PhD Program in Computational Mechanics and Advanced Materials
XXVIII cycle

Shape-memory materials:
constitutive modeling for advanced applications

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Outline

- Goals of my work
- Shape-memory alloys:
  - ➢ SMA preliminaries
  - ➢ Constitutive modeling
  - ➢ Implicit and explicit algorithms for SMA constitutive model
  - ➢ UMAT / VUMAT semi-automatic generator
  - ➢ Gradient structures for SMA: full thermomechanical coupling
- Shape-memory polymers:
  - ➢ SMP preliminaries
  - ➢ New phenomenological constitutive model
- Conclusions and future developments

Challenge

- **Human needs** are in continuous evolution → Medicine, safety, industry, comfort, domotic, …

- Science and technology are inceasingly pushed

Shape memory materials

- Shape-memory materials are a mean to promote **advancements**:
    - response to external stimuli
    - simpler designs and actuation mechanisms than conventional ones
    - more compact
    - more efficient

- Example **applications** in:
    - aerospace and mechanics: morphing wings, actuators, valves, switches
    - medicine: stents, catheters, surgical instruments
    - civil and mechanical engineering: sensors, dampeners
    - … many others …

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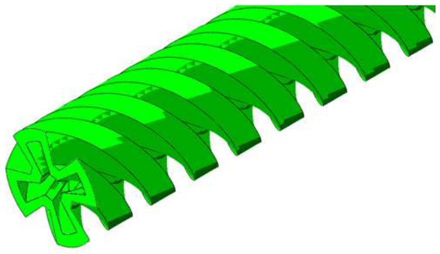
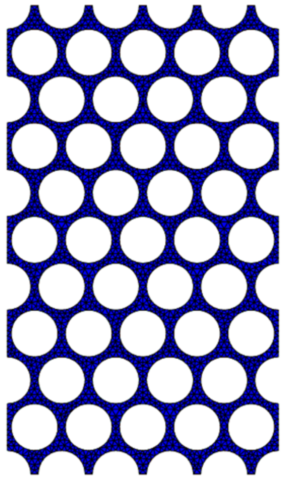
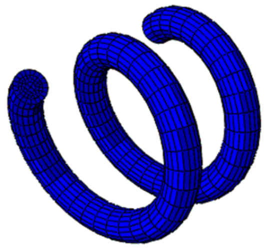
Computer-based simulations

- **Virtual simulations** are very helpful, often even necessary, to develop new solutions and products



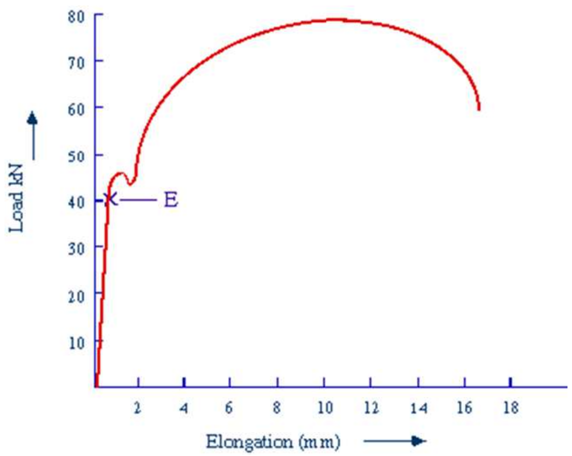


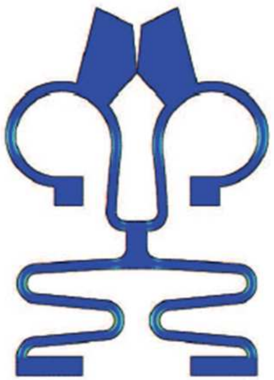


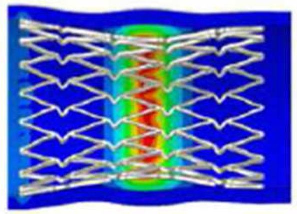
- A fundamental part of the numerical simulation is **material constitutive modeling**
- Robust and effective material models and algorithms need to be developed, to be used in complex simulations
- The research field is wide open regarding **advanced materials** behavior

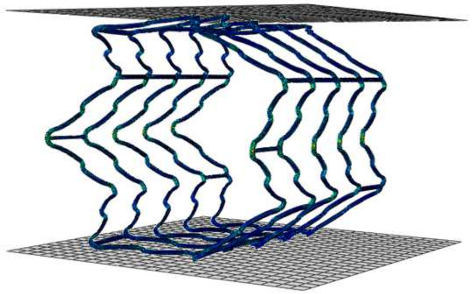
Material modeling

1. Experimental data on material behavior
2. Development of mathematical model based on both experimental data and commonly accepted theories and assumptions
3. Calibration of the model parameters over the initial experimental data
4. Validation of the model with different and more complex experimental data: comparison of numerical vs experimental curves









Goal

- My work has been dealing with the development and numerical testing of advanced **constitutive models** for **shape-memory alloys** and **shape-memory polymers**

- The aim is to provide engineers and researchers with an effective tool to use within FEA simulations

- Simulation of real-life applications in biomedical and industrial fields: e.g. medical devices, actuators, dampeners, wave filters

- Comparison with experimental data

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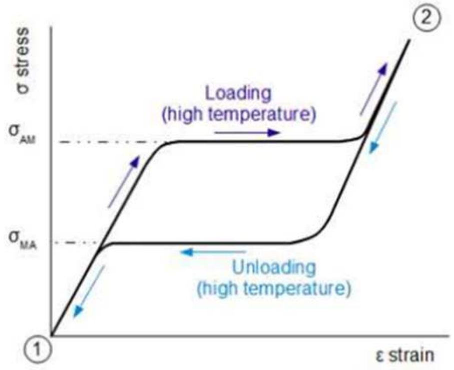
Part 1

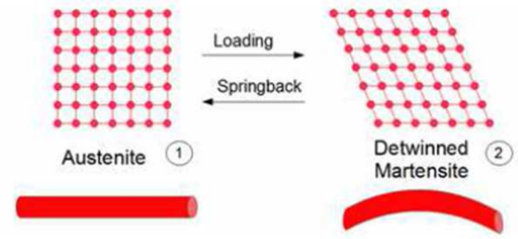
Shape memory alloys

SMA properties

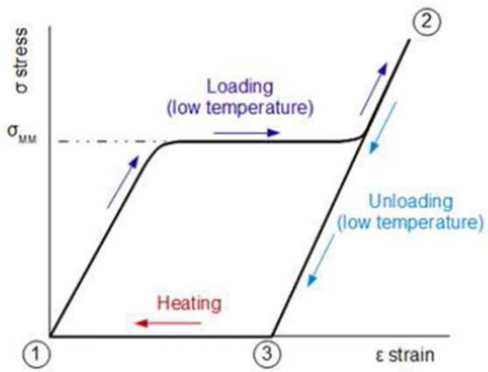
- Peculiar materials presenting **superelasticity** and **shape memory effect**

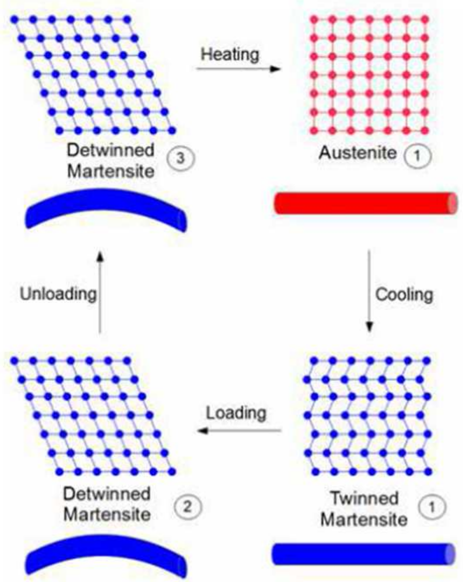
Superelasticity:





Shape memory effect:

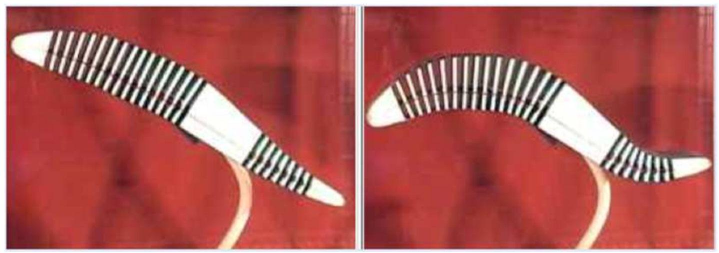
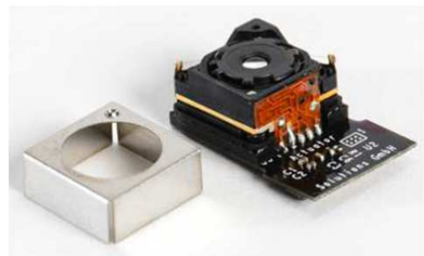




SMA applications

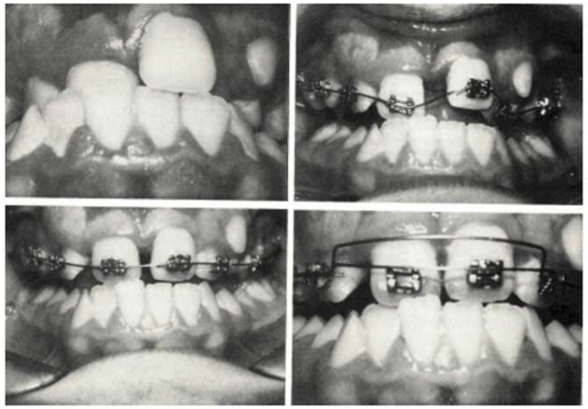
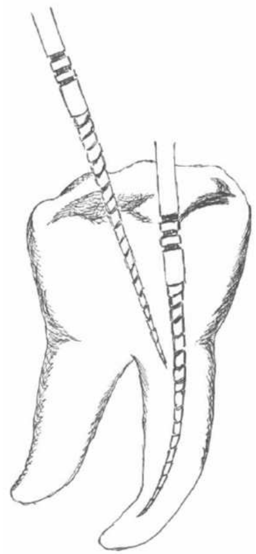
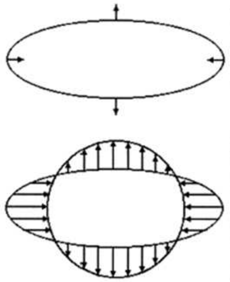
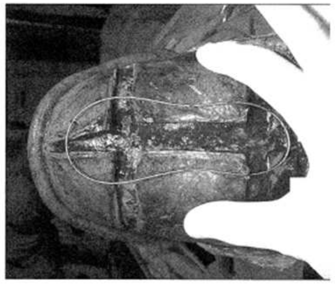
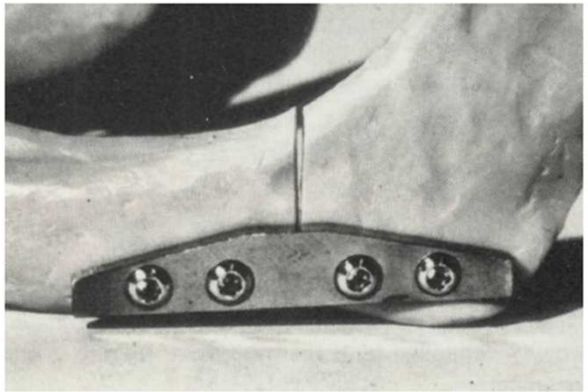
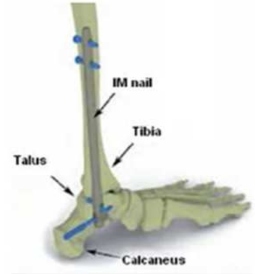
- Applications in different fields
  - Valves
  - Actuators
  - Switches
  - Blinds
  - Morphing structures
  - Stents and stent-grafts
  - Flexible surgical instruments
  - Catheter guides
  - …

