Mississippi State University: Center for Advanced Vehicular Systems

Tribology and Friction of Soft Materials: Mississippi State Case Study

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Advanced Materials: Models and Methods Forum
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MISSISSIPPI STATE UNIVERSITY

JAMES WORTH BAGLEY COLLEGE OF ENGINEERING MISSISSIPPI STATE UNIVERSITY

CAVS

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Outline

1. Background of Mississippi State U.

2. MSU/CAVS Capabilities

3. Overall Strategy for Polymer Research

4. Multiscale Material Modeling

5. Case Study

6. Summary

Mississippi State University:
Center for Advanced Vehicular Systems

www.cavs.msstate.edu

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CAVS

Bagley College of Engineering Degree Programs

Mechanical Engineering

Industrial Engineering

Software Engineering (Undergraduate only)

Applied Physics (Graduate only)

Aerospace Engineering

Electrical Engineering

Biological Engineering

Computer Science

Mississippi State University Athletics
www.mstateathletics.com

Computational Engineering (Graduate only)

Biomedical Engineering (Graduate only)

Chemical Engineering

Civil Engineering

Computer Engineering

CAVS Today

CAVS STRENGTH: People (about 250)

Faculty: 47

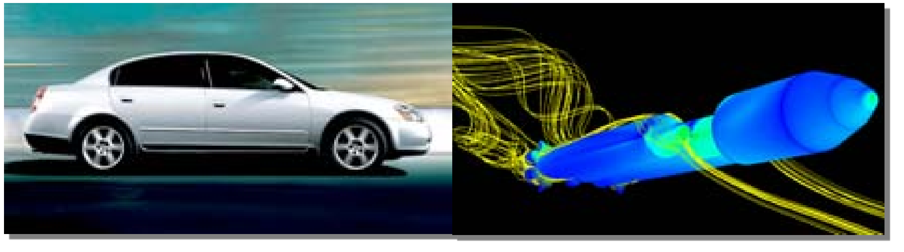
Staff: 58

Graduate students: 85

Undergraduate students: 79

CAVS GOAL: Become the nation's premier interdisciplinary high-performance ***vehicular*** computing research facility.

NEXT STEPS: CAVS has a central focus on computational engineering to serve as our differentiator. We have now broadened the domain definition of the term "vehicular." We are in the process of defining areas of research which are needed to complement the central focus.



CAVS / MSU Capabilities

- **Materials Characterization Facilities**

  X-Ray CT Scan, High performance FEG-SEM, EVO–SEM, TALYSURF CLI 2000, Hysitron Nanoindenter, Axiovert Optical Microscope, Particle Size Analyzer, Spectroscopy, …

- **High Temperature Characterization Facilities**

  TGA, DSC, DMA, Dilatometer, Microwave Sintering Furnace, Arburg Powder Injection Molding, Randcastle–Extruder, Powder Compaction Machine, …

- **Mechanical Properties - Testing Facilities**

  Hopkinson Bar setup (compression, tension, and torsion), Instron (50 kN, and 100 kN load capacity), Biaxial Instron, MTS (5-25 kN load capacity), Hardness Tester, Structural Test Systems, …

- **Computational capabilities**

  SunFire X2200 M2 (2048 Opteron proc.), IBM x335 Linux Supercluster (384 Pentium IV proc.), IBM x300 Linux Supercluster (1038 Pentium proc.), UltraSparc SUN

Websites:

http://www.cavs.msstate.edu/cavs4capabilities.php

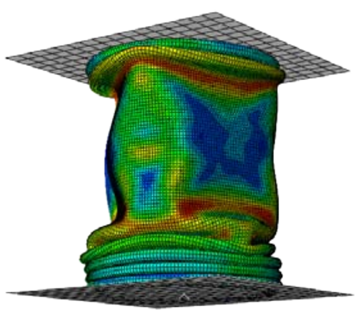
http://www.dial.msstate.edu/cap/Analytical%20Services%20Laboratory%20Web%20Page%20August%202006.html

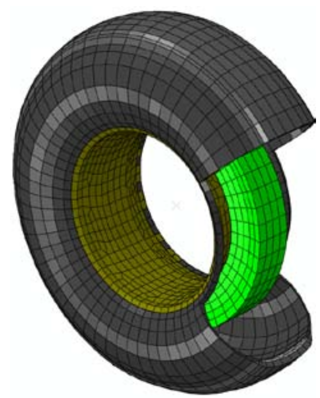
http://emcenter.msstate.edu

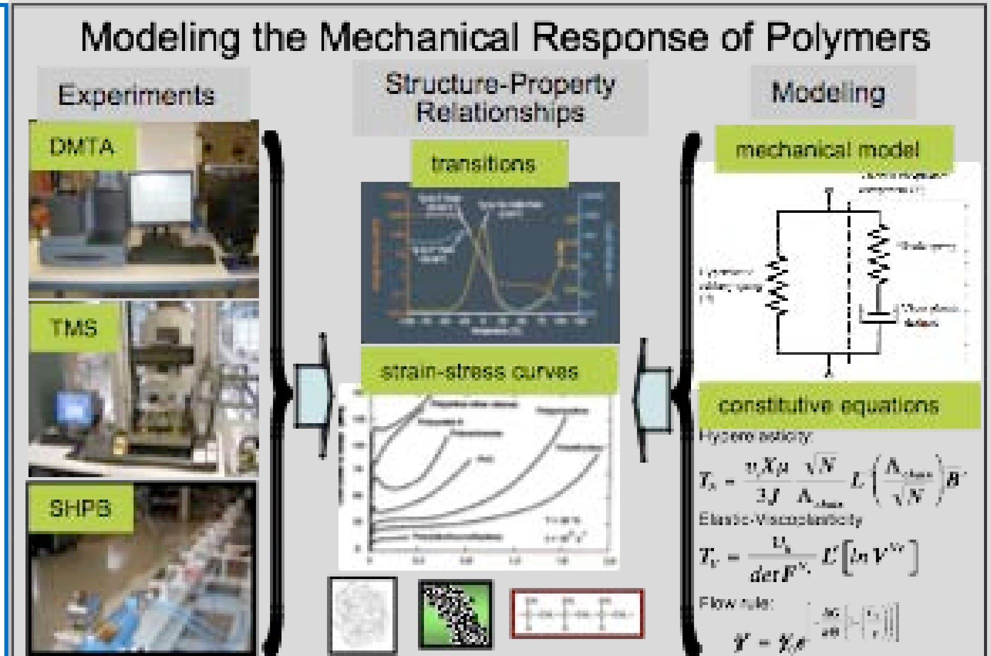
Polymer Overall Strategy (1)

Motivation

1. Increase the reliability and safety involving designing with polymeric materials for the automotive industry.
2. Better understanding of the mechanical response of polymers
3. Building a material database and developing material models for these materials







Goals

A. Develop material database capturing structure-property relationships for thermoplastics, elastomers, foams, and fabrics.

B. Develop internal state variable (ISV) material model. Model will be calibrated using database and verified / validated for a range of strain rates and temperatures.

Materials

Plastics:

Polycarbonate (PC)
Acrylonitrile Butadiene Styrene (ABS)
Polypropylene (PP)

Rubbers

Natural rubber
Santoprene (Vulcanized Elastomer)
Styrene Butadiene Rubber (SBR)

Foams

Polypropylene Foam
Polyurethane Foam

Fabrics

Kevlar
Nylon

Polymer Overall Strategy (2)

Experiments

Mechanical Tests

- Low to High strain rates
- Temperatures below/above Tg
- Volumetric testing, relaxation, dissipation, strain paths, stress state)
- Impact tests
- Fatigue tests

Mechanical / Fatigue tests
- Test at different strain rates, temperature, Hz (stress/strain ratios, cyclic loading to failure)

Micro-structural studies
- Failure mechanisms (crack initiation / growth)

Materials

PLASTICS
Polycarbonate (PC)
Polypropylene (PP)
ABS

RUBBERS
Natural Rubber
Santoprene
SBR
TPU

FOAMS
PP foam
PU foam

Modeling / Simulation

ISV material model (improved):
- Identification / Calibration
- FEA Implementation (ABAQUS,)
- Verification

Fatigue model:
- Identification / Calibration
- FEA Implementation (ABAQUS,)
- Verification

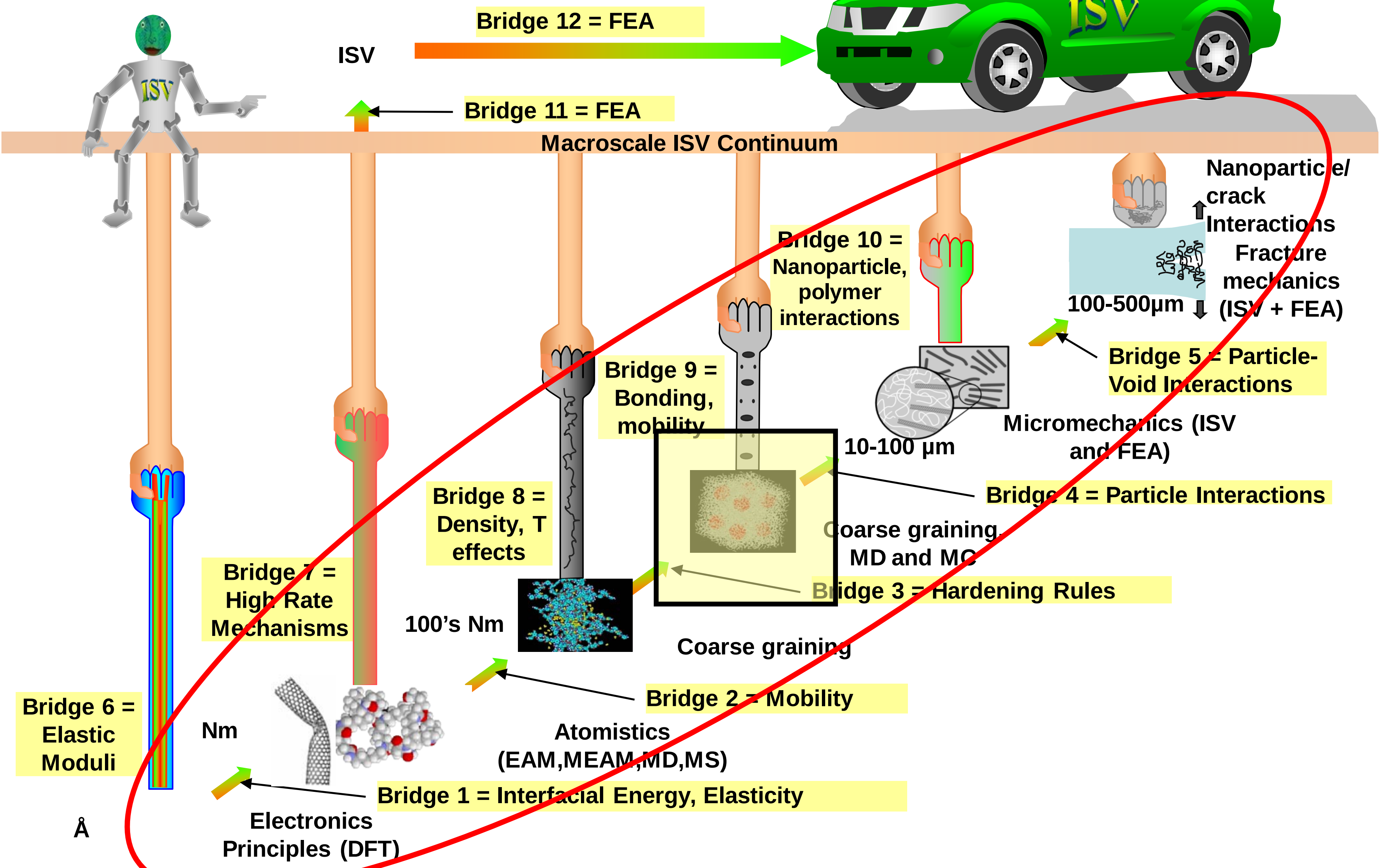
ISV material model:
- Identification / Calibration
- FEA Implementation (ABAQUS,)
- Verification

Fatigue model:
- Identification / Calibration
- FEA Implementation (ABAQUS)
- Verification

Work supported by:
TARDEC (DoD)
American Chemistry Council
DOE

People: **Faculty (8), Staff (3), PhD (3), UG (10)**

Multiscale Polymer Modeling



Studying Polymers with Molecular Dynamics

Typical terms in
Inter-atomic potential

Bond angle

$$E_{bs}(r) = \sum_{atoms}\{k_r(r-r_0)^2\}$$ ← Bond stretching

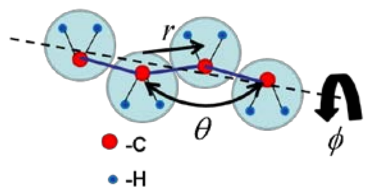
$$E_{be}(\text{¸}) = \sum_{atoms}\{k_{\text{¸}}(\text{¸}-\text{¸}_0)^2\}$$

$$E_{to}(\square) = \sum_{atoms}\{V_1\cos\square + V_2\cos 2\square + V_3\cos 3\square + V_6\cos 6\square\}$$

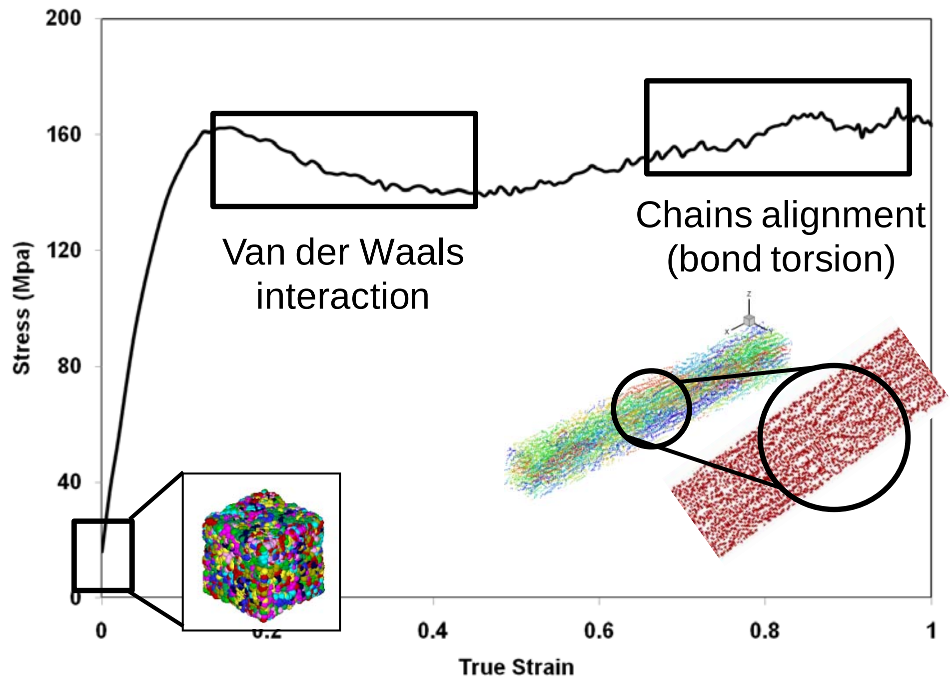
$$E_{vw}(\bar{r}) = \sum_{nobonded}\{A(\bar{r})^{-12} - C(\bar{r})^{-6}\}$$

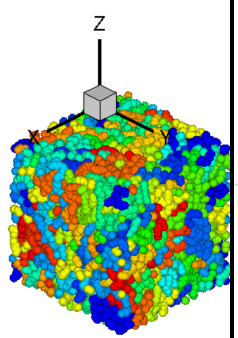
Bond torsion

Van der Waals

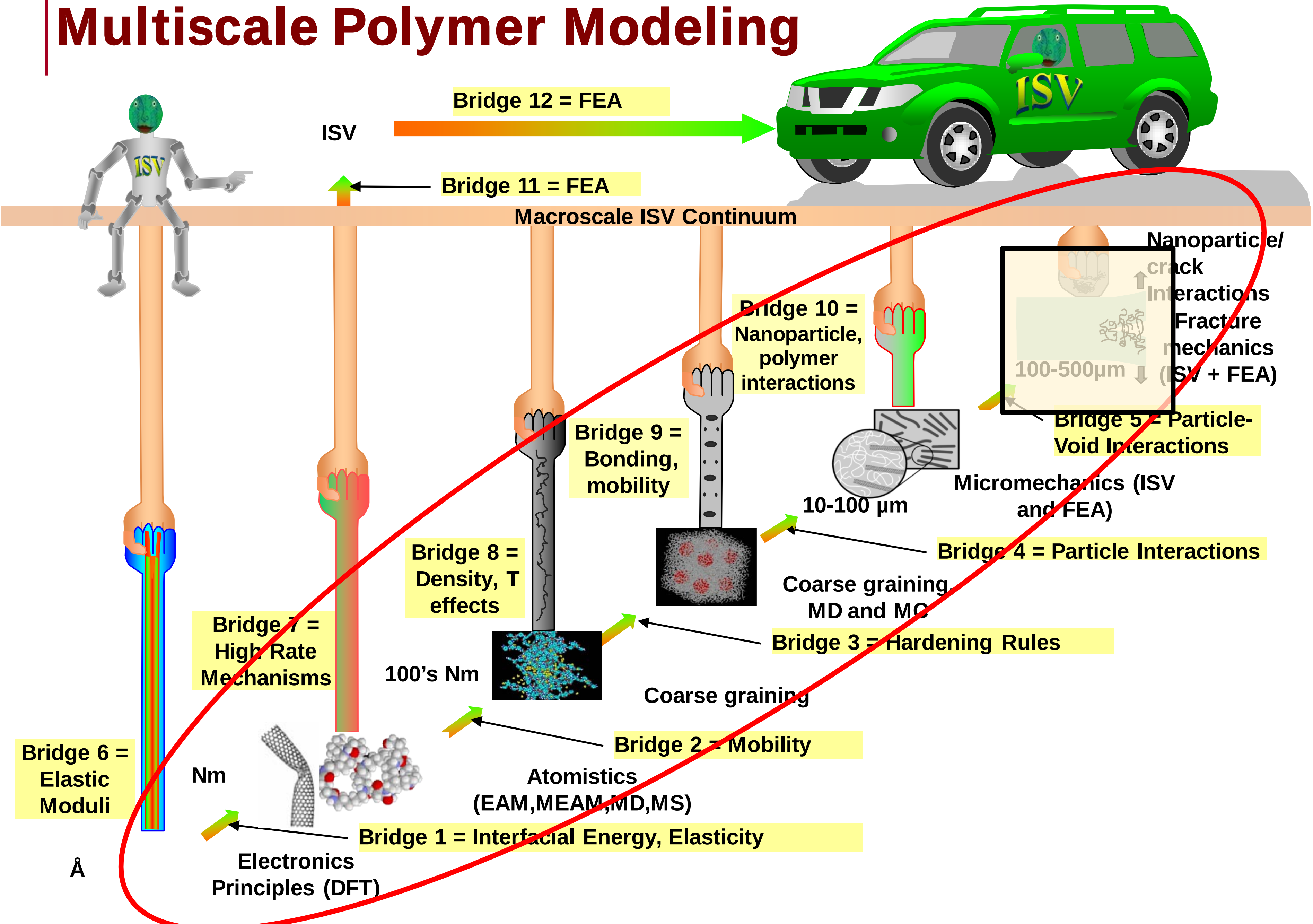


Nanoscopic specimen of idealized
Linear amorphous polyethylene under
uniaxial tension (T=100K, nc=200, n_monomers=1000)

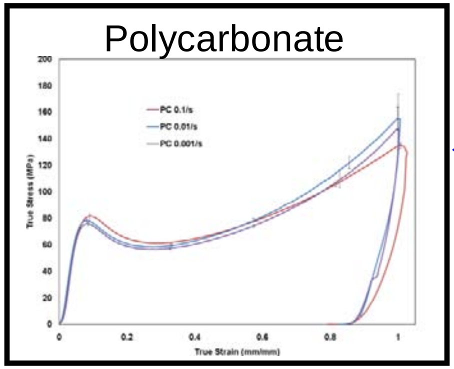




Multiscale Polymer Modeling



Methodology Applied to Model Mechanical Response of Polymers

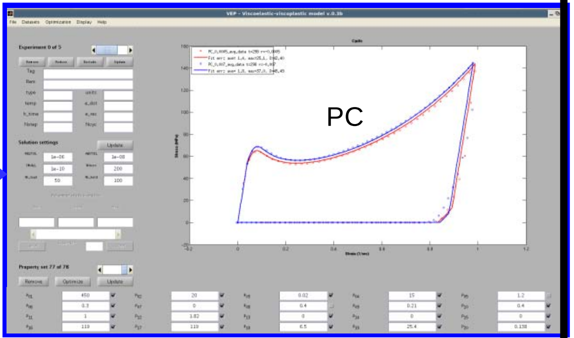


EXPERIMENTAL DATA

ISV MATERIAL MODEL

3-D Constitutive Equations
+ Numerical Integration Procedure

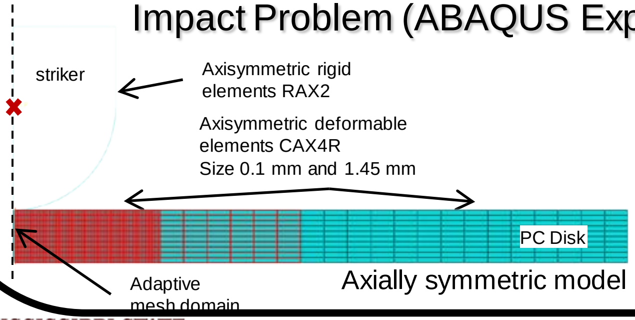
fitting algorithm developed for MATLAB



1-D Constitutive Equations

MODEL CALIBRATION TOOL

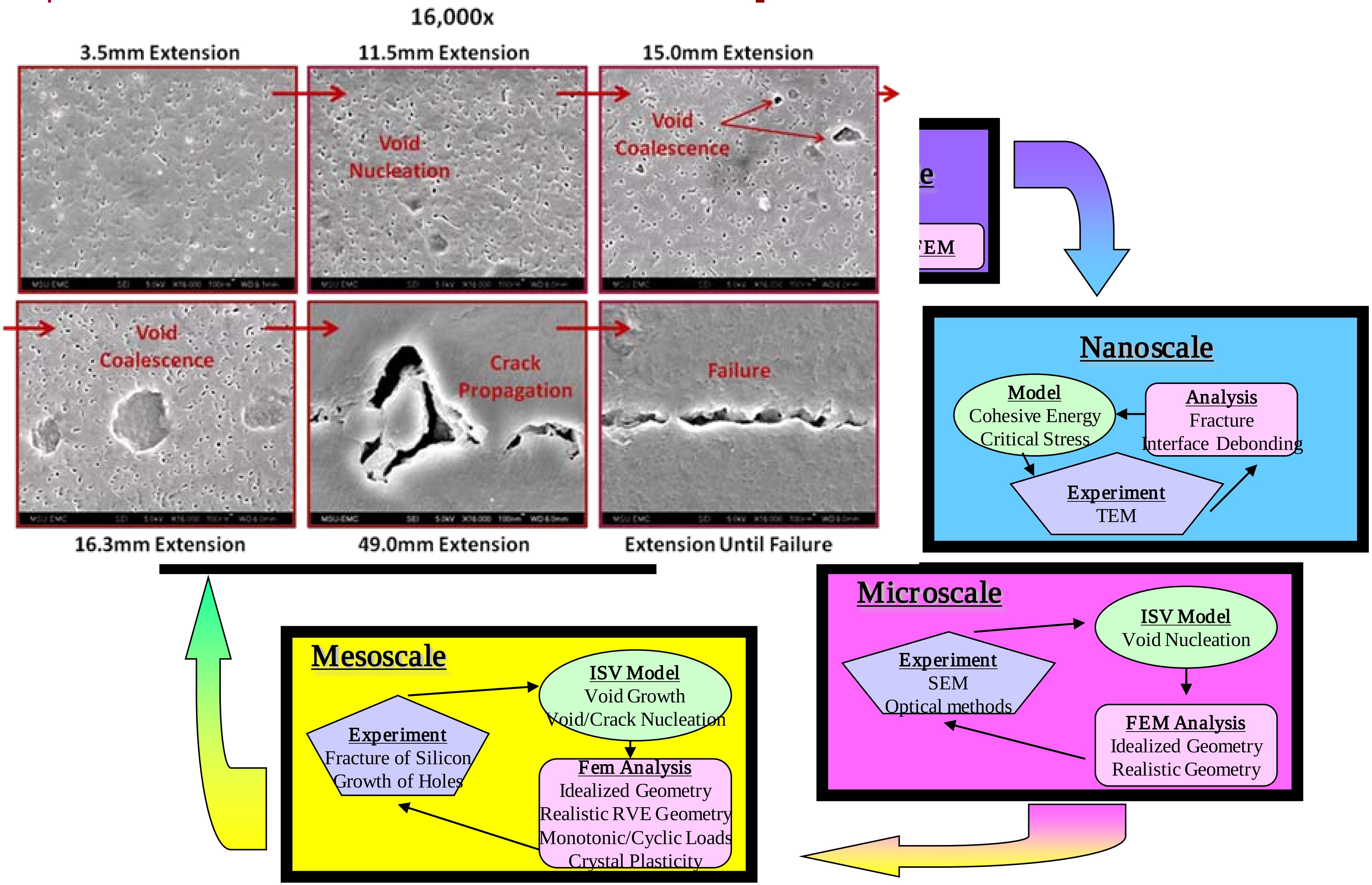
Impact Problem (ABAQUS Explicit)



FEA

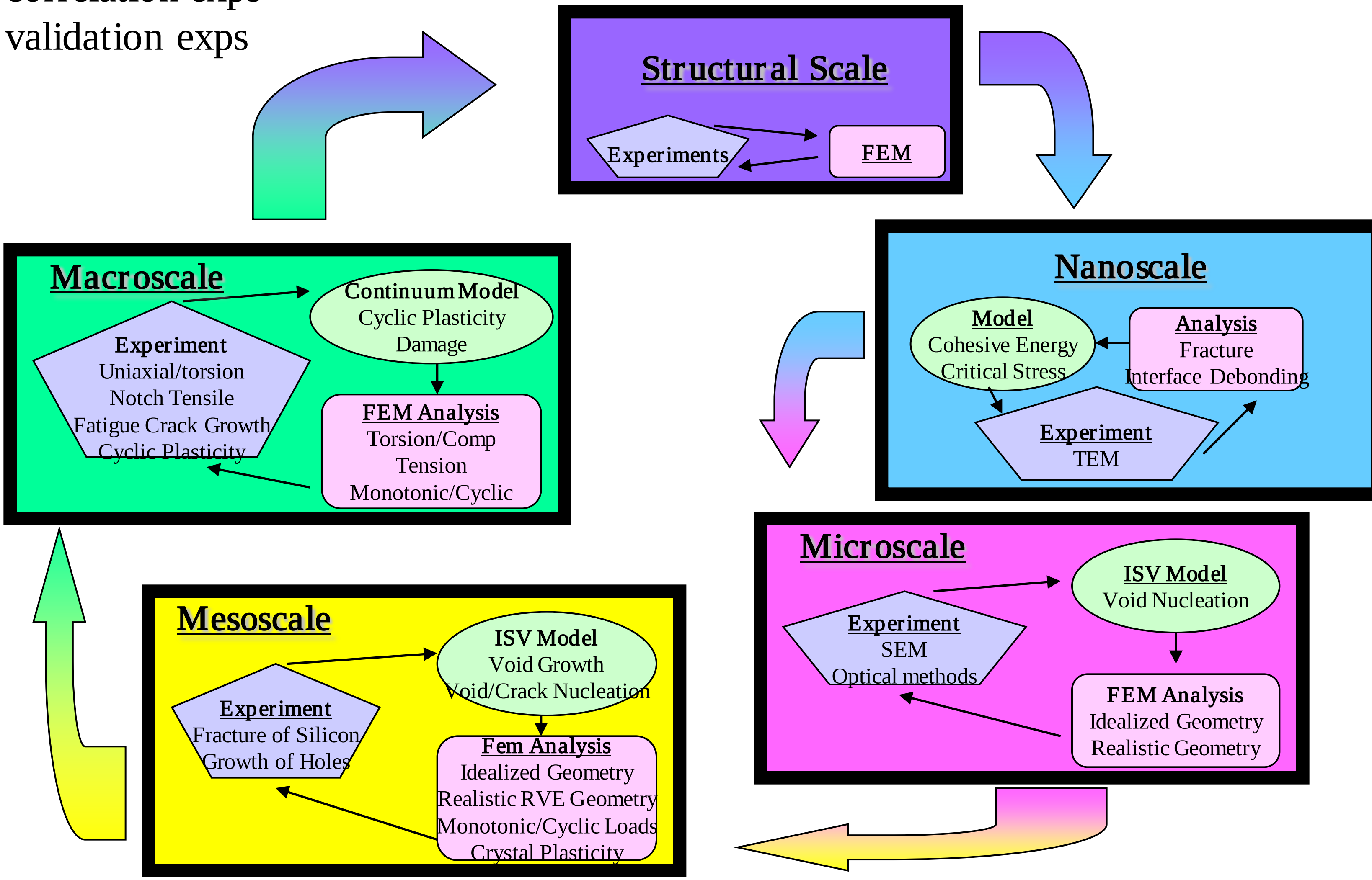
Numerical Implementation in FEM Codes

Multiscale Experiments



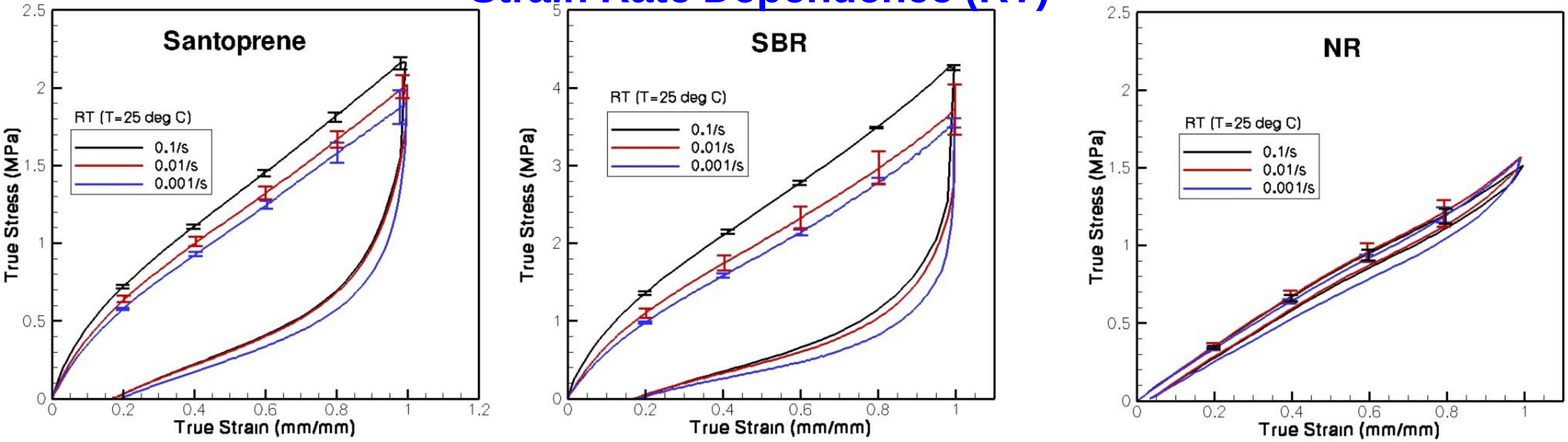
Multiscale Experiments

1. Exploratory exps
2. Model correlation exps
3. Model validation exps

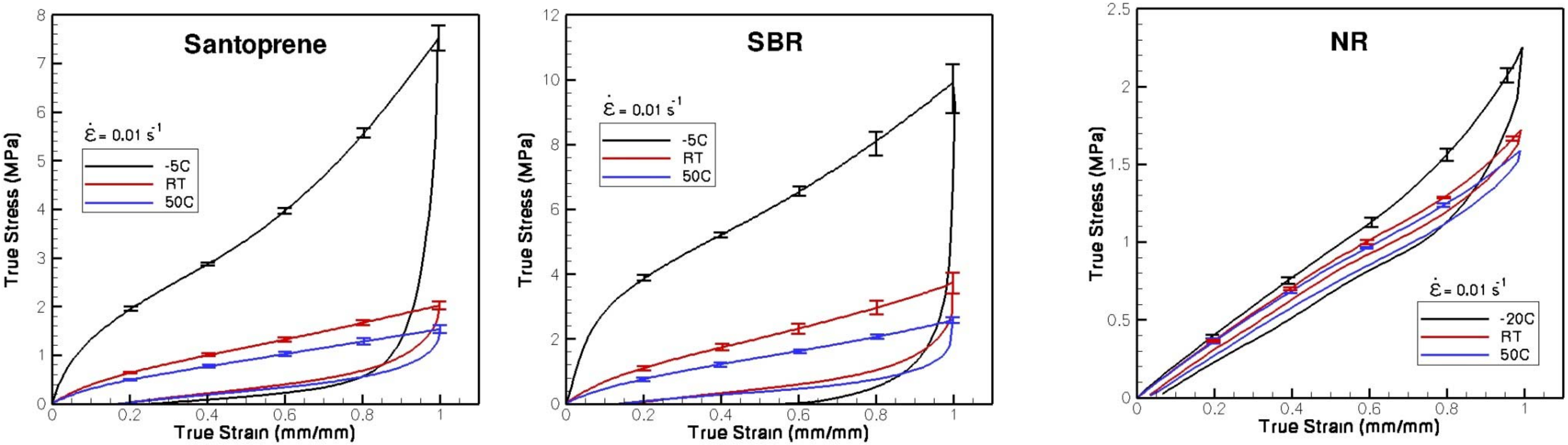


Compression Tests Results – Rubbers

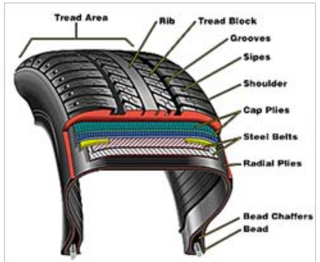
Strain Rate Dependence (RT)



Temperature Dependence (0.01 /s)

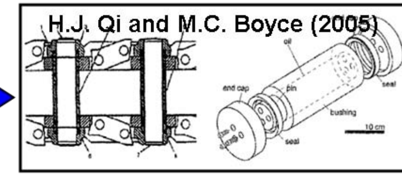


MSU / CAVS Case Study



rubber tire

Michelin's PAX run-flat tire



Goals

A. Capture experimentally the mechanical properties of Thermoplastic Polyurethane (TPU)

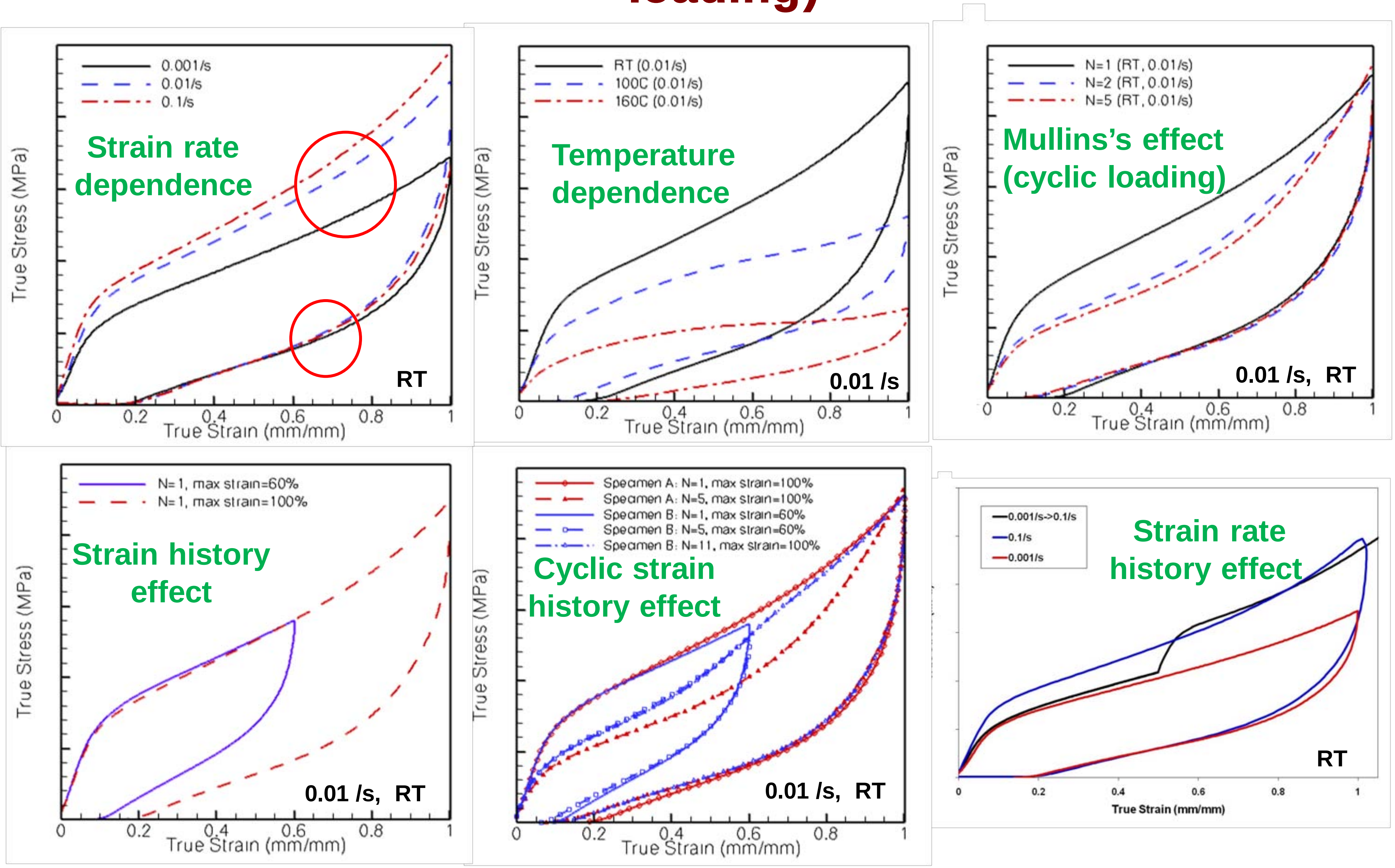
B. Develop an internal state variable (ISV) material model for this material.

C. Develop a preliminary multiscale fatigue model to predict the failure of real structural component

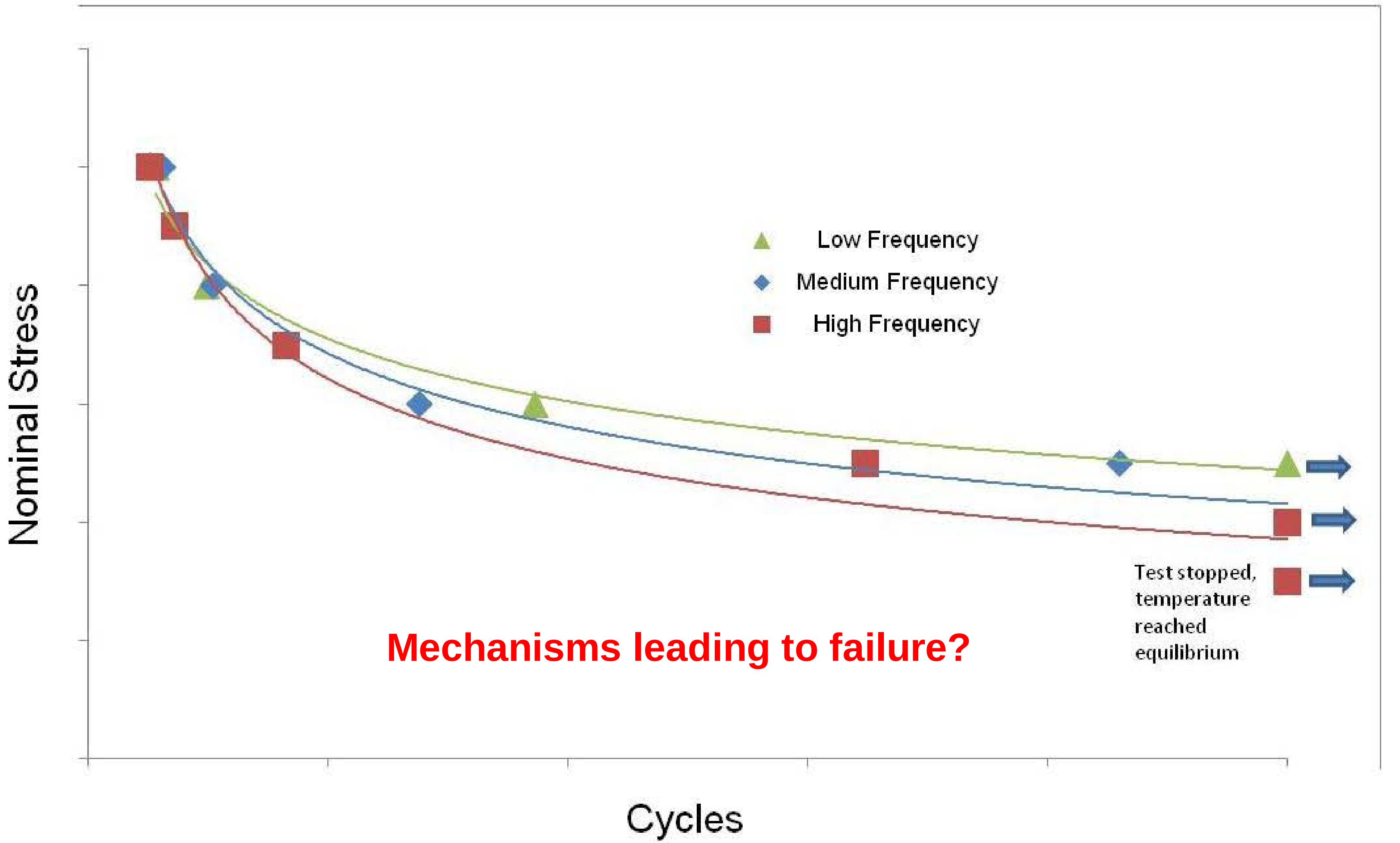
Approach

- Carry out experiments using current testing methodologies:
  - Dynamic Mechanical Analyzer (DMA)
  - Thermogravimetric Analysis (TGA)
  - X-Ray Diffraction (XRD)
  - INSTRON (tensile and compressive testing)
- Develop ISV material model
  Develop a model calibration procedure (MATLAB)
  Model implementation in finite element code (ABAQUS).
- Develop a Multiscale Fatigue Model
- Perform finite element analysis to understand/improve the the performance of a structural component design

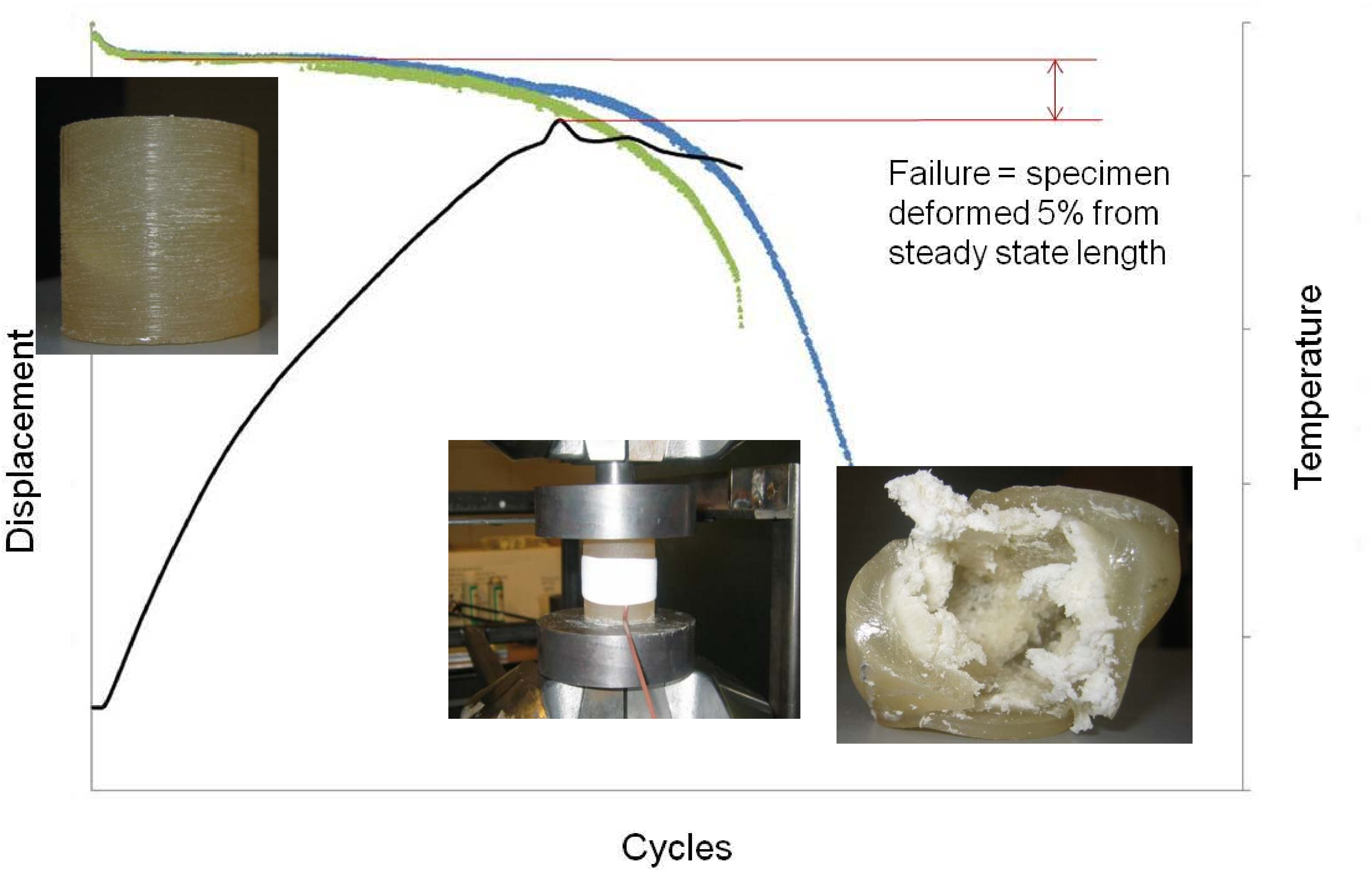
Mechanical Behavior at the Coupon Level (monotonic loading)



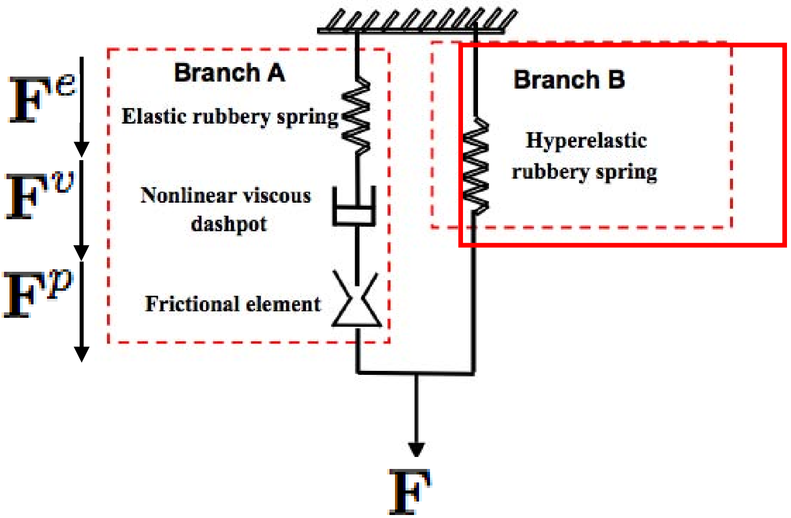
Stress – Life With Frequency Effects



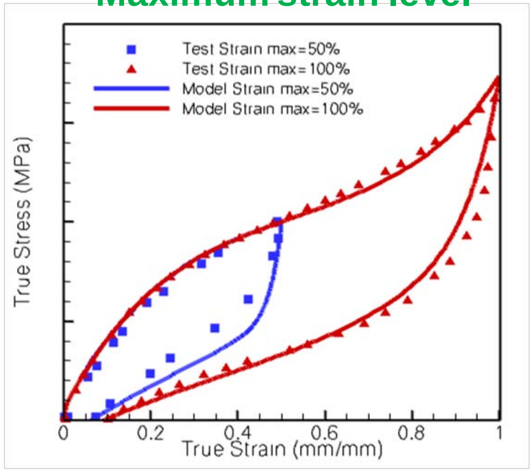
Fatigue Behavior: Internal Heat Build-up Leads to Failure



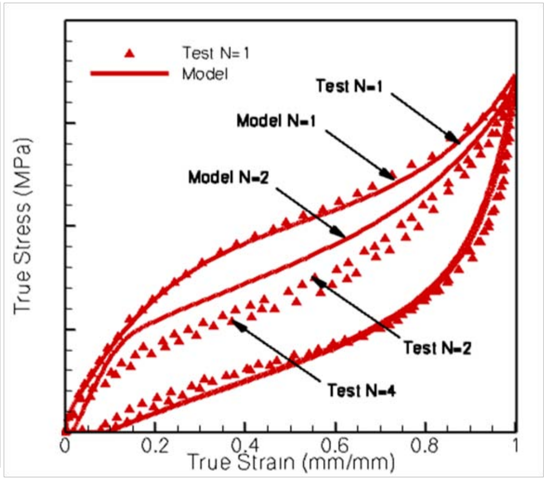
ISV Material Model Prediction



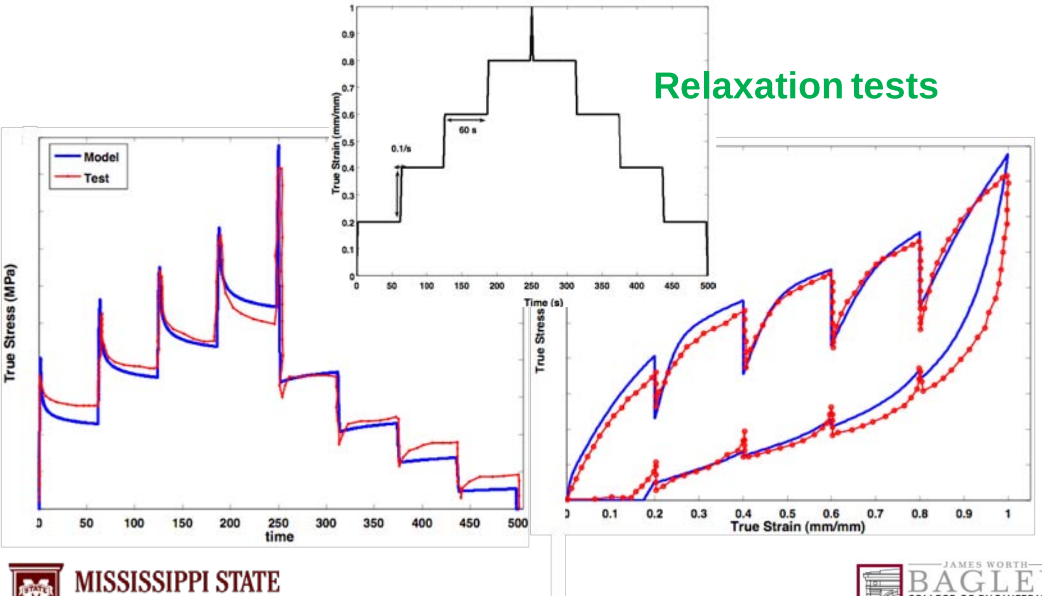
Maximum strain level

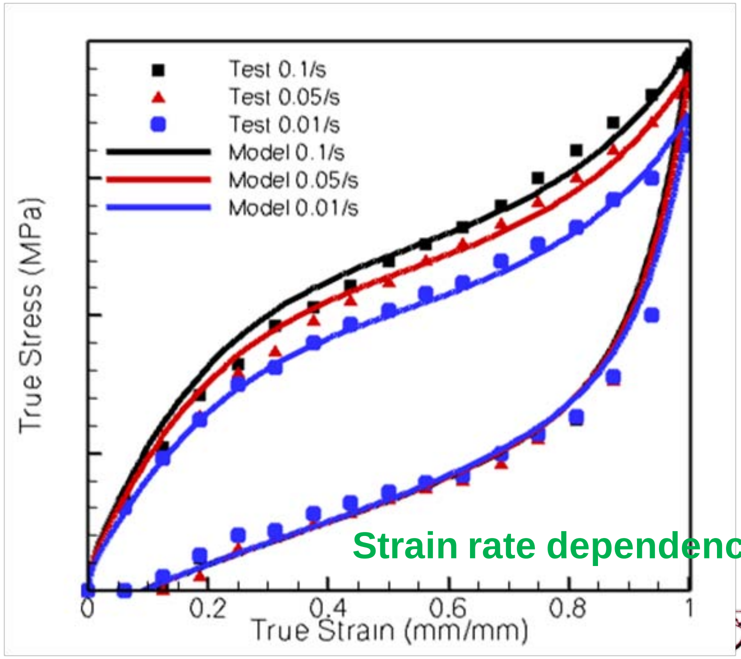


Mullins' effect



Relaxation tests





Strain rate dependence

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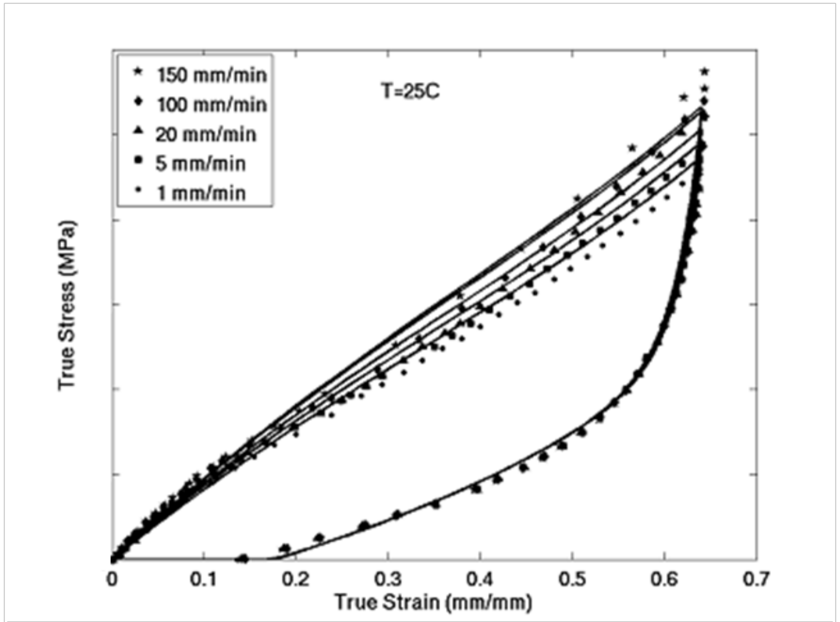
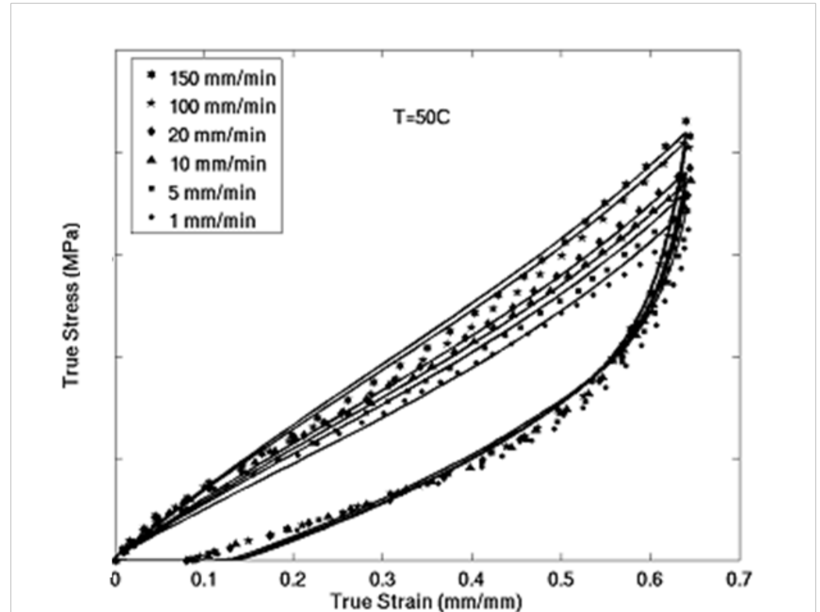
