

THE NEXT GENERATION OF SHAPE MEMORY ALLOY FEA MODELS: DEVELOPMENT OF A USER MATERIAL SUBROUTINE FOR IMPROVED SIMULATION OF TRANSFORMATION-PLASTICITY COUPLING EFFECTS

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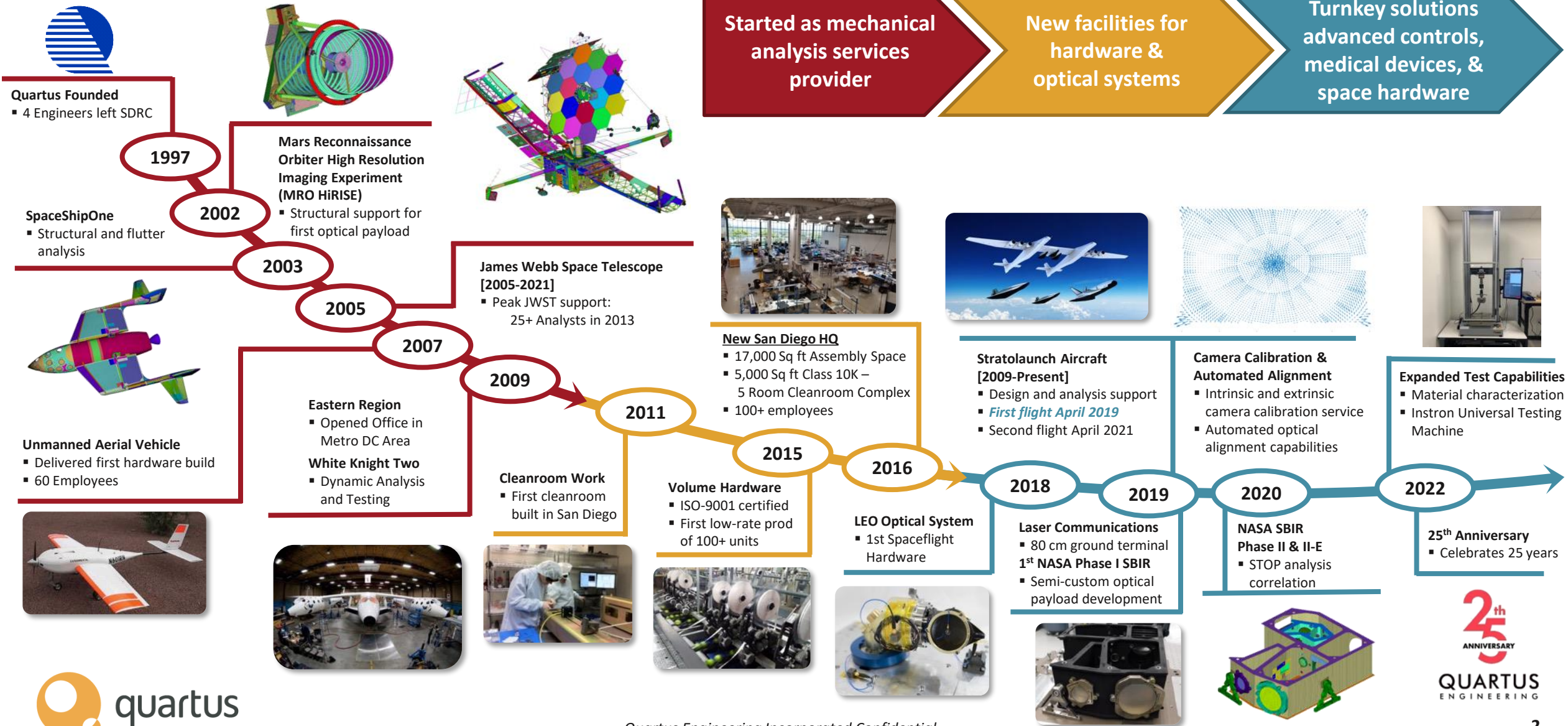
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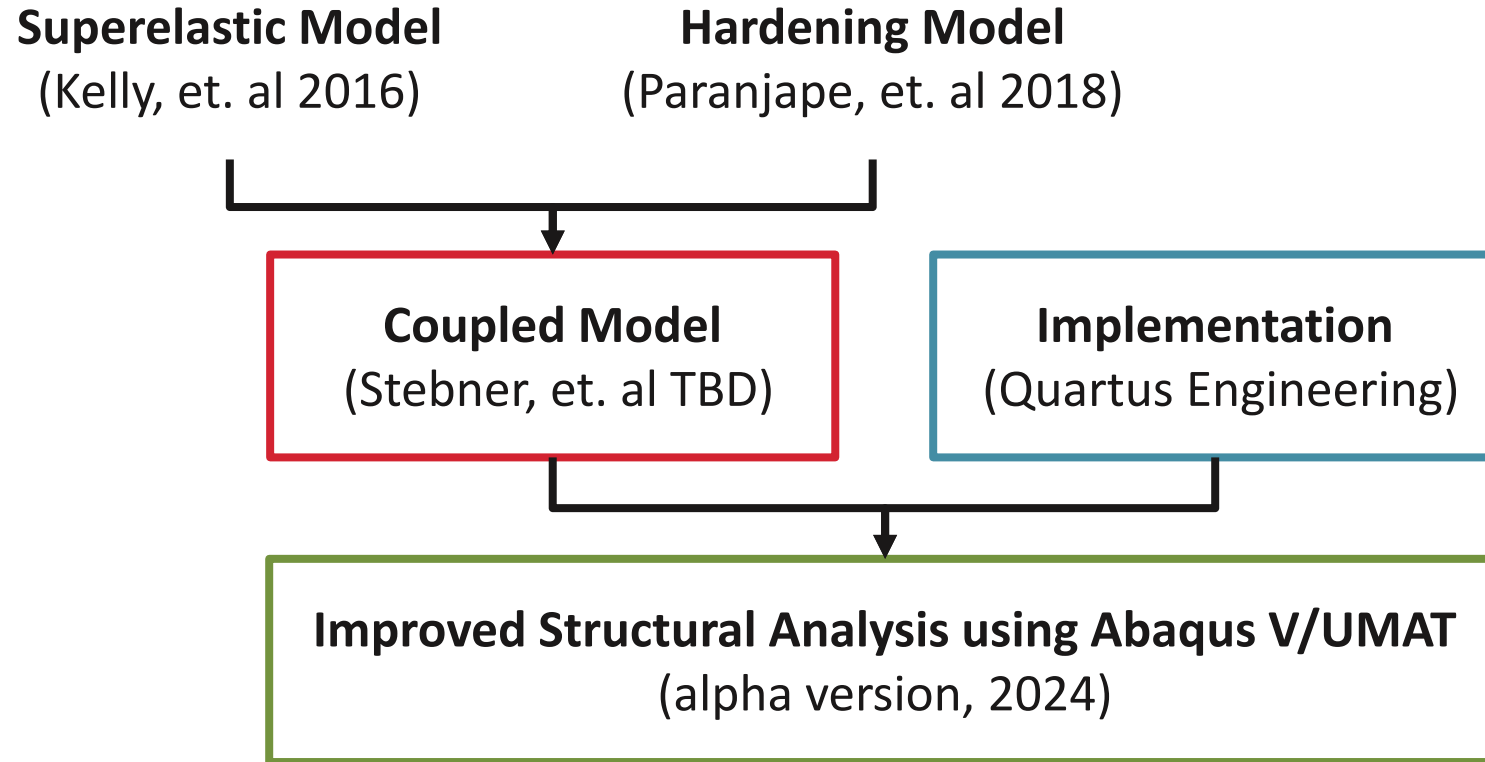
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WHO IS QUARTUS?



NEW MODEL TO IMPROVE STRUCTURAL ANALYSIS OF SHAPE MEMORY ALLOYS



COUPLED MODEL: FEATURES

Nonlinear minimization problem:

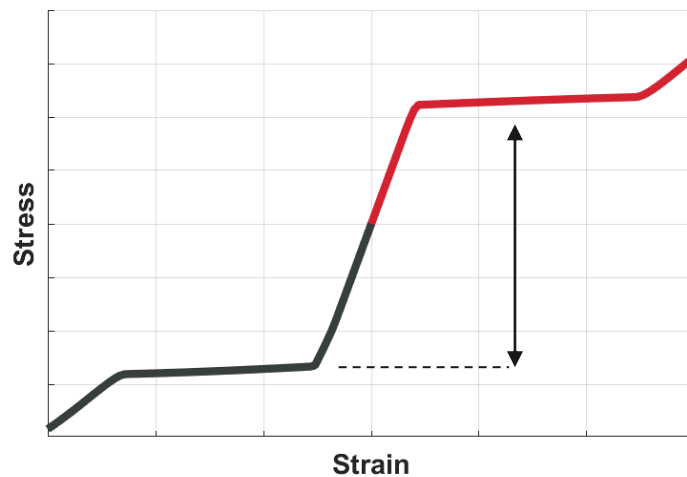
$$\frac{\partial W}{\partial U} - \frac{\partial D}{\partial \dot{U}} \in 0$$

Growth kinetics:

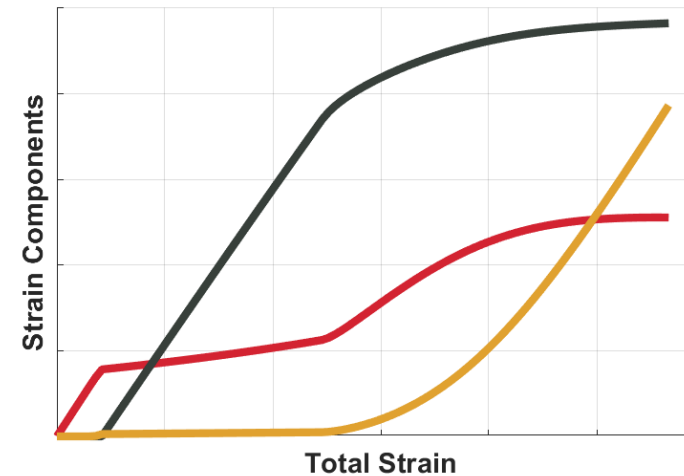
$$D = d_\lambda^{cr} |\dot{\lambda}| + \lambda d_{\varepsilon_m}^{cr} |\dot{\varepsilon}_m|$$

Gibb's Free Energy:

$$W = \frac{1}{2}(\varepsilon - \lambda\varepsilon_m - \varepsilon_p) : C(\lambda) : (\varepsilon - \lambda\varepsilon_m - \varepsilon_p) + \lambda L \frac{\theta - \theta_c}{\theta_c} - c_p(\lambda)\theta \ln\left(\frac{\theta}{\theta_c}\right) + \lambda g_i(\varepsilon_m) + g_s(\lambda\varepsilon_m) + g_\lambda(\lambda) + g_h(a, r) + g_c(\lambda\varepsilon_m, \varepsilon_p)$$



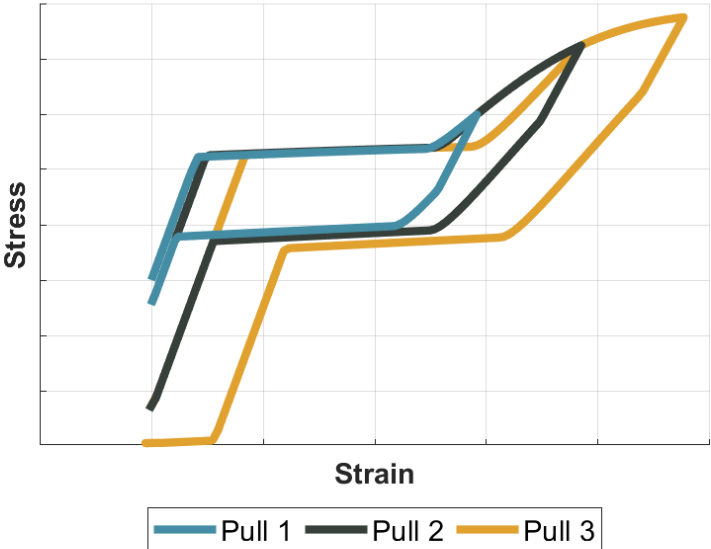
— Tension — Compression



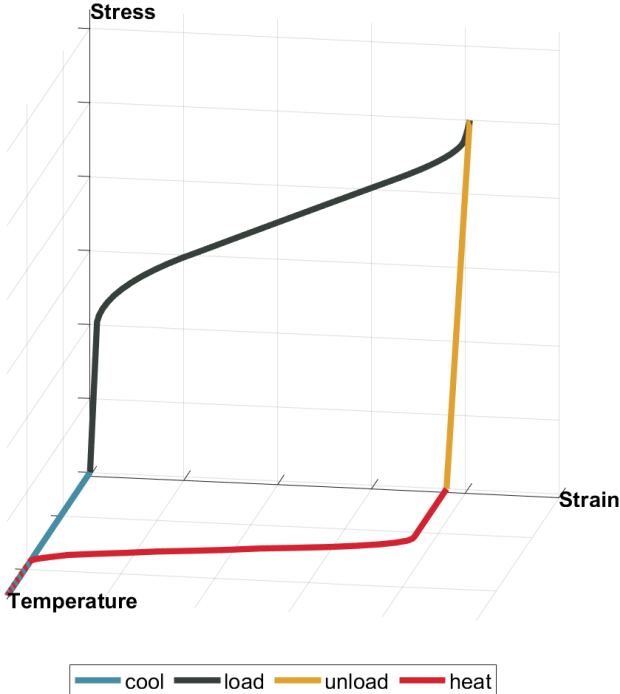
— Elastic — Transformation — Plastic

COUPLED MODEL: CAPABILITIES

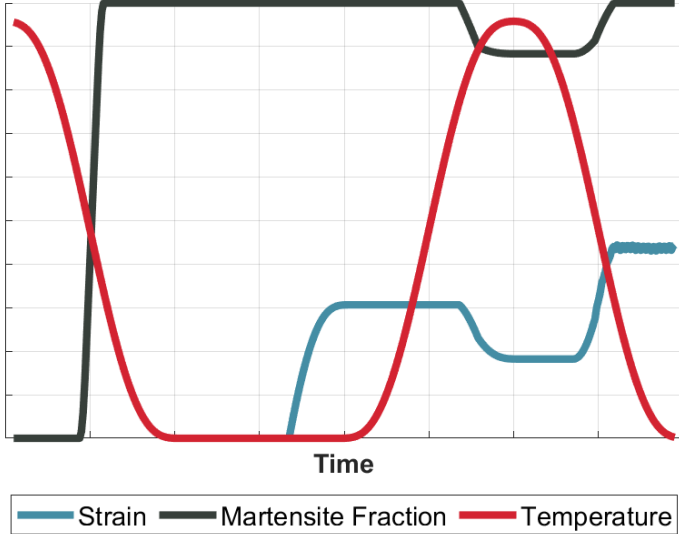
Superelasticity and Stress Ratcheting



Shape Memory



Actuation



IMPLEMENTATION: SOLVING THE PROBLEM

Formulation constrained optimization problem:

Use Intel MKL TRNLSP unconstrained optimization solver

1. Formulate the Lagrange equation based on which state variables are evolving

Predictor:

1. Incoming strain increment is assumed to be elastic
 - Evaluate intermediate stress state
 - Evaluate derivative of free energy
2. Check for inelastic evolution

Corrector:

1. Solve the nonlinear constrained optimization problem
 - Seed the nonlinear solver with elastic state variable results
 - If any constraints are violated, update and resolve new set of equations
2. Return stress and state at end of increment!

The constrained optimization problem:

$$\text{minimize} \quad \frac{\partial W}{\partial U} - \frac{\partial D}{\partial \dot{U}}$$

$$\text{subjected to} \quad \text{trace}(\varepsilon_m) = 0$$

$$g_i \leq 0$$

$$0 \leq \lambda \leq 1$$

$$\frac{\partial W}{\partial \lambda} \dot{\lambda} \geq 0$$

$$\frac{1}{\lambda} \frac{\partial W}{\partial \varepsilon_m} : \dot{\varepsilon}_m \geq 0$$

$$\Lambda \geq 0$$

$$\text{Stress} \quad \frac{\partial W}{\partial \varepsilon} = \sigma = \mathbb{C} : (\varepsilon - \lambda \varepsilon_m - \varepsilon_p)$$

$$\text{Phase evolution} \quad \dot{\lambda} = 0 \text{ for } \left| \frac{\partial W}{\partial \lambda} \right| < d_\lambda^{cr}$$

$$\dot{\varepsilon}_m = 0 \text{ for } \left| \frac{1}{\lambda} \frac{\partial W}{\partial \varepsilon_m} \right| < d_{\varepsilon_m}^{cr}$$

$$\text{Hardening evolution} \quad U_h = 0 \text{ for } \Lambda U_h \cdot \frac{dU_h}{dU_h} < 1$$

IMPLEMENTATION: USABILITY AND ORGANIZATION

- Custom types and interfaces are implemented to perform tensor operations like standard elementary coding math operations which reduces implementation errors and improves readability.

$$A: B = A_{ij}B_{ij}$$

A.ddot.B

$$A: C = A_{ij}B_{ijkl}$$

A.ddot.C

$$\bar{A} = A_{ij} - \frac{1}{3}A_{kk}$$

dev(A)

$$g_c = -k|\varepsilon_p|^m \varepsilon_p: \lambda \varepsilon_m$$

-k*mag(ep)**m * (ep.ddot.(lam*em))

- Code is modular to improve reusability and organization

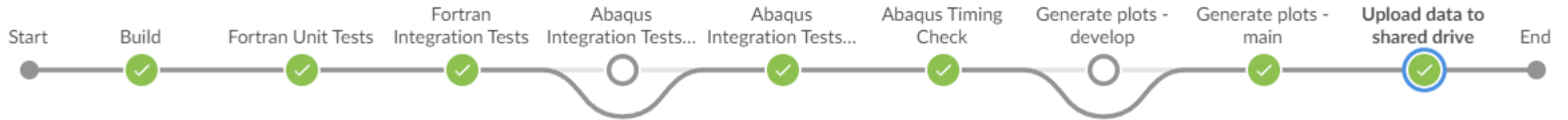
use tensor

use math, only : minimize

use hypersurfaces, only : coupling

IMPLEMENTATION: QA TESTING

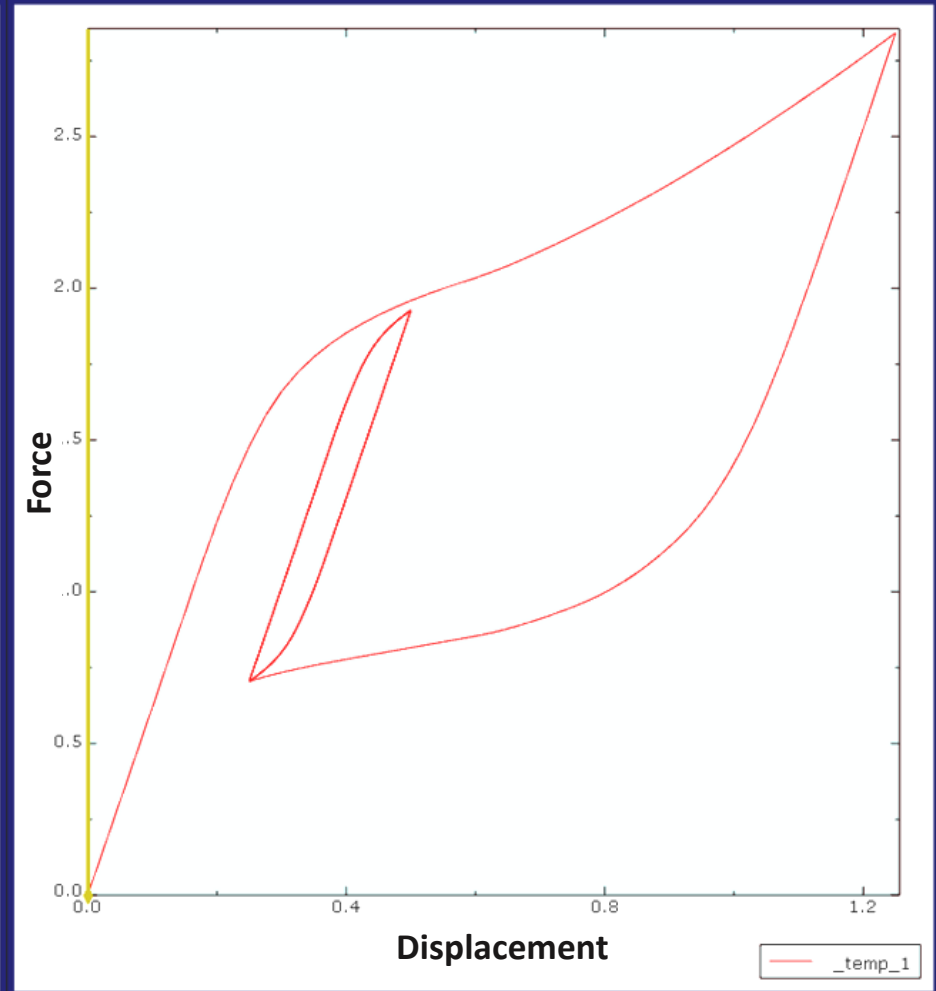
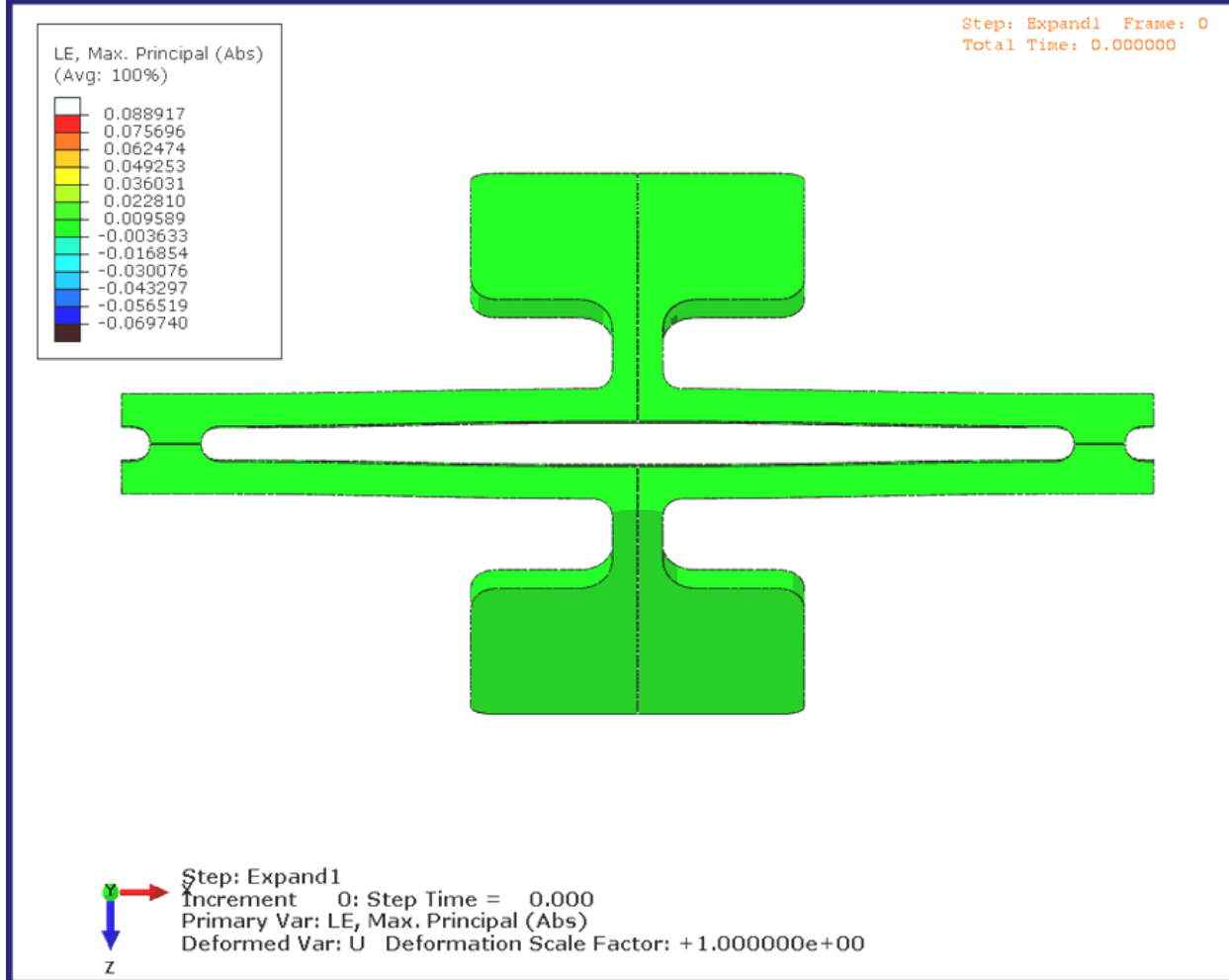
- Testing, automated in Jenkins



- **Build Test:** No compile errors
 - **Fortran Unit Tests:** Individual functions are tested for correctness
 - **Fortran Integration Tests:** Select cases are tested against an analytical solution
 - **FEA (Abaqus) Integration Tests:** Select cases are tested against an analytical solution for a unit cube
 - **Abaqus Timing:** ensure code changes did not make the code slower
 - **Generate plots:** archive results
- Additional testing
 - Arbitrary inputs (strain, stress, temperature, material constants) can be generated with a simple json input file and be used to compute an analytical solution and compare against Fortran/Abaqus depending

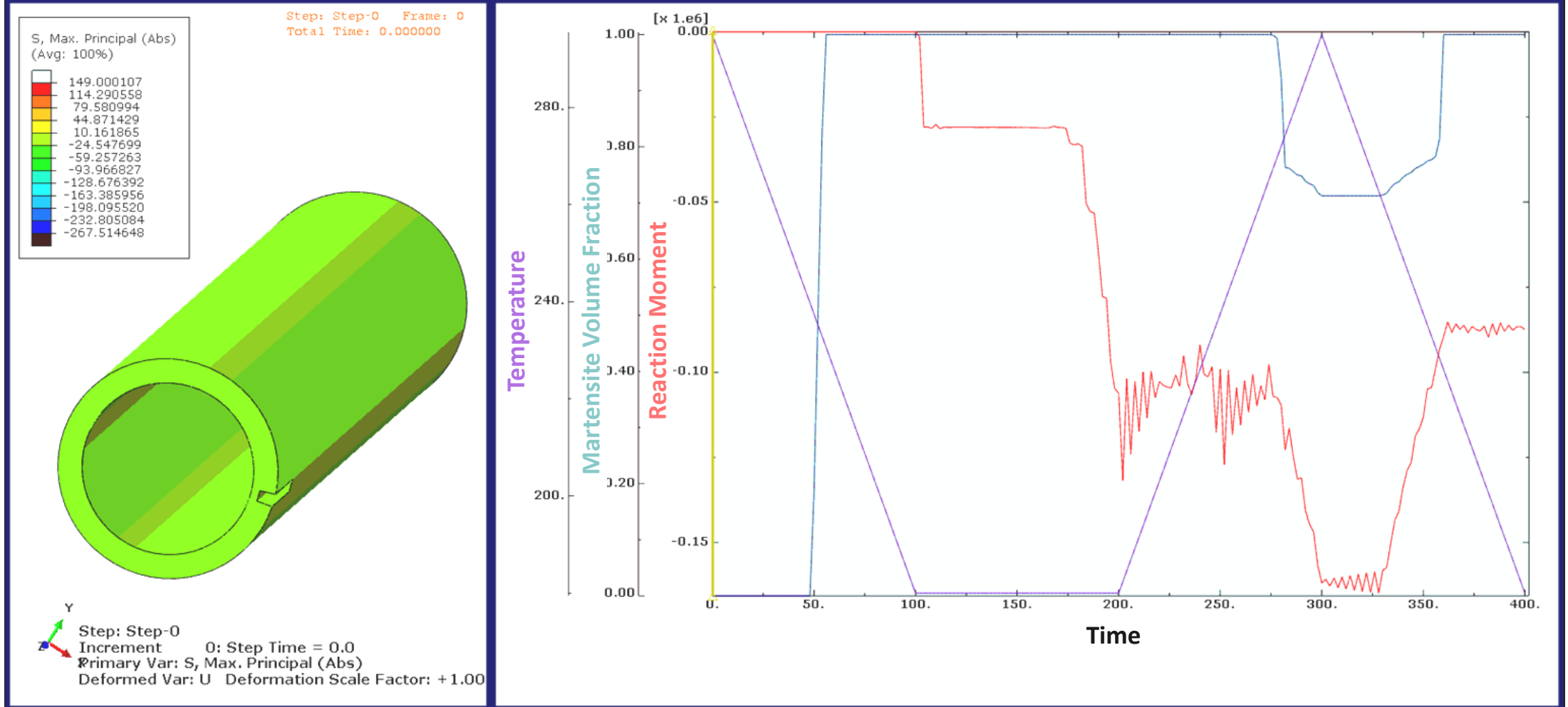
DEMONSTRATION: DIAMOND SURROGATE

Force vs Displacement

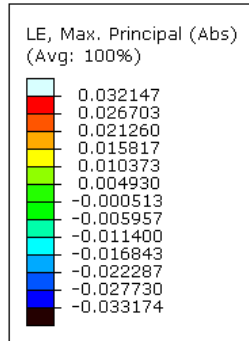


DEMONSTRATION: TORQUE TUBE ACTUATION

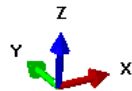
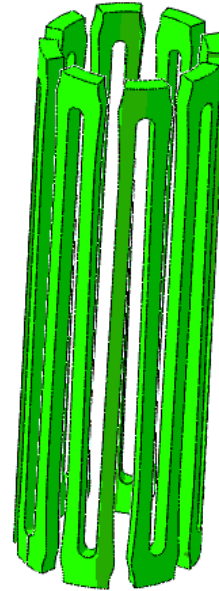
Temperature, Martensite Fraction and Reaction Moment vs Time



DEMONSTRATION: STENT



Step: Expand Frame: 0
Total Time: 0.000000



Step: Expand
Increment 0: Step Time = 0.000
Primary Var: LE, Max. Principal (Abs)
Deformed Var: U Deformation Scale Factor: +1.000000e+00

CONCLUSION

- Future Work
 - Replace Cazacu yield surface theory with Brunson
 - Optimized code for speed
 - Write adjacent program to automate calibration and minimize tests
- Overview
 - Available for use in Abaqus as a UMAT or VUMAT
 - New model is micro-mechanical inspired
 - Anisotropic
 - Tunable Tension-Compression Asymmetry
 - Coupled thermal-mechanical loading
 - Coupled phase transformation – plasticity



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