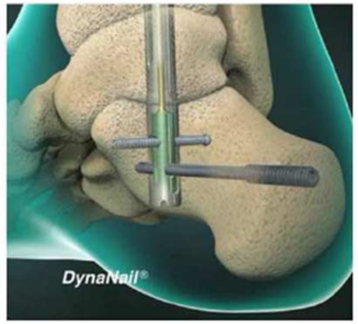


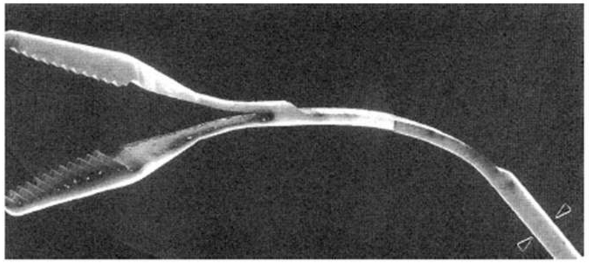



SMA applications

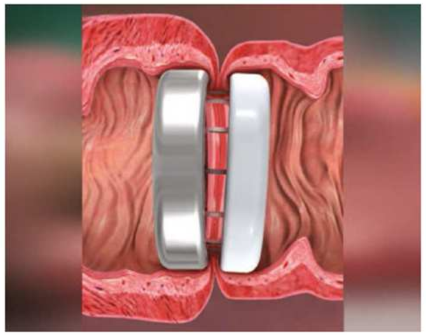
- In particular, in the biomedical field:










Auricchio F., **Boatti E.**, Conti M., Chapter 11 in *Shape memory alloy engineering: for aerospace, structural and other applications*, 2014

Auricchio F., **Boatti E.**, Conti M., Chapter 12 in *Shape memory alloy engineering: for aerospace, structural and other applications*, 2014

SMA constitutive modeling

- Modeling routes: micro, micro-macro, macro
- **Souza-Auricchio model** is a robust and relatively simple 3D phenomenological model

Continuous formulation

Input variables: $\varepsilon,\ \theta$

Internal variable: $\boldsymbol{e}^{\mathrm{tr}}$

Saturation constraint: $\|\boldsymbol{e}^{\mathrm{tr}}\| \le \epsilon_L$

Free energy:

$$\psi(\varepsilon, \mathbf{e}^{\mathrm{tr}}, \theta) := c\theta(1-\log\theta) + \frac{1}{2}(\varepsilon-\mathbf{e}^{\mathrm{tr}}):\mathbb{C}(\varepsilon-\mathbf{e}^{\mathrm{tr}}) + \frac{H}{2}|\mathbf{e}^{\mathrm{tr}}|^2 + f(\theta)|\mathbf{e}^{\mathrm{tr}}| + I(\mathbf{e}^{\mathrm{tr}}).$$

Constitutive equations:

$$p = \partial_\theta \psi = Kv,$$
$$\boldsymbol{s} = \partial_{\boldsymbol{e}} \psi = 2G(\boldsymbol{e}-\mathbf{e}^{\mathrm{tr}}),$$
$$s = -\partial_\theta \psi = -f'(\theta)|\mathbf{e}^{\mathrm{tr}}| + c\log\theta - c,$$
$$\boldsymbol{X} = -\partial_{\boldsymbol{e}^{\mathrm{tr}}} \psi = \boldsymbol{s} - H\boldsymbol{e}^{\mathrm{tr}} - f(\theta)\partial|\mathbf{e}^{\mathrm{tr}}| - \partial I(\mathbf{e}^{\mathrm{tr}})$$

Von Mises yield condition: $F = \|\boldsymbol{X}\| - R_Y$

Flow rule: $\dot{e}^{tr} = \xi \dfrac{\partial F}{\partial \boldsymbol{X}} = \xi \dfrac{\boldsymbol{X}}{\|\boldsymbol{X}\|}$

Consistency and Kuhn-Tucker conditions: $\xi \ge 0,\quad F \le 0,\quad \xi F = 0$

Souza et al., *Eur. J. Mech A/Solids,* 1998
Auricchio and Petrini, *IJMNE*, 2004

SMA numerical algorithm: implicit

Discrete formulation

Implicit algorithm

Given quantities: $\boldsymbol{\varepsilon}, T, \boldsymbol{e}_n^{\text{tr}}, \ell_n$

Compute trial state:

$$\xi_{TR} = 0;$$
$$\boldsymbol{e}_{TR}^{\text{tr}} = \boldsymbol{e}_n^{\text{tr}}$$
$$\ell_{TR} = 0$$
$$\boldsymbol{s}_{TR} = 2G\left(\boldsymbol{e} - \boldsymbol{e}_{TR}^{\text{tr}}\right)$$
$$\boldsymbol{X}_{TR} = \boldsymbol{s}_{TR} - f(\theta)\frac{\boldsymbol{e}_{TR}^{\text{tr}}}{\|\boldsymbol{e}_{TR}^{\text{tr}}\|} - h\boldsymbol{e}_{TR}^{\text{tr}}$$
$$F_{TR} = \|\boldsymbol{X}_{TR}\| - R_Y$$

IF $F_{TR} \leq tol$ THEN

Elastic step:

$$\xi = \xi_{TR};\ \boldsymbol{e}^{\text{tr}} = \boldsymbol{e}_{TR}^{\text{tr}};\ \ell = \ell_{TR};\ \boldsymbol{s} = \boldsymbol{s}_{TR};\ \boldsymbol{X} = \boldsymbol{X}_{TR}$$

ELSE

Inelastic PT1 step

Initialize:

$$k = 0$$
$$\boldsymbol{h}^{(0)} = \left\{\boldsymbol{e}^{tr(0)}, \xi^{(0)}\right\} = \left\{\boldsymbol{e}_{TR}^{\text{tr}}, \xi_{TR}\right\}$$

REPEAT

$$\boldsymbol{s}^{(k)} = 2G\left(\boldsymbol{e} - \boldsymbol{e}^{tr(k)}\right)$$
$$\boldsymbol{X}^{(k)} = \boldsymbol{s}^{(k)} - f(\theta)\frac{\boldsymbol{e}^{tr(k)}}{\|\boldsymbol{e}^{tr(k)}\|} - h\boldsymbol{e}^{tr(k)}$$

Solve system $\boldsymbol{Q}^{(k)} = \begin{pmatrix} \boldsymbol{e}^{tr(k)} - \boldsymbol{e}_n^{\text{tr}} - \xi^{(k)}\dfrac{\boldsymbol{X}^{(k)}}{\|\boldsymbol{X}^{(k)}\|} \\ \|\boldsymbol{X}^{(k)}\| - R_Y \end{pmatrix} = \boldsymbol{0}$

via Newton-Raphson procedure to find:

$$\boldsymbol{h}^{(k+1)} = \left\{\boldsymbol{e}^{tr(k+1)}, \xi^{(k+1)}\right\} = \boldsymbol{h}^{(k)} + \Delta\boldsymbol{h}^{(k)} = \boldsymbol{h}^{(k)} - \left[\nabla_h \boldsymbol{Q}^{(k)}\right]^{-1}\boldsymbol{Q}^{(k)}$$
$$k = k + 1$$

UNTIL $\|\Delta\boldsymbol{h}^{(k-1)}\| < tol_{NR}$

Resulting quantities:

$$\boldsymbol{e}_{PT1}^{\text{tr}} = \boldsymbol{e}^{tr(k)}$$
$$\xi_{PT1} = \xi^{(k)}$$

IF $\|\boldsymbol{e}_{PT1}^{\text{tr}}\| \leq \epsilon_L$ THEN

$$\xi = \xi_{PT1}$$
$$\boldsymbol{e}^{\text{tr}} = \boldsymbol{e}_{PT1}^{\text{tr}}$$
$$\ell = \ell_{TR}$$
$$\boldsymbol{s} = 2G\left(\boldsymbol{e} - \boldsymbol{e}^{\text{tr}}\right)$$
$$\boldsymbol{X} = \boldsymbol{s} - f(\theta)\frac{\boldsymbol{e}^{\text{tr}}}{\|\boldsymbol{e}^{\text{tr}}\|} - h\boldsymbol{e}^{\text{tr}}$$

ELSE

Inelastic PT2 step

Initialize:

$$k = 0$$
$$\boldsymbol{h}^{(0)} = \left\{\boldsymbol{e}^{tr(0)}, \xi^{(0)}, \ell^{(0)}\right\} = \left\{\boldsymbol{e}_{TR}^{\text{tr}}, \xi_{TR}, \ell_{TR}\right\}$$

REPEAT

$$\boldsymbol{s}^{(k)} = 2G\left(\boldsymbol{e} - \boldsymbol{e}^{tr(k)}\right)$$
$$\boldsymbol{X}^{(k)} = \boldsymbol{s}^{(k)} - \left(f(\theta) + \ell^{(k)}\right)\frac{\boldsymbol{e}^{tr(k)}}{\|\boldsymbol{e}^{tr(k)}\|} - h\boldsymbol{e}^{tr(k)}$$

Solve system $\boldsymbol{Q}^{(k)} = \begin{pmatrix} \boldsymbol{e}^{tr(k)} - \boldsymbol{e}_n^{\text{tr}} - \xi^{(k)}\dfrac{\boldsymbol{X}^{(k)}}{\|\boldsymbol{X}^{(k)}\|} \\ \|\boldsymbol{X}^{(k)}\| - R_Y \\ \|\boldsymbol{e}^{tr(k)}\| - \epsilon_L \end{pmatrix} = \boldsymbol{0}$

via Newton-Raphson procedure to find:

$$\boldsymbol{h}^{(k+1)} = \left\{\boldsymbol{e}^{tr(k+1)}, \xi^{(k+1)}, \ell^{(k+1)}\right\} = \boldsymbol{h}^{(k)} + \Delta\boldsymbol{h}^{(k)} = \boldsymbol{h}^{(k)} - \left[\nabla_h \boldsymbol{Q}^{(k)}\right]^{-1}\boldsymbol{Q}^{(k)}$$
$$k = k + 1$$

UNTIL $\|\Delta\boldsymbol{h}^{(k-1)}\| < tol_{NR}$

Resulting quantities:

$$\boldsymbol{e}_{PT2}^{\text{tr}} = \boldsymbol{e}^{tr(k)}$$
$$\xi_{PT2} = \xi^{(k)}$$
$$\ell_{PT2} = \ell^{(k)}$$

END IF

END IF

Explicit algorithm motivation

Why are explicit algorithms useful ??

- highly non-linear simulations
- fully-coupled analyses
- dynamic analyses
- >1.000.000 DoFs

… above all, when implicit fails !

