q_h - q], \dot{q}_h\rangle_{\mathcal{Q}} \\
&+\langle \mathrm{D}_q\mathcal{E}(t,q_h) - \mathrm{D}_q\mathcal{E}(t,q) + \mathrm{D}_q^2\mathcal{E}(t,q)[q - q_h], \dot{q}\rangle_{\mathcal{Q}} \\
&+2 \underbrace{\langle \mathrm{D}_q\mathcal{E}(t,q_h) - \mathrm{D}_q\mathcal{E}(t,q), \dot{q}_h - \dot{q}\rangle_{\mathcal{Q}}}_{\overset{\text{(VI)}}{\leq} \langle \mathrm{D}_q\mathcal{E}(t,q_h), v_h - \dot{q}\rangle_{\mathcal{Q}} + \Psi(v_h - \dot{q}) \overset{\text{(CC)}}{\leq} C(h^\alpha + \|q_h - q\|_{\mathcal{Q}}^2)\|\dot{q}\|_{\mathcal{Q}} + \langle \mathbf{B}_h q, \dot{q}\rangle_{\mathcal{Q}}}
\end{aligned}$$

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By differentiation, we get

$$\dot{\gamma} \overset{\textbf{(E1)-(E3)}}{\leq} C\left(h^\alpha\|\dot{q}\|_{\mathcal{Q}} + \left(\|\dot{q}\|_{\mathcal{Q}} + \|\dot{q}_h\|_{\mathcal{Q}}\right)\|q - q_h\|^2_{\mathcal{Q}}\right) + 2\langle \mathbf{B}_h q, \dot{q}\rangle_{\mathcal{Q}}$$

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By differentiation, we get

$$\dot{\gamma} \overset{\substack{\text{Thm.}\\ \text{M\&T'04}}}{\leq} C\left(h^\alpha + \tfrac{\gamma}{\kappa}\right) + 2\langle \mathbf{B}_h q, \dot{q}\rangle_{\mathcal{Q}}$$

$$\Downarrow \text{ Mult. by } \mathrm{e}^{-Ct/\kappa} + \text{Int.}$$

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

$$\Downarrow \text{ (G1)}$$

$$\|q_h(t) - q(t)\|_{\mathcal{Q}}^2 \leq \mathrm{e}^{Ct/\kappa}\left(\tfrac{C}{\kappa}\|q_h(0) - q(0)\|_{\mathcal{Q}}^2 + (\kappa + 2C^{\mathbf{B}})h^\alpha\right)$$

Lemma

Assume that **(E1)-(E3)**, **(D1)-(D3)** *hold. Then there exists* $C_0 > 0$ *such that for all* $h \in (0, h_0]$, *we have* $q_h(0) \in \mathcal{S}_h(0)$ *and*

$$\|q_h(0) - q(0)\|_{\mathcal{Q}} \le C_0 h^{\alpha/2} \quad \text{with} \quad \alpha = \min\{\alpha_1, 2\alpha_2, \alpha_3\}.$$

Proof: We deduce from $\mathcal{E}(0, q(0)) + \frac{\kappa}{2}\|\widehat{q} - q(0)\|_{\mathcal{Q}}^2 \le \mathcal{E}(0, \widehat{q}) + \Psi(\widehat{q} - q(0))$ that

$$\begin{aligned}\frac{\kappa}{2}\|q_h(0) - q(0)\|_{\mathcal{Q}}^2 &\le \mathcal{E}(0, \mathbf{P}_h q(0)) - \mathcal{E}(0, q(0)) + \Psi((\mathbf{P}_h - \mathbf{Id})q(0)) \\ &\le \langle \mathrm{D}_q\mathcal{E}(0, q(0)), (\mathbf{P}_h - \mathbf{Id})q(0)\rangle_{\mathcal{Q}} + \mathcal{I} + \Psi((\mathbf{P}_h - \mathbf{Id})q(0))\end{aligned}$$

where

$$\begin{aligned}\mathcal{I} &\stackrel{\text{def}}{=} \int_0^1 \langle \mathrm{D}_q\mathcal{E}(0, q(0) + s(\mathbf{P}_h - \mathbf{Id})q(0)) - \mathrm{D}_q\mathcal{E}(0, q(0)), (\mathbf{P}_h - \mathbf{Id})q(0)\rangle_{\mathcal{Q}}\,\mathrm{d}s \\ &\le C^{\kappa}\big(\|(\mathbf{P}_h - \mathbf{Id})q(0)\|_{\mathcal{Q}}^2 + \|(\mathbf{P}_h - \mathbf{Id})q(0)\|_{\mathcal{X}}^2\big)\end{aligned}$$

