On the existence and error bounds for space-time discretizations of a 3D model for shape-memory alloys

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DFG Research Center MATHEON
Mathematics for key technologies

Weierstraß-Institut für Angewandte Analysis und Stochastik

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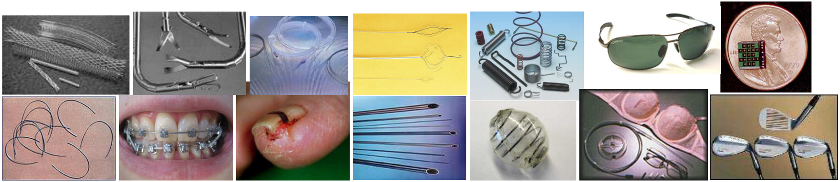
Shape-Memory Alloys are used today in real life:



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

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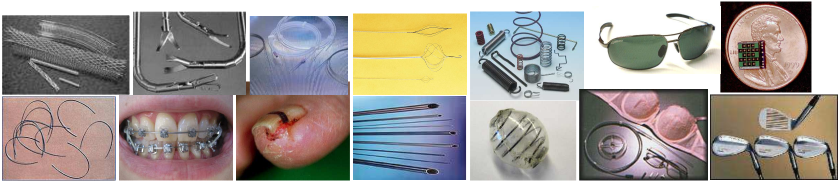

WHY? Because their have the following properties:

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

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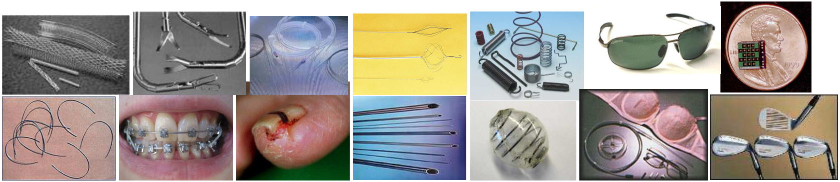

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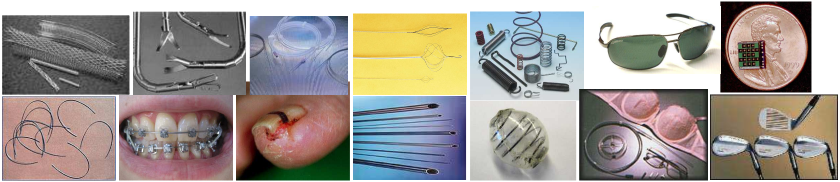

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$\Longrightarrow$ Souza-Auricchio model for shape-memory alloys[1]

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State variables

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

$z : \Omega \to Z$ phase indicator

Applied field

$\ell_{\mathrm{appl}} : [0, T] \to \mathcal{F}^*$ mechanical loading

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

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

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

(S) $\mathcal{E}(t, u(t), z(t)) \le \mathcal{E}(t, \tilde{u}, \tilde{z}) + \mathcal{D}(z(t), \tilde{z})$ for all $(\tilde{u}, \tilde{z}) \in \mathcal{F} \times \mathcal{Z}$

(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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$z : \Omega \to Z$ phase indicator

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$\ell_{\rm appl} : [0, T] \to \mathcal{F}^*$ mechanical loading

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

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If $\mathcal{D}(z_1, z_2) = \Psi(z_2 - z_1)$ and $\mathcal{E}(t, \cdot) : \mathcal{F} \times \mathcal{Z} \to \mathbb{R}_\infty$ 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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- $\mathcal{X}$: Banach space such that $\mathcal{Q} \subset \mathcal{X} \subset \mathcal{Q}'$
- $\mathcal{E} : [0, T] \times \mathcal{Q} \to \mathbb{R}$: the energy functional

(E1) $\mathcal{E} \in \mathrm{C}^3([0, T] \times \mathcal{Q})$

(E2) $\mathcal{E}(t, \cdot)$ is κ-uniformly convex

(E3) $\exists c,\ C > 0 \ : \ \forall \widehat{q} \in \mathcal{Q} \ \ c\|\widehat{q}\|^2_{\mathcal{Q}} - C \leq \mathcal{E}(t, \widehat{q}) \leq C\|\widehat{q}\|^2_{\mathcal{Q}} + C$

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  (D2) $\forall q_1, q_2 \in \mathcal{Q} : \;\Psi(q_1 + q_2) \leq \Psi(q_1) + \Psi(q_2)$