- previously, there was no explicit algorithm implementation for Souza-Auricchio SMA model

SMA numerical algorithm: explicit

Discrete formulation

Explicit algorithm

Given quantities: $\boldsymbol{\varepsilon}, T, \boldsymbol{e}_n^{\mathrm{tr}}, \xi_n, \ell_n$

Compute trial state:

$$\xi_{TR} = 0$$
$$\boldsymbol{e}_{TR}^{\mathrm{tr}} = \boldsymbol{e}_n^{\mathrm{tr}}$$
$$\ell_{TR} = 0$$
$$\boldsymbol{s}_{TR} = 2G\left(\boldsymbol{e} - \boldsymbol{e}_{TR}^{\mathrm{tr}}\right)$$
$$\boldsymbol{X}_{TR} = \boldsymbol{s}_{TR} - f(\theta)\frac{\boldsymbol{e}_{TR}^{\mathrm{tr}}}{\|\boldsymbol{e}_{TR}^{\mathrm{tr}}\|} - h\boldsymbol{e}_{TR}^{\mathrm{tr}}$$
$$F_{TR} = \|\boldsymbol{X}_{TR}\| - R_Y$$

IF $F_{TR} \leq tol$ THEN

Elastic step:

$$\xi = \xi_{TR};\ \boldsymbol{e}^{\mathrm{tr}} = \boldsymbol{e}_{TR}^{\mathrm{tr}};\ \ell = \ell_{TR};\ \boldsymbol{s} = \boldsymbol{s}_{TR};\ \boldsymbol{X} = \boldsymbol{X}_{TR}$$

ELSE

Inelastic step:

Compute ξ_{PT1} via Eq. $\xi_{PT1} = \xi^{(0)} + \delta\xi^{(0)} = \xi^{(0)} - \left(\left.\frac{dF}{d\xi}\right|^{(0)}\right)^{-1} F^{(0)}$

$$\boldsymbol{e}_{PT1}^{\mathrm{tr}} = \boldsymbol{e}_n^{\mathrm{tr}} + \xi_{PT1}\frac{\boldsymbol{X}_{TR}}{\|\boldsymbol{X}_{TR}\|}$$

IF $\|\boldsymbol{e}_{PT1}^{\mathrm{tr}}\| \leq \epsilon_L$ THEN

$$\xi = \xi_{PT1}$$
$$\boldsymbol{e}^{\mathrm{tr}} = \boldsymbol{e}_{PT1}^{\mathrm{tr}}$$
$$\ell = \ell_{TR}$$
$$\boldsymbol{s} = 2G\left(\boldsymbol{e} - \boldsymbol{e}^{\mathrm{tr}}\right)$$
$$\boldsymbol{X} = \boldsymbol{s} - f(\theta)\frac{\boldsymbol{e}^{\mathrm{tr}}}{\|\boldsymbol{e}^{\mathrm{tr}}\|} - h\boldsymbol{e}^{\mathrm{tr}}$$

ELSE

Saturation step:

$$\boldsymbol{e}^{\mathrm{tr}} = \boldsymbol{e}_{PT2}^{\mathrm{tr}} = \epsilon_L\frac{\boldsymbol{e}_{PT1}^{\mathrm{tr}}}{\|\boldsymbol{e}_{PT1}^{\mathrm{tr}}\|}$$

Compute $\ell = \ell_{PT2}$ via Eq. $\ell_{PT2} = \left(-R_Y\frac{\boldsymbol{e}_{PT2}^{\mathrm{tr}} - \boldsymbol{e}_n^{\mathrm{tr}}}{\|\boldsymbol{e}_{PT2}^{\mathrm{tr}} - \boldsymbol{e}_n^{\mathrm{tr}}\|} + 2G\left(\boldsymbol{e} - \boldsymbol{e}_{PT2}^{\mathrm{tr}}\right) - f(\theta) - h\boldsymbol{e}_{PT2}^{\mathrm{tr}}\right) : \frac{\boldsymbol{e}_{PT2}^{\mathrm{tr}}}{\|\boldsymbol{e}_{PT2}^{\mathrm{tr}}\|}$

$$\boldsymbol{s} = 2G\left(\boldsymbol{e} - \boldsymbol{e}^{\mathrm{tr}}\right)$$
$$\boldsymbol{X} = \boldsymbol{s} - \left(f(\theta) + \ell\right)\frac{\boldsymbol{e}^{\mathrm{tr}}}{\|\boldsymbol{e}^{\mathrm{tr}}\|} - h\boldsymbol{e}^{\mathrm{tr}}$$

END IF

END IF

Scalet G., **Boatti E.**, Ferraro M., Mercuri V., Hartl D., Auricchio F.; paper submitted

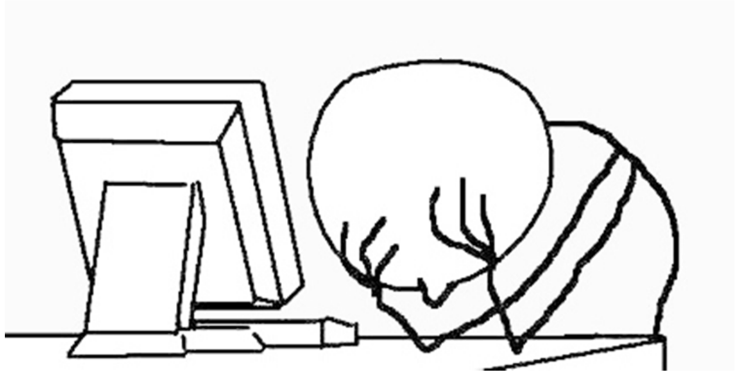
Semi-automatic subroutine generator

Problem: how to implement algorithms in commercial FEA software?

- Abaqus **user material subroutines** can be used to customize the material behavior
- UMAT for Abaqus Standard solver, VUMAT for Abaqus Explicit solver

Solution:

- FORTRAN → relatively lower-level computer language



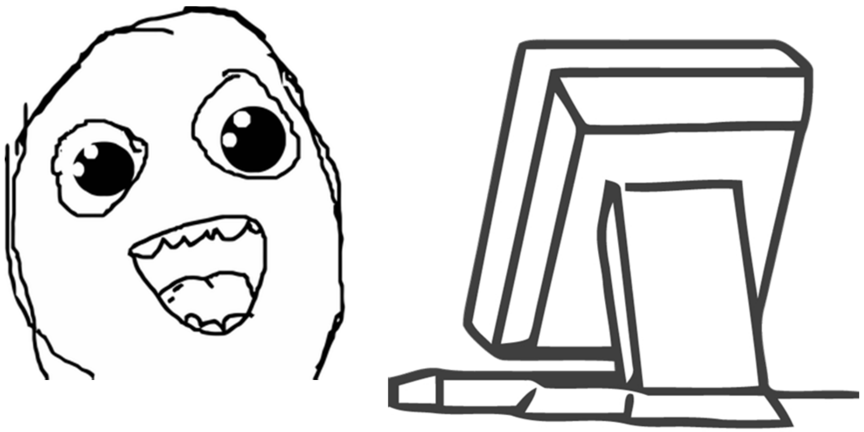
- **AceGen** → high-level intuitive and optimized language, very similar to Mathematica code

Korelc, *Theor. Comp. Science*, 1997
Korelc, *Eng. with Comp.*, 2002

Semi-automatic subroutine generator

- I developed a procedure for **semi-automatic UMAT/VUMAT generation**:

1. Write AceGen code
2. Perform optimized automatic translation of AceGen code into FORTRAN subroutine
3. Embed FORTRAN subroutine in UMAT/VUMAT user subroutine
4. Call UMAT/VUMAT in Abaqus analysis



Semi-automatic subroutine generator

```fortran
c-----------------------------------------------------------------------c
c        ******** UMAT USER SUBROUTINE ----> ELASTICITY ********        c
c                                                                       c
c           INPUT: material properties (PROPS), strain (STRAN)          c
c          OUTPUT: stress (STRESS), material tangent matrix (DDSDDE)    c
c                                                                       c
c                PROPS(1) = Young's Modulus                             c
c                PROPS(2) = Poisson's coefficient                       c
c                                                                       c
c-----------------------------------------------------------------------c
c-----------------------------------------------------------------------c
!  UMAT PARAMETERS
!
      SUBROUTINE UMAT(STRESS, STATEV, DDSDDE, SSE, SPC, SCD, RPL,DDSDDT,
     *                DRPLDE ,DRPLDT , STRAN, DSTRAN, TIME, DTIME, TEMP,
     *                DTEMP, PREDEF, DPRED, CMNAME, NDI, NSHR, NTENS,
     *                NSTATV, PROPS, NPROPS, COORDS, DROT, PNEWDT,
     *                CELENT, DFGRD0, DFGRD1, NOEL, NPT, LAYER, KSPT,
     *                KSTEP, KINC)
!
      implicit real*8(a-h,o-z)
      parameter (nprecd=2)
!      INCLUDE 'aba_param_dp.inc'
!
      CHARACTER*80 CMNAME
!
      DIMENSION STRESS(NTENS), STATEV(NSTATV), DDSDDE(NTENS,NTENS),
     *        DDSDDT(NTENS), DRPLDE(NTENS), STRAN(NTENS),
     *          DSTRAN(NTENS), TIME(2), PREDEF(1), DPRED(1),
     *          PROPS(NPROPS), COORDS(3), DROT(3,3), DFGRD0(3,3),
     *          DFGRD1(3,3)
```

UMAT HEADER

```fortran
c-----------------------------------------------------------------------c
!  SUBROUTINE PARAMETERS
!
      DIMENSION v(5001)
```

PARAMETERS OF THE AUTOMATICALLY GENERATED SUBROUTINE

```fortran
c-----------------------------------------------------------------------c
!  CALL OF ELASTICITY SUBROUTINE
!
      STRAN=STRAN+DSTRAN
!
      call Test(v,PROPS,STRAN,STRESS,DDSDDE)
```

CALL OF AUTOMATICALLY GENERATED SUBROUTINE

```fortran
c-----------------------------------------------------------------------c
!  END OF UMAT SUBROUTINE
      return
      end
c-----------------------------------------------------------------------c
!  ELASTICITY SUBROUTINE
      SUBROUTINE Test(v,matprop,ee,ss,DssDee)
      IMPLICIT NONE
      INTEGER i01,i02
      DOUBLE PRECISION v(5001),matprop(2),ee(6),ss(6),DssDee(6,6)
      v(33)=ee(1)+ee(2)+ee(3)
      v(32)=1d0/(1d0-2d0*matprop(2))
      v(31)=1d0/(1d0+matprop(2))
      v(34)=matprop(1)*v(31)
      v(15)=matprop(2)*v(32)*v(34)
      v(23)=v(15)*v(33)
      v(17)=v(34)/2d0
      v(27)=v(15)+v(34)
      ss(1)=v(23)+ee(1)*v(34)
      ss(2)=2d0*ee(2)*v(17)+v(23)
      ss(3)=v(23)+ee(3)*v(34)
        ...
```

AUTOMATICALLY GENERATED SUBROUTINE

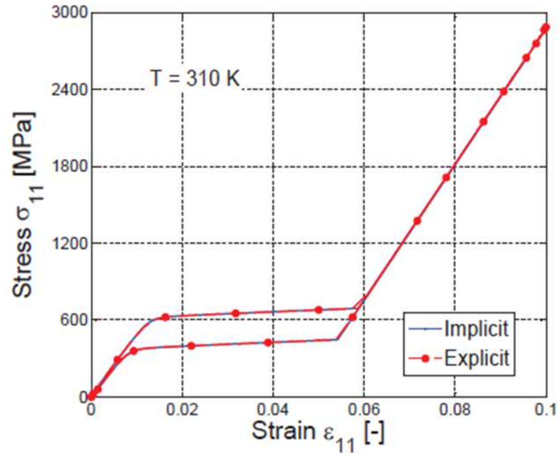
Comparison implicit vs explicit

Results

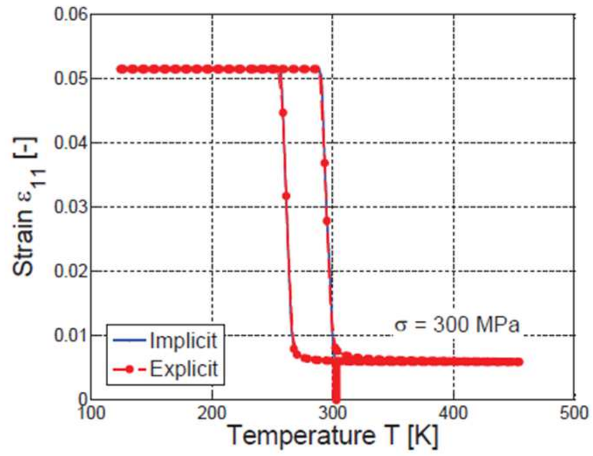
Uniaxial tests:

- superelasticity (1)
- temperature cycling (2)
- shape memory (3)

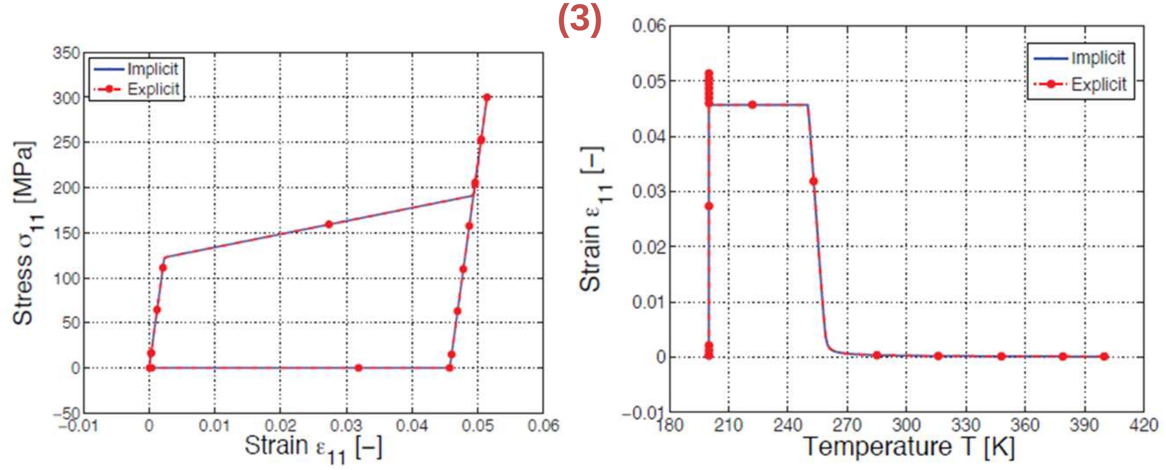
(1)



(2)

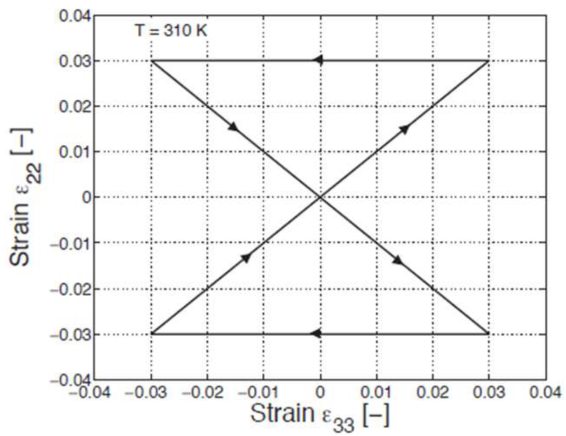


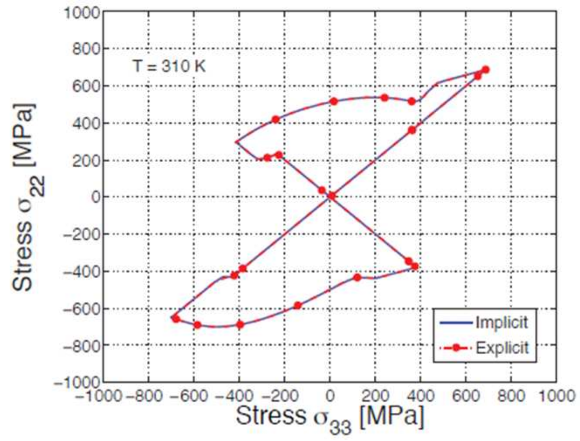
(3)



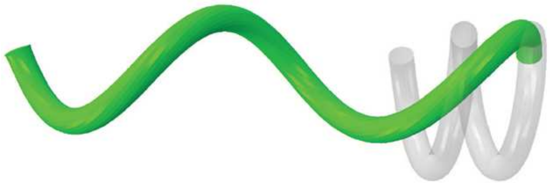
Comparison implicit vs explicit

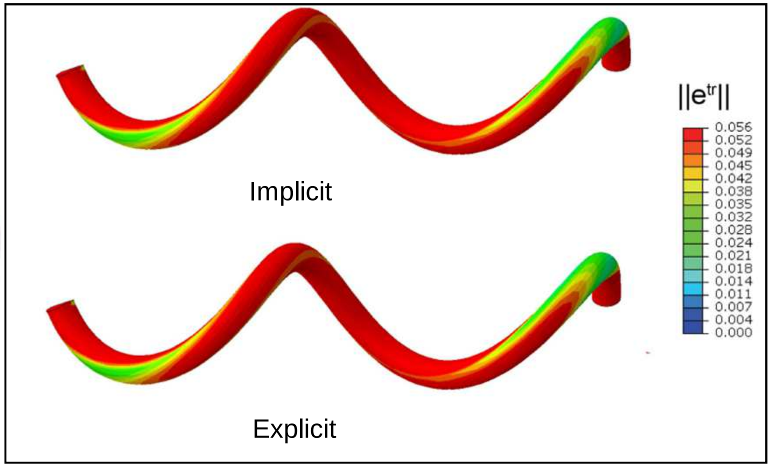
Biaxial hourglass test

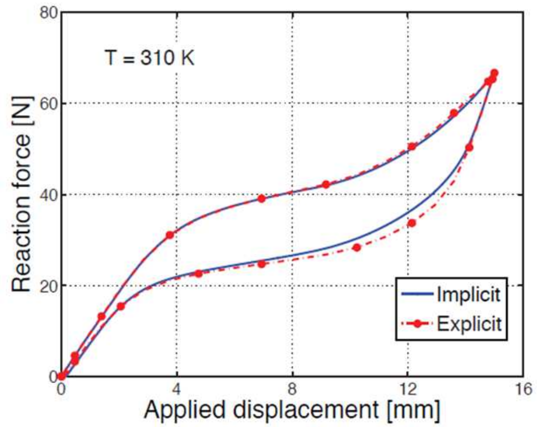




Pseudoelastic spring test

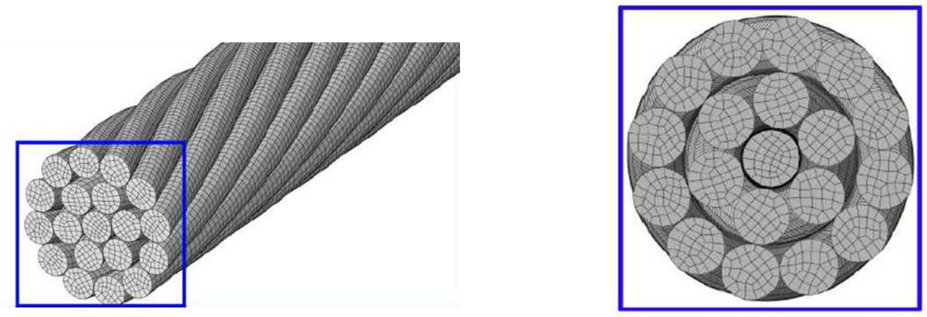


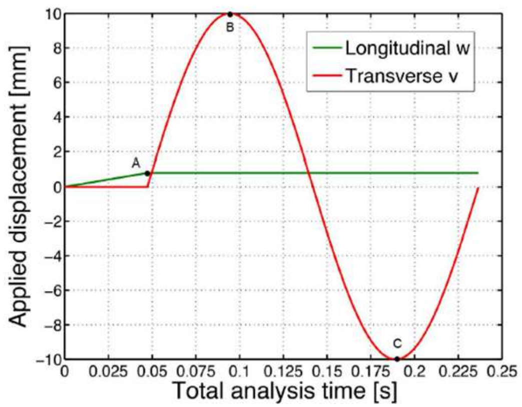


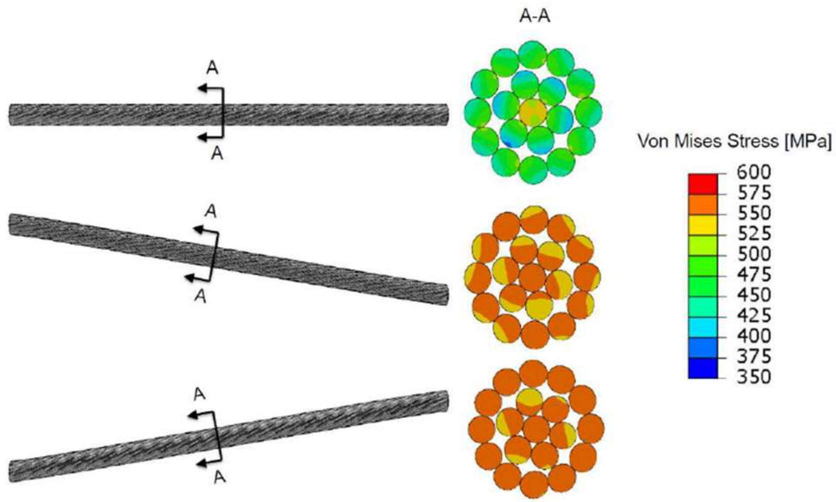


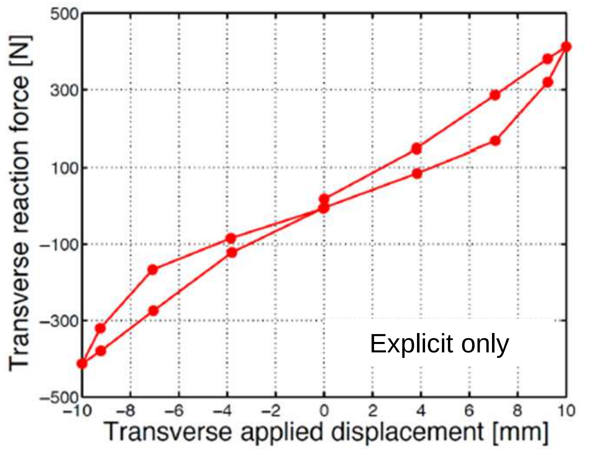
Comparison implicit vs explicit

Pseudoelastic cable test







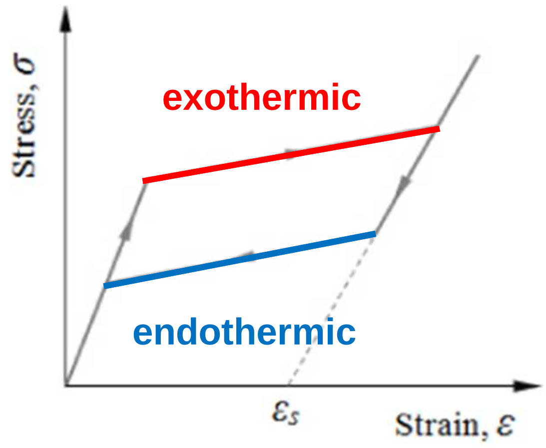


Implicit fails!

Gradient structures for SMA

(in collaboration with prof. Ulisse Stefanelli, University of Vienna)

Motivation:



- Full thermomechanical coupling: **exo- and endothermic effects** during transformations are taken into account

- New variational formulation based on the General Equations for Non-Equilibrium Reversible-Irreversible Coupling (GENERIC) formalism

$$\partial_{\dot{y}}\mathcal{K}(t, y; \dot{y}) - \partial\mathcal{S}(y) \ni \mathbf{0},$$

Full system:

$$\nabla \cdot \mathbb{C}(\boldsymbol{\varepsilon}(\boldsymbol{u}) - \boldsymbol{e}^{\mathrm{tr}}) + \boldsymbol{f} = \mathbf{0},$$

$$\left(c - \theta f''(\theta)\,|\boldsymbol{e}^{tr}|\right)\dot{\theta} + \nabla \cdot \boldsymbol{q} = R|\dot{\boldsymbol{e}}^{\mathrm{tr}}| + \theta f'(\theta)\,|\boldsymbol{e}^{\mathrm{tr}}|^{\cdot},$$

$$R\partial|\dot{\boldsymbol{e}}^{\mathrm{tr}}| + H\boldsymbol{e}^{\mathrm{tr}} + f(\theta)\partial|\boldsymbol{e}^{\mathrm{tr}}| + \partial I(\boldsymbol{e}^{\mathrm{tr}}) \ni 2G(\boldsymbol{e}(\boldsymbol{u}) - \boldsymbol{e}^{\mathrm{tr}})$$

- Semi-implicit time-discretization proved **unconditionally stable and convergent**

Auricchio F., **Boatti E.**, Reali A., Stefanelli U., *CMAME*, 2015

Gradient structures for SMA

Algorithm:

Starting data: $\{\boldsymbol{e}_i, \theta_i^{\rm e}\} \in \mathbb{R}^{3\times3}_{\rm dev} \times \mathbb{R}_+$ and $\{\boldsymbol{e}^{\rm tr}_{i-1}, \theta_{i-1}\} \in \mathbb{R}^{3\times3}_{\rm dev} \times \mathbb{R}_+$

Define $\boldsymbol{e}^{\rm tr}_{i,0} = \boldsymbol{e}^{\rm tr}_{i-1}$.

while $k \geq 1,\ |\theta_{i,k}-\theta_{i,k-1}|/\theta_{i,k} \geq tol,\ and\ |\boldsymbol{e}^{\rm tr}_{i,k}-\boldsymbol{e}^{\rm tr}_{i,k-1}|/|\boldsymbol{e}^{\rm tr}_{i,k}| \geq tol$ **do**

Solve the **thermal subproblem**
given $\{\theta_i^{\rm e}, \theta_{i-1}, \boldsymbol{e}^{\rm tr}_{i-1}\} \in \mathbb{R}_+ \times \mathbb{R}_+ \times \mathbb{R}^{3\times3}_{\rm dev}$ and $\boldsymbol{e}^{\rm tr}_{i,k-1} \in \mathbb{R}^{3\times3}_{\rm dev}$
find $\theta_{i,k} > 0$ solving

$$\gamma_\eta(\boldsymbol{y}_{i-1})\theta_i - \frac{\tau_i\lambda}{\theta_i} = -\frac{\tau_i\lambda}{\theta_i^{\rm e}} + \gamma_\eta(\boldsymbol{y}_{i-1})\theta_{i-1}$$
$$+ R_Y|\boldsymbol{e}^{\rm tr}_i - \boldsymbol{e}^{\rm tr}_{i-1}| + \theta_i f_*'(\theta_i)\partial|\boldsymbol{e}^{\rm tr}_i|_\eta{:}(\boldsymbol{e}^{\rm tr}_i - \boldsymbol{e}^{\rm tr}_{i-1})$$

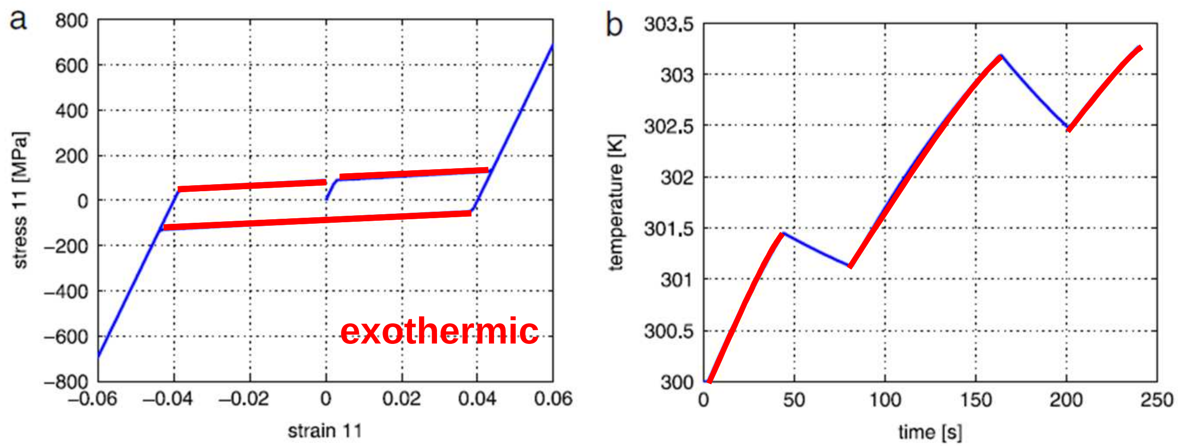
Solve the **mechanical subproblem**
given $\{\boldsymbol{e}_i, \theta_{i,k}\} \in \mathbb{R}^{3\times3}_{\rm dev} \times \mathbb{R}_+$ and $\boldsymbol{e}^{\rm tr}_{i-1} \in \mathbb{R}^{3\times3}_{\rm dev}$
find $\boldsymbol{e}^{\rm tr}_{i,k} \in \mathbb{R}^{3\times3}_{\rm dev}$ solving

$$R_Y\partial|\boldsymbol{e}^{\rm tr}_i - \boldsymbol{e}^{\rm tr}_{i-1}| + (H+2G)\boldsymbol{e}^{\rm tr}_i + f(\theta_i)\partial|\boldsymbol{e}^{\rm tr}_i| \ni 2G\boldsymbol{e}_i$$

end

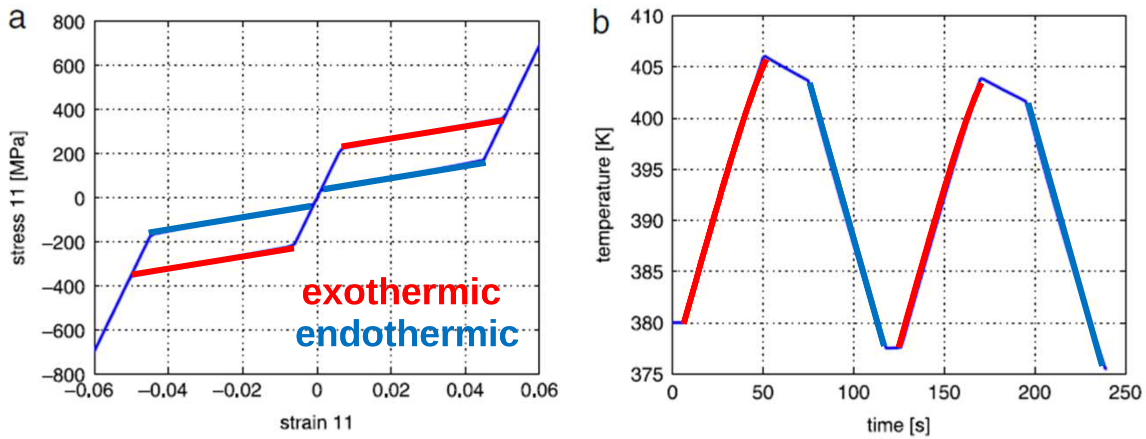
Gradient structures for SMA

Martensitic condition:



$$\vartheta_e = \vartheta_0 = 300\ K$$

Austenitic condition:



$$\vartheta_e = \vartheta_0 = 380\ K$$

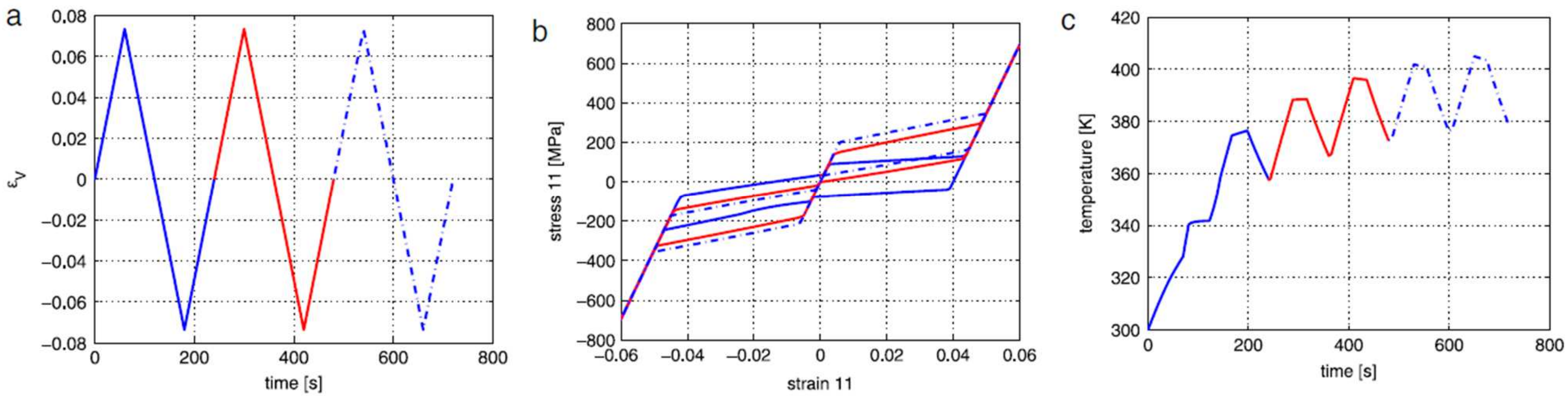
Gradient structures for SMA

Material parameters

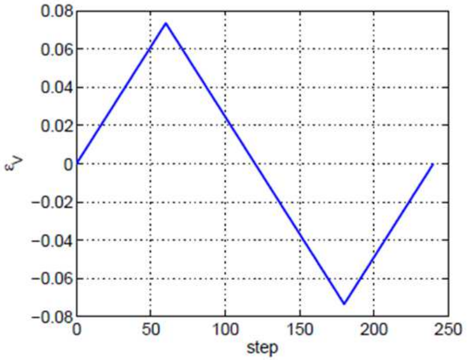
Symbol	Value	Unit	Description
E	45 000	MPa	Young's modulus
ν	0.3	–	Poisson's coefficient
K	37 500	MPa	Bulk modulus
G	17 308	MPa	Shear modulus
R	110	MPa	Critical stress
β	4.49	MPa/K	Coefficient of function f
H	1000	MPa	Hardening constant
θ_{tr}	343	K	Martensite finish temperature
ϵ_L	0.049	–	Saturation strain limit
θ_0	300	K	Initial temperature
θ^e	390	K	External temperature
c	3.22	MPa/K	Specific heat
λ	2×10^3	(MPa K)/s	Heat exchange coefficient
ρ	31	K	Parameter in the definition of f
tol	10^{-6}	–	Tolerance

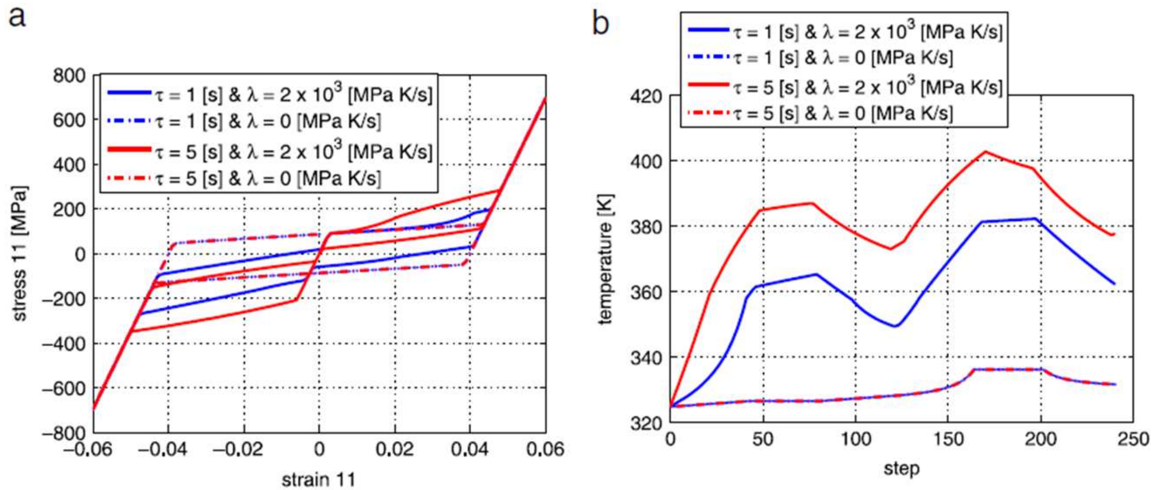
Gradient structures for SMA

3 tractions/compressions:



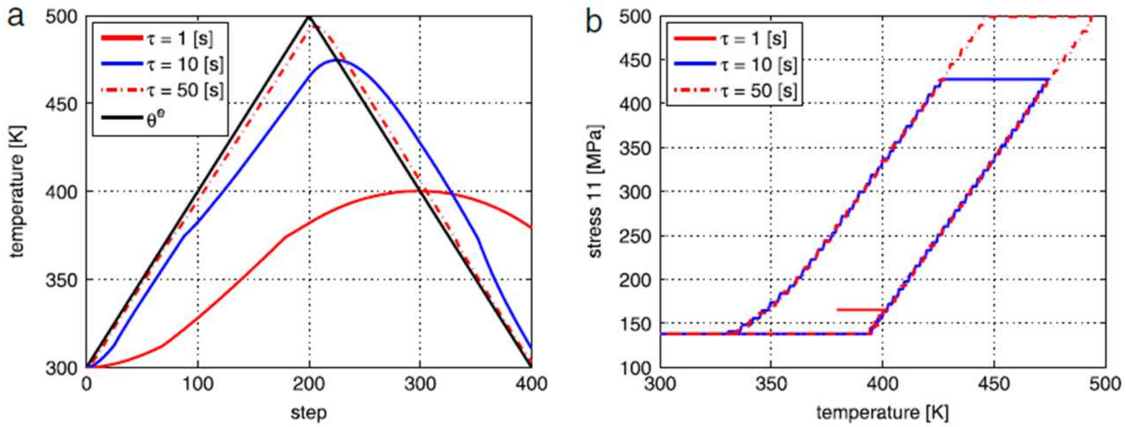
Traction/compression test with varying *step time* and *heat exchange coefficient*:





Gradient structures for SMA

External temperature increase/decrease at constant strain:



Part 2
Shape memory polymers

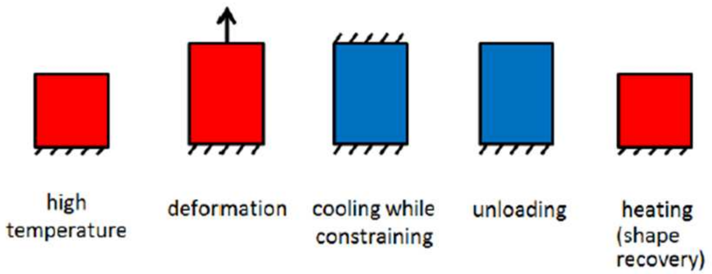
UNIVERSITÀ DI PAVIA DICAr

IUSS Scuola Universitaria Superiore Pavia

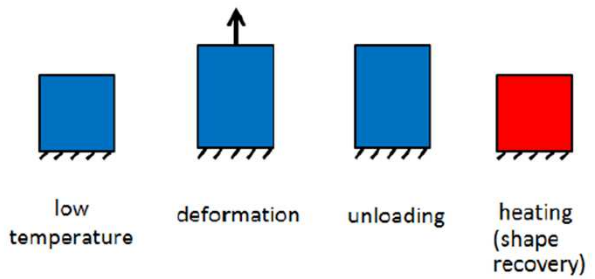
SMP properties

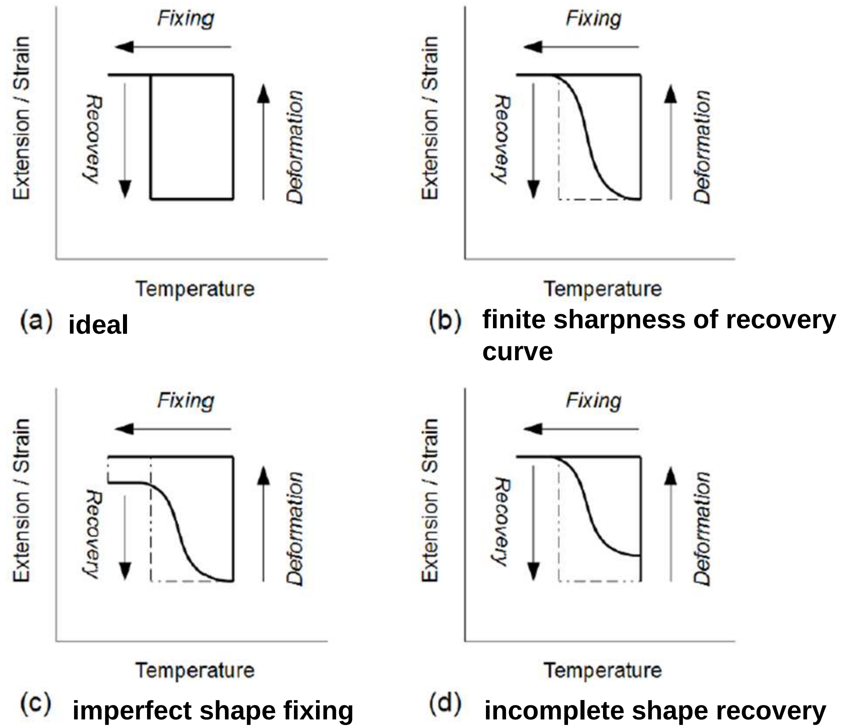
- Ability to store a **temporary** shape and to recover their **original** shape upon an external stimulus
- Thermo-responsive SMP are the most common: physical or chemical switches activate/deactivate according to temperature
- Shape-fixing procedure + heating to trigger shape recovery

1) high-temperature shape fixing + recovery



2) low-temperature shape fixing + recovery

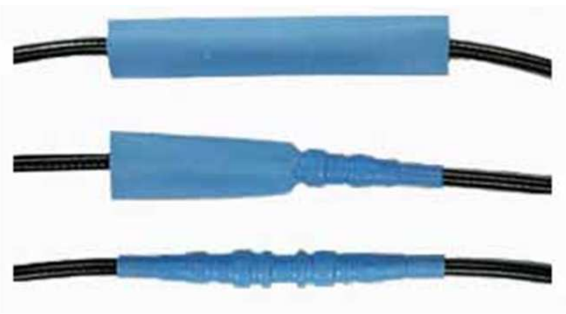


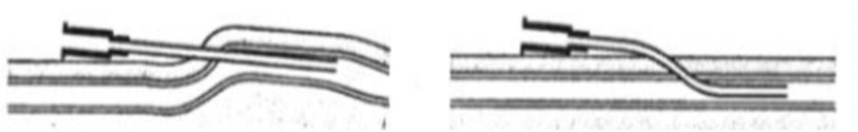


SMP applications

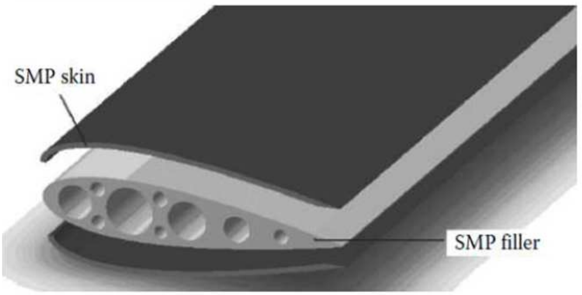
- Applications in different fields:

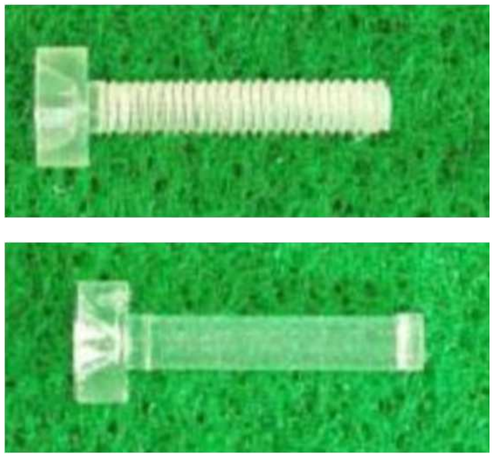
  - Heat shrinkable tubes
  - Toys and items
  - Soft grippers
  - Smart fabrics
  - Cardiovascular stents
  - Wound closure stitches
  - Drug delivery systems
  - Damping systems
  - Deployable and morphing structures
  - Food packaging
  - Fasteners
  - …

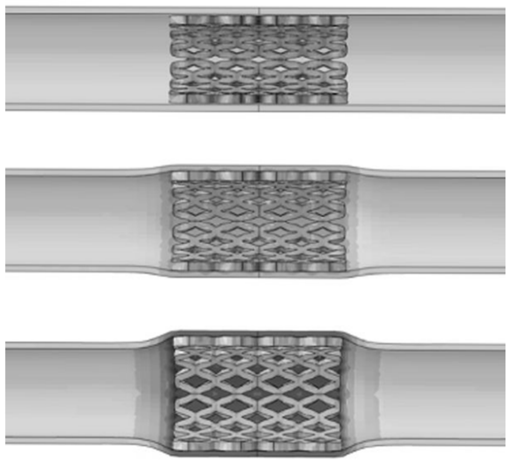




Intravenous syringe cannula







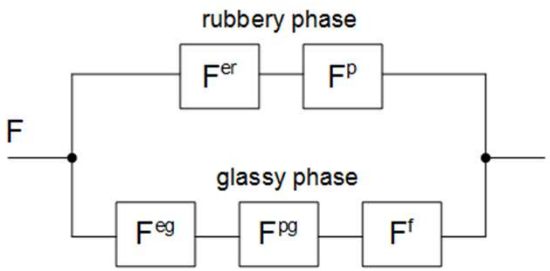
3D finite-strain model for SMP

- Modeling routes: standard thermo-viscoelastic models, or phenomenological models based on the concept of phase transition

<u>New 3D finite-strain phenomenological model for SMP</u>

Continuous formulation

Decompositions:



$$\mathbf{F} = \mathbf{F}^g \mathbf{F}^f$$

frozen deformation

$$\mathbf{F}^g = \mathbf{F}^{eg} \mathbf{F}^{pg}$$

glassy phase deformation

$$\mathbf{F} = \mathbf{F}^r \mathbf{F}^p$$

permanent deformation

$$\mathbf{F}^r = \mathbf{F}^{er}$$

rubbery phase deformation

- the frozen deformation gradient models the amount of deformation stored during the high-temperature shape fixing
- the glassy phase deformation gradient is divided into an elastic part and a plastic part; the plastic part represents the amount of deformation stored during the low-temperature shape fixing
- the permanent deformation gradient represents the irrecoverable deformation and therefore it simulates the incomplete shape recovery
- the deformation gradient of the rubbery phase is purely elastic

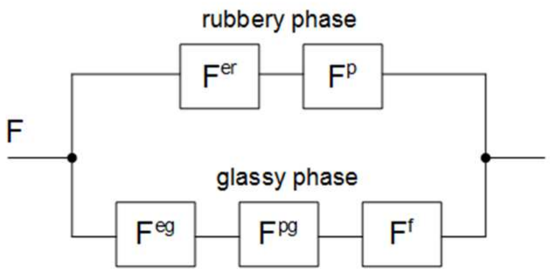
3D finite-strain model for SMP

- Modeling routes: standard thermo-viscoelastic models, or phenomenological models based on the concept of phase transition

New 3D finite-strain phenomenological model for SMP

Continuous formulation

Decompositions:



$$\mathbf{F} = \mathbf{F}^g \mathbf{F}^f$$

frozen deformation

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glassy phase deformation

$$\mathbf{F} = \mathbf{F}^r \mathbf{F}^p$$

permanent deformation

$$\mathbf{F}^r = \mathbf{F}^{er}$$

rubbery phase deformation

Free energy:

$$\Psi = z^g \Psi^g + (1 - z^g) \Psi^r$$

$$\Psi^g = \Psi^{eg} + \Psi^{pg}$$

$$\Psi^{pg} = \frac{1}{2} h \|\mathbf{E}^{pg}\|^2$$

$$\Psi^{eg} = \frac{\lambda^g}{2} [\mathrm{tr}\,(\mathbf{E}^{eg})]^2 + \mu^g \mathrm{tr}\,(\mathbf{E}^{eg2})$$

$$\Psi^r = \Psi^{er}$$

$$\Psi^{er} = \frac{\lambda^r}{2} [\mathrm{tr}\,(\mathbf{E}^{er})]^2 + \mu^r \mathrm{tr}\,(\mathbf{E}^{er2})$$

3D finite-strain model for SMP

Input variables: θ $\mathbf{F}$

State variables: z^g $\mathbf{F}^{pg}$ $\mathbf{F}^f$ $\mathbf{F}^p$

Evolution equations:

$$z^g = \begin{cases} 1 & \text{if } \theta \leq \theta_t - \Delta\theta \\ \dfrac{1}{1+\exp\left[2w\left(\theta-\theta_t\right)\right]} & \text{if } \theta_t - \Delta\theta < \theta < \theta_t + \Delta\theta \\ 0 & \text{if } \theta \geq \theta_t + \Delta\theta \end{cases}$$

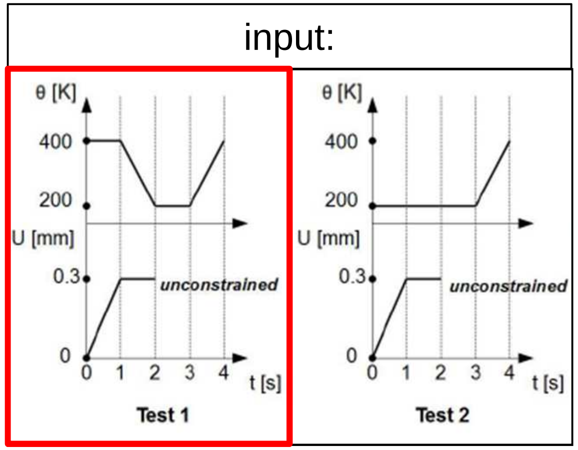
$$\mathbf{F}^{pg} = \begin{cases} \text{evolves according to assigned flow rule} & \begin{array}{c} \text{if} \quad \theta \leq \theta_t - \Delta\theta \\ \text{OR} \\ \text{if} \quad \theta_t - \Delta\theta < \theta < \theta_t + \Delta\theta \quad \text{and} \quad \dot{\theta} < 0 \end{array} \\ \mathbb{1} & \text{otherwise} \end{cases}$$

$$\mathbf{F}^f = \begin{cases} \boxed{c}\,(\mathbf{F} - \mathbb{1}) + \mathbb{1} & \text{if} \quad \theta > \theta_t + \Delta\theta \\ \text{constant} & \text{otherwise} \end{cases}$$

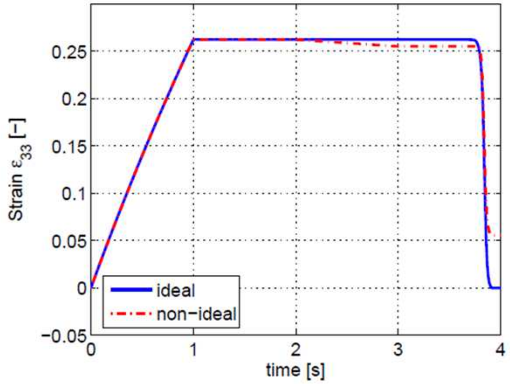
$$\mathbf{F}^p = \begin{cases} \boxed{c^p}\,(\mathbf{F}^f + \mathbf{F}^{pg} - 2\cdot\mathbb{1}) + \mathbb{1} & \text{if} \quad \{\, \theta \leq \theta_t + \Delta\theta \quad \text{and} \quad \|\mathbf{E}^p\|^{\cdot} \geq 0 \,\} \\ \text{constant} & \text{otherwise} \end{cases}$$

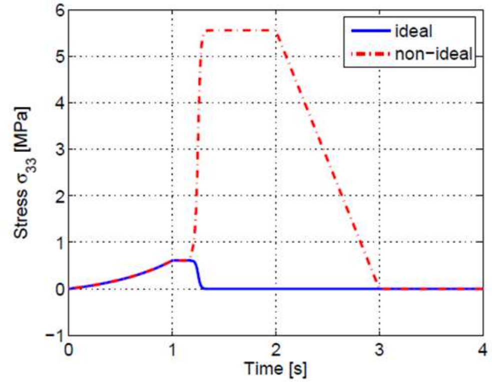
Boatti E., Scalet G., Auricchio F., under review

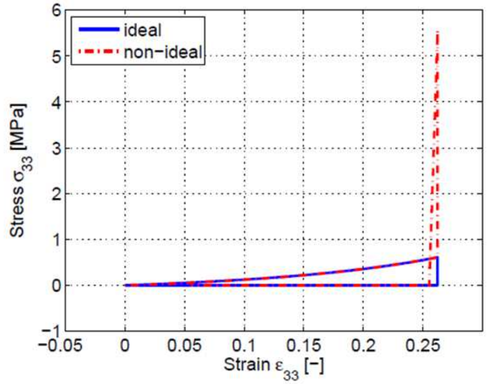
SMP numerical test: uniaxial

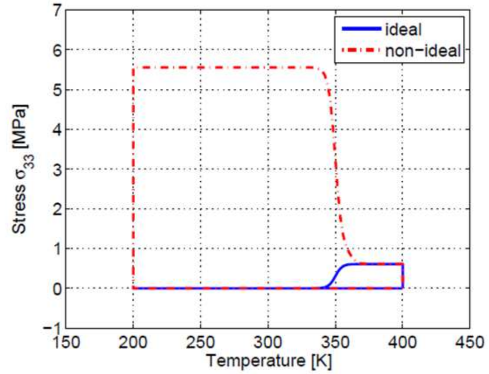


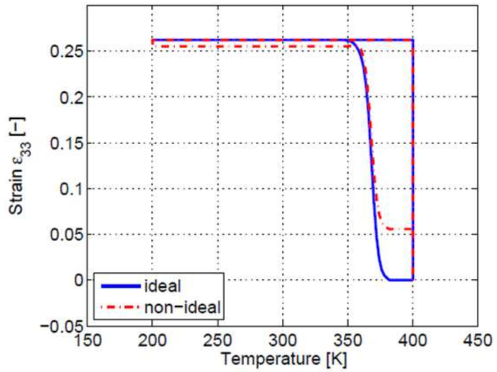
High temp. shape fixing



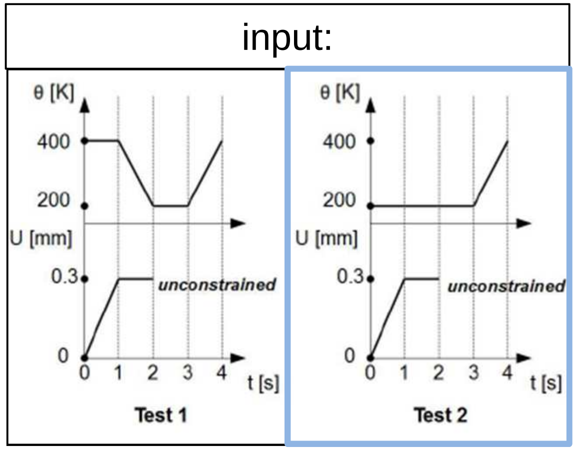




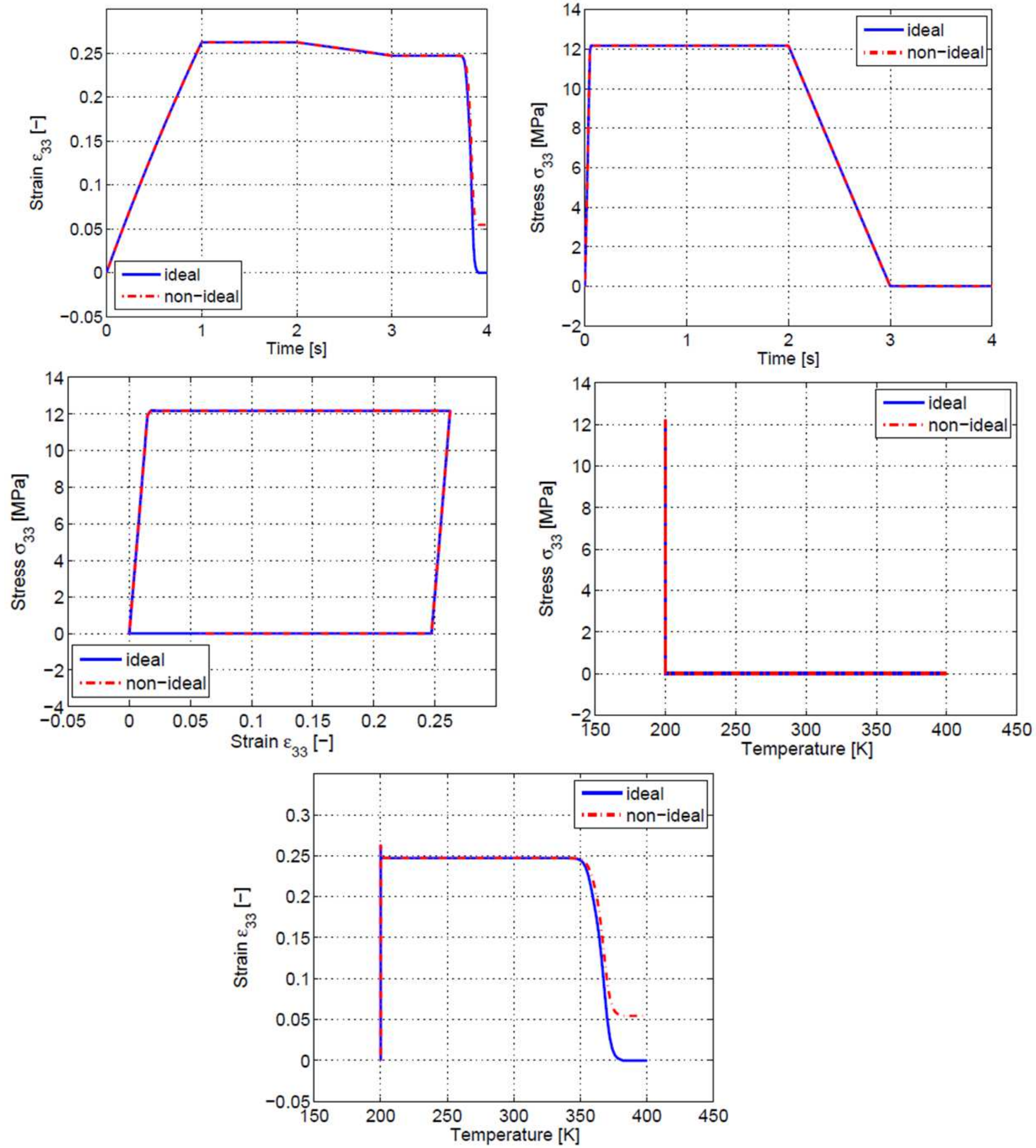




SMP numerical test: uniaxial

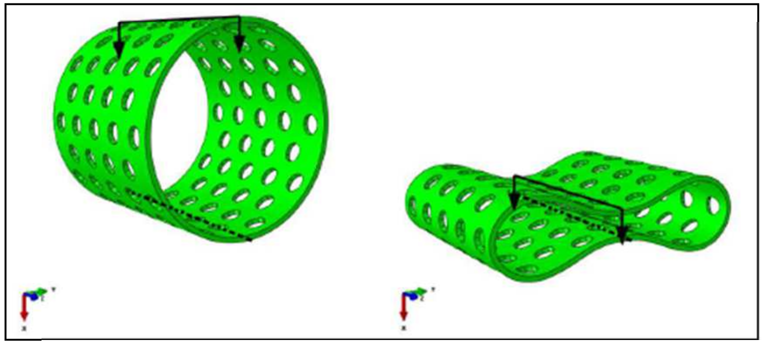


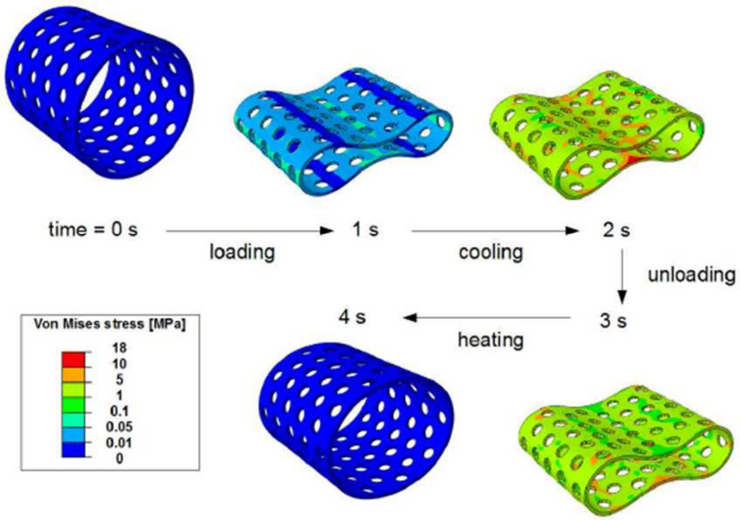
Low temp. shape fixing

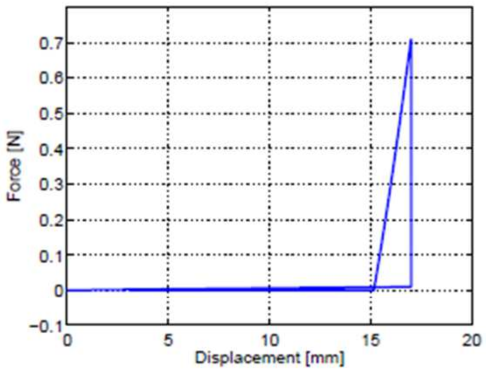


SMP numerical test: stent

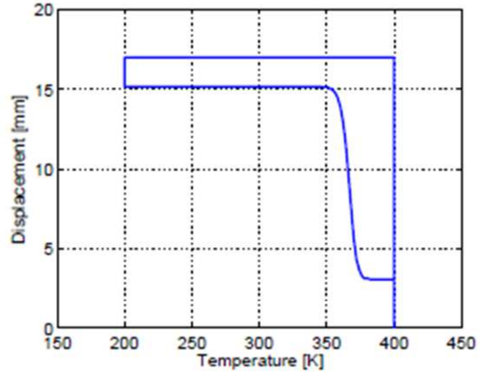
(non-ideal)



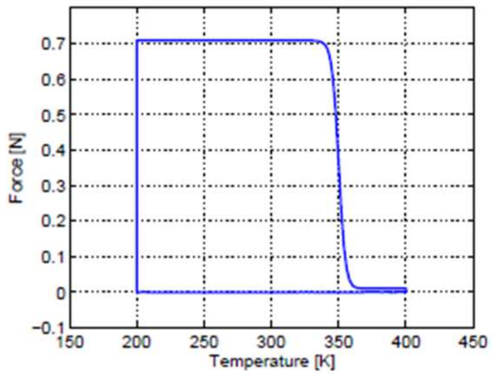




(a)



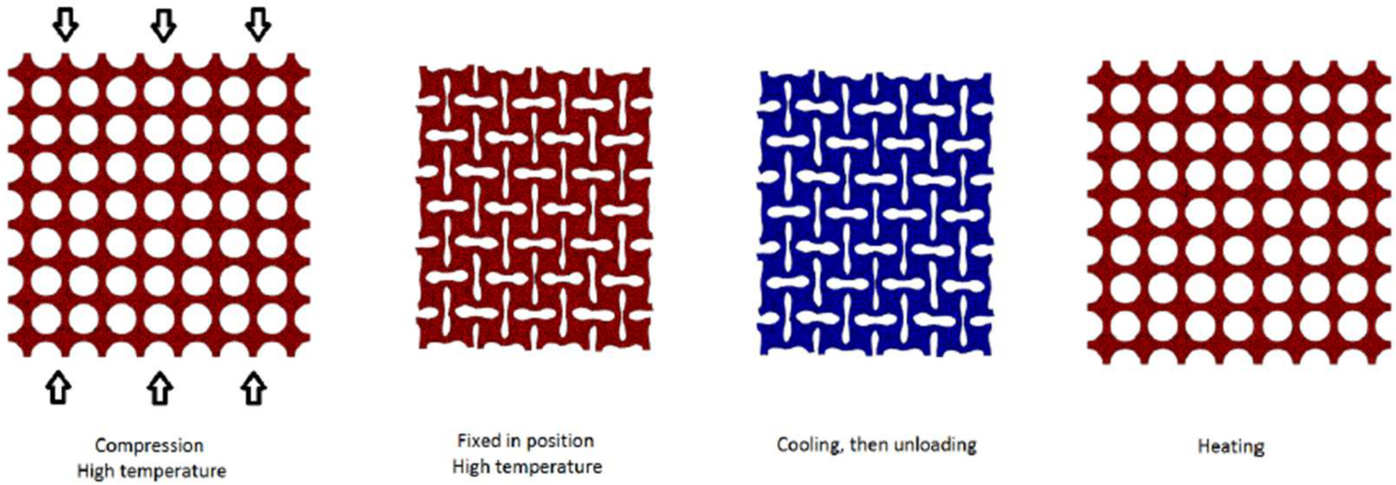
(b)

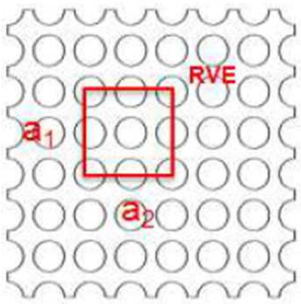


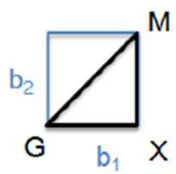
(c)

SMP numerical test: phononic crystal

Tunable phononic crystals (in collaboration with prof. Katia Bertoldi, Harvard University)







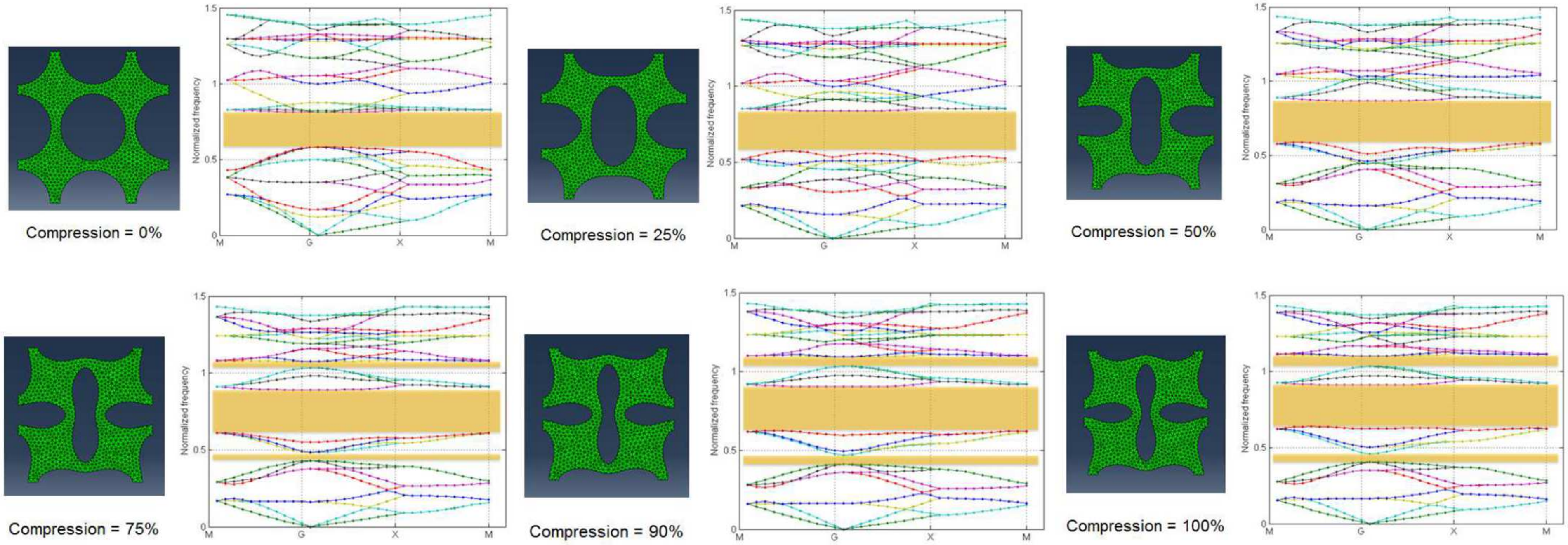
$$b_1 = 2\pi \frac{a_2 \times z}{\|z\|^2}$$

$$b_2 = 2\pi \frac{z \times a_1}{\|z\|^2}$$

$$z = a_1 \times a_2$$

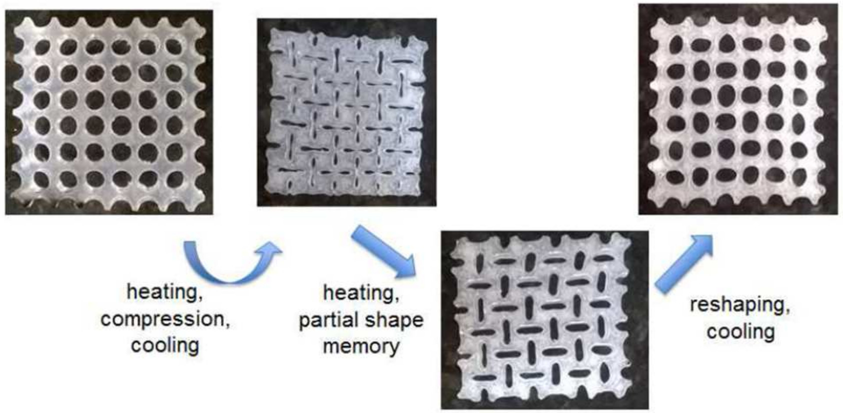
- RVE and irreducible Brillouin zone in the reciprocal lattice

SMP numerical test: phononic crystal



- Dispersion diagrams obtained through the Bloch wave analysis
- The band gaps change with compression
- We have a tunable wave filter

Experiments:



Conclusions

- New modeling and algorithmic tools have been proposed for SMA and SMP
- A fast and effective semi-automatic procedure to create user material subroutine for ABAQUS has been presented
- The possibility to simulate real-life applications has been demonstrated

Related publications:

- Auricchio F., **Boatti E.**, Conti M. “SMA biomedical applications”, Chapter 11 in *Shape memory alloy engineering: for aerospace, structural and other applications,* editors: A. Concilio, L. Lecce, publisher: Elsevier, 2014
- Auricchio F., **Boatti E.**, Conti M. “SMA cardiovascular applications and computer-based design”, Chapter 12 in *Shape memory alloy engineering: for aerospace, structural and other applications*, editors: A. Concilio, L. Lecce, publisher: Elsevier, 2014
- Ferraro M., Auricchio F., **Boatti E.**, Scalet G., Conti M., Morganti S., Reali A. “An efficient finite element framework to assess flexibility performances of SMA self-expandable carotid artery stents”, Journal of Functional Biomaterials, 2015
- Auricchio F., **Boatti E.**, Reali A., Stefanelli U. “Gradient structures for the thermomechanics of shape-memory materials”, CMAME, 2015
- Scalet G., **Boatti E.**, Ferraro M., Mercuri V., Hartl D., Auricchio F. “Explicit finite element implementation of a shape memory alloy constitutive model and associated analyses”, submitted
- **Boatti E.**, Scalet G., Auricchio F. “A three-dimensional finite-strain phenomenological model for shape-memory polymers: formulation, numerical simulations, and comparison with experimental data”, under review

Future developments

- Develop the finite-strain version of the SMA fully-coupled thermomechanical model
- Extend the SMA fully-coupled thermomechanical model implementation to the space non-homogeneous case
- Test the explicit algorithm of SMA Souza-Auricchio model in dynamic conditions
- Improve the phenomenological SMP consitutive model by adding viscoelastic effects

…

Thank you