Lemma

Assume that $q(0) \in \mathcal{S}(0)$, **(D1)** *and* **(D3)** *hold. Then we have* $\mathrm{D}_q\mathcal{E}(0, q(0)) \in \mathrm{Lin}(\mathcal{Q}, \mathcal{X}')$ *and* $\|\mathrm{D}_q\mathcal{E}(0, q(0))\|_{\mathrm{Lin}(\mathcal{Q},\mathcal{X}')} \leq C^{\Psi}$.

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$$\frac{\kappa}{2}\|q_h(0) - q(0)\|_{\mathcal{Q}}^2 \le \mathcal{E}(0, \mathbf{P}_h q(0)) - \mathcal{E}(0, q(0)) + \Psi((\mathbf{P}_h - \mathbf{Id})q(0))$$

$$\le C^{\kappa}\left(\|(\mathbf{P}_h - \mathbf{Id})q(0)\|_{\mathcal{Q}}^2 + \|(\mathbf{P}_h - \mathbf{Id})q(0)\|_{\mathcal{X}}^2\right) + 2C^{\Psi}\|(\mathbf{P}_h - \mathbf{Id})q(0)\|_{\mathcal{X}}$$

$$\overset{\textbf{(P1)}}{\le} C^{\kappa}\|(\mathbf{P}_h - \mathbf{Id})q(0)\|_{\mathcal{Q}}^2 + C^{\kappa}(C_1^{\mathbf{P}})^2 h^{2\alpha_1}\|q(0)\|_{\mathcal{Q}}^2 + 2C^{\Psi}C_1^{\mathbf{P}} h^{\alpha_1}\|q(0)\|_{\mathcal{Q}}$$

Lemma

Assume that $q(0) \in \mathcal{S}(0)$, **(D1)** *and* **(D3)** *hold. Then we have* $\mathrm{D}_q\mathcal{E}(0, q(0)) \in \mathrm{Lin}(\mathcal{Q}, \mathcal{X}')$ *and* $\|\mathrm{D}_q\mathcal{E}(0, q(0))\|_{\mathrm{Lin}(\mathcal{Q},\mathcal{X}')} \leq C^{\Psi}$.

$$\frac{\kappa}{2}\|q_h(0)-q(0)\|^2_{\mathcal{Q}} \leq \mathcal{E}(0, \mathbf{P}_h q(0)) - \mathcal{E}(0, q(0)) + \Psi((\mathbf{P}_h-\mathbf{Id})q(0))$$
$$\leq C^{\kappa}\|(\mathbf{P}_h-\mathbf{Id})q(0)\|^2_{\mathcal{Q}} + C^{\kappa}(C_1^{\mathbf{P}})^2 h^{2\alpha_1}\|q(0)\|^2_{\mathcal{Q}} + 2C^{\Psi}C_1^{\mathbf{P}} h^{\alpha_1}\|q(0)\|_{\mathcal{Q}}$$

It remains to evaluate $\|(\mathbf{P}_h-\mathbf{Id})q(0)\|_{\mathcal{Q}}$

$$\frac{\kappa}{2}\|(\mathbf{P}_h-\mathbf{Id})q(0)\|^2_{\mathcal{Q}} \leq C \underbrace{\langle \mathbf{A}(\mathbf{P}_h-\mathbf{Id})q(0), (\mathbf{P}_h-\mathbf{Id})q(0)\rangle_{\mathcal{Q}}}_{=\langle(\mathbf{P}_h^*\mathbf{A}-\mathbf{A}\mathbf{P}_h)(\mathbf{P}_h-\mathbf{Id})q(0),q(0)\rangle_{\mathcal{Q}}+\langle\mathbf{A}(\mathbf{P}_h-\mathbf{Id})\mathbf{P}_h q(0),q(0)\rangle_{\mathcal{Q}}-\langle\mathbf{A}(\mathbf{P}_h-\mathbf{Id})q(0),q(0)\rangle_{\mathcal{Q}}}$$
$$+C\|(\mathbf{P}_h-\mathbf{Id})q(0)\|^2_{\mathcal{X}} + 2C^{\Psi}\|(\mathbf{P}_h-\mathbf{Id})q(0)\|_{\mathcal{X}}$$

$$\overset{\textbf{(P1)-(P3)}}{\Longrightarrow} \|(\mathbf{P}_h-\mathbf{Id})q(0)\|^2_{\mathcal{Q}} \leq C_0 h^{\alpha} \text{ with } \alpha = \min\{\alpha_1, 2\alpha_2, \alpha_3\}.$$

Theorem

Assume that **(E1)-(E3)**, **(D1)-(D3)** *hold. Then there exists* $C_* > 0$ *such that* $q(0) \in \mathcal{S}(0)$, *we have*

$$\|q_{\tau,h}(t) - q(t)\|_{\mathcal{Q}} \le C_* \left(h^{\alpha/2} + \sqrt{\tau}\right)$$

with $\alpha = \min\{\alpha_1, 2\alpha_2, \alpha_3\}$.

State variables

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

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

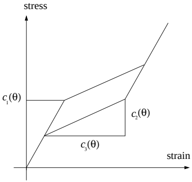
Applied field

$\ell_{\mathrm{appl}} \in \mathrm{C}^3([0,T],\mathcal{F}^*)$ 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 $W(\mathbf{e}(u),z,\nabla z) = \frac{1}{2}\mathbb{C}(\mathbf{e}(u)-z):(\mathbf{e}(u)-z) + H_{\mathrm{SoAu}}(z) + \nu|\nabla z|^2$

- $\mathbf{e}(u) = \frac{1}{2}(\nabla u + \nabla u^{\mathsf{T}})$: 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



Dissipation distance: $\Psi(z_2-z_1) = \int_\Omega \rho|z_2-z_1|\,\mathrm{d}x$

Notations: $\mathcal{Q} = \mathcal{F}\times\mathcal{Z}$ and $q=(u,z)$

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Regularized version of H_{SoAu}:

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

Dissipation distance: $\Psi(z_2{-}z_1) = \int_\Omega \rho|z_2{-}z_1|\,\mathrm{d}x$

Theorem (Existence and uniqueness)

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

For $\delta > 0$ the solutions are unique since $\mathcal{E} \in \mathrm{C}^3([0,T]\times \mathrm{H}^1(\Omega))$.

Since $\mathcal{E}(t,\cdot) : \mathcal{F} \times \mathcal{Z} \to \mathbb{R}_\infty$ convex, then **(S)&(E)** is equivalent to

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$$0 \in \partial\Psi(\dot{q}(t)) + \mathrm{D}_q\mathcal{E}(t, q(t))$$

Since $\mathcal{E}(t,\cdot) : \mathcal{F} \times \mathcal{Z} \to \mathbb{R}_\infty$ convex, then **(S)&(E)** is equivalent to

$$0 \in \partial\Psi(\dot{q}) + \mathbf{A}q + \mathrm{D}_q\mathcal{H}_{\mathrm{SoAu}}(q) - \mathbf{l}(t)$$

- $\partial\Psi(\dot{q}) \overset{\text{def}}{=} (0, \partial\Psi(\dot{z}))^{\mathsf{T}}$
- $\mathcal{H}_{\mathrm{SoAu}}(q) \overset{\text{def}}{=} (0, H_{\mathrm{SoAu}}(z) + \frac{c_2}{2}|z|^2)^{\mathsf{T}}$
- $\mathbf{l}(t) \overset{\text{def}}{=} (\ell(t), 0)^{\mathsf{T}}$
- $\mathbf{A} \overset{\text{def}}{=} \begin{pmatrix} -\mathrm{div}(\mathbb{C}\mathbf{e}(\cdot)) & \mathrm{div}\,(\mathbb{C}(\cdot)) \\ -\mathbb{C}(\mathbf{e}(\cdot)) & \mathbb{C}(\cdot) - \nu\Delta(\cdot) + \frac{c_2}{2}\mathbf{Id}(\cdot) \end{pmatrix}$

Theorem

There exists $C_*^{\mathrm{SoAu}} > 0$ such that for all $h \in (0,1]$, we have

$$\|q_{\tau,h}(t) - q(t)\|_{\mathcal{Q}} \leq C_*^{\mathrm{SoAu}}\left(\sqrt{h} + \sqrt{\tau}\right) \text{ for all } t \in [0,T].$$

- understand the limit when $\nu \longrightarrow 0$ (formation of microstructure)
- include rate-dependent effects like a heat equation
- develop the theory to include other multifunctional materials (ferroelectric materials, magnetostrictive materials)

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Thank you for your attention !

Papers on line: `http://www.wias-berlin.de/people/petrov`