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  - **(D3)** $\exists C_\Psi > 0 \; \forall \widehat{q} \in \mathcal{X} : \;\Psi(\widehat{q}) \leq C_\Psi \|\widehat{q}\|_{\mathcal{X}}$
- $\mathcal{S}(t) \stackrel{\text{def}}{=} \left\{ q \in \mathcal{Q} \,\middle|\, \forall \widehat{q} \in \mathcal{Q} : \mathcal{E}(t, q) \leq \mathcal{E}(t, \widehat{q}) + \Psi(\widehat{q} - q) \right\}$: the stable states

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We consider the *doubly nonlinear evolution equation*

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

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

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

Remark: (S)&(E) $\Longleftrightarrow$ **(DI)**

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

Space-Time Discretization

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

where $q_k^{\tau,h} = (u_k^{\tau,h}, z_k^{\tau,h})$ and $\widehat{q}^h = (\widehat{u}^h, \widehat{z}^h)$

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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. $t \in [0, T]$.*

Finite-element spaces $\mathcal{F}_h \subset \mathcal{F}$ and $\mathcal{Z}_h \subset \mathcal{Z}$ with $\mathcal{Q}_h = \mathcal{F}_h \times \mathcal{Z}_h$
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Theorem (Mielke&Theil'04)

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

The **central condition** for our approximation result is the following:

(CC) $\forall E>0\ \exists C>0\ \exists h_0>0\ \forall h\in[0,h_0]\ \forall(t,\bar q_h)\in[0,T]\times\mathcal{Q}_h$ with $\mathcal{E}(t,\bar q_h)\le E\ \forall w\in\mathcal{Q}\ \exists v_h\in\mathcal{Q}_h$: $\langle \mathrm{D}_q\mathcal{E}(t,\bar q_h), v_h-w\rangle_{\mathcal{Q}}+\Psi(v_h-w)\le Ch^{\alpha}\|w\|_{\mathcal{Q}}$

Theorem

*Assume that **(E1)**, **(D1)**, **(D2)** and **(CC)** hold. Then there exists* $C>0$ *such that for all* $h\in[0,h_0]$ *and all* $q_h(0)\in\mathcal{S}_h(0)$,
$\forall t\in[0,T]\ \forall\tau\in(0,T]:\|q_{\tau,h}(t)-q(t)\|_{\mathcal{Q}}\le C\big(h^{\alpha/2}+\sqrt{\tau}+\|q_h(0)-q(0)\|_{\mathcal{Q}}\big)$

Sketch of proof: Let us remark that

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

Define now

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

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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

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

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

By differentiation, we get

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

$\Downarrow$ Int. + Gronwall

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

$\Downarrow$ (G1)

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

We consider now that the energy has the following form

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

(H1)
$\mathbf{A} \in \mathrm{Lin}(\mathcal{Q},\mathcal{Q}')$ is a symmetric operator
$\mathcal{H} \in C^3(\mathcal{Q},\mathbb{R})$ is convex and $\mathrm{D}_q\mathcal{H} \in \mathrm{C}^{1,\mathrm{Lip}}(\mathcal{Q};\mathcal{X}')$
$\mathbf{l} \in \mathrm{C}^1([0,T];\mathcal{X}')$

Let $\mathbf{P}_h : \mathcal{Q} \to \mathcal{Q}_h$ be a linear operator such that there exist $C_{\mathbf{P}}^{(i)} > 0$ 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) $\|(\mathbf{P}_h - \mathbf{I})v\|_{\mathcal{X}} \le C_{\mathbf{P}}^{(1)} h^{\alpha_1}\|v\|_{\mathcal{Q}}$

(P2) $\|(\mathbf{P}_h^*\mathbf{A} - \mathbf{A}\mathbf{P}_h)v\|_{\mathcal{Q}'} \le C_{\mathbf{P}}^{(2)} h^{\alpha_2}\|v\|_{\mathcal{Q}}$

(P3) $\|(\mathbf{P}_h - \mathbf{I})v_h\|_{\mathcal{Q}} \le C_{\mathbf{P}}^{(3)} h^{\alpha_3}\|v_h\|_{\mathcal{Q}}$

Lemma

Assume that ***(H1)***, ***(E2)***, ***(D3)*** *hold. Then* ***(CC)*** *holds with* $\alpha = \min\{\alpha_1, \alpha_2, \alpha_3\}$ *i.e.* $\|q_{\tau,h}(t) - q(t)\|_{\mathcal{Q}} \leq C(h^{\alpha/2} + \sqrt{\tau} + \|q_h(0) - q(0)\|_{\mathcal{Q}})$

Idea of the proof: Use **(D3)** and **(P1)-(P3)**.

On the other hand, we have

Lemma

Assume that ***(H1)***, ***(E2)***, ***(D1)-(D3)*** *hold. Then there exists* $C > 0$ *such that for all* $h \in (0, h_0]$, *we have* $q_h(0) \in \mathcal{S}_h(0)$ *and*

$$\|q_h(0) - q(0)\|_{\mathcal{Q}} \leq Ch^{\beta/2} \quad \textit{with} \quad \beta = \min\{\alpha_1, 2\alpha_2, \alpha_3\}.$$

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.

Theorem

Assume that ***(H1)****,* ***(E2)****,* ***(D1)****-****(D3)*** *hold. Then there exists* $C > 0$ *such that* $q(0) \in \mathcal{S}(0)$*, we have*

$$\forall h \in [0, h_0] \; \exists q_h(0) \in \mathcal{S}_h(0) \; \forall t \in [0, T] \; \forall \tau \in (0, T] :$$

$$\|q_{\tau,h}(t) - q(t)\|_{\mathcal{Q}} \leq C\left(h^{\alpha/2} + \sqrt{\tau}\right) \quad \textit{with} \quad \alpha = \min\{\alpha_1, \alpha_2, \alpha_3\}$$

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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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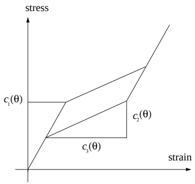
- $\mathbf{e}(u) = \frac{1}{2}(\nabla u + \nabla u^{\mathsf{T}})$: infinitesimal strain
- $\mathbb{C}$: elasticity tensor
- $H_{\mathrm{SoAu}}(z) = c_1|z| + \frac{c_2}{2}|z|^2 + \chi_{\{|z|\le c_3\}}(z)$
  - c_1: activation threshold
  - c_2: hardening in the martensitic regime
  - c_3: maximal transformation strain



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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 $\mathcal{E} \in \mathrm{C}^3([0,T]\times \mathrm{H}^1(\Omega))$.

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

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

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

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

Then our problem can be rewritten as follows

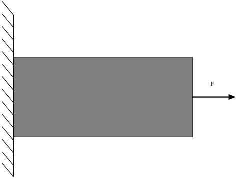
$$\mathbf{A}q + \partial\Psi(\dot q) + \mathrm{D}_q\mathcal{H}_{\mathrm{SoAu}}(q) - \mathbf{l}(t) \ni 0$$

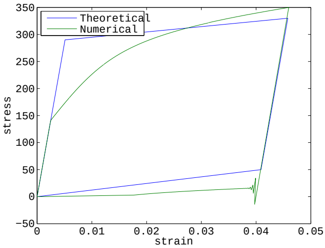
where $\partial\Psi(\dot q) \overset{\mathrm{def}}{=} (0,\partial\Psi(\dot z))^{\mathsf T}$, $\mathcal{H}_{\mathrm{SoAu}}(q) \overset{\mathrm{def}}{=} (0, H_{\mathrm{SoAu}}(z))^{\mathsf T}$, $\mathbf{l}(t) \overset{\mathrm{def}}{=} (\ell(t),0)^{\mathsf T}$
and

$$\mathbf{A} \overset{\mathrm{def}}{=} \begin{pmatrix} -\mathrm{div}(\mathbb{C}e(\cdot)) & \mathrm{div}\,(\mathbb{C}(\cdot)) \\ -\mathbb{C}(e(\cdot)) & \mathbb{C}(\cdot)-\sigma\Delta(\cdot)\end{pmatrix}$$

$$\Longrightarrow \|q(t){-}q_{\tau,h}(t)\|_{\mathcal{Q}} \le C(\sqrt{h}{+}\sqrt{\tau})$$

- We have developed a FE simulation tools (2D and 3D)





- include rate-dependent effects like a heat equation
- develop the theory to include other multifunctional materials (ferroelectric materials, magnetostrictive materials)

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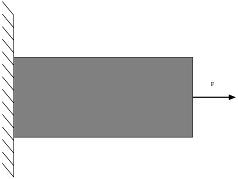

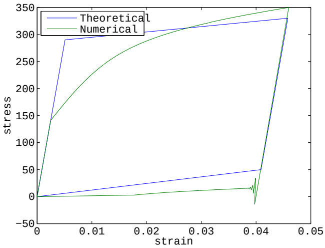

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Thank you for your attention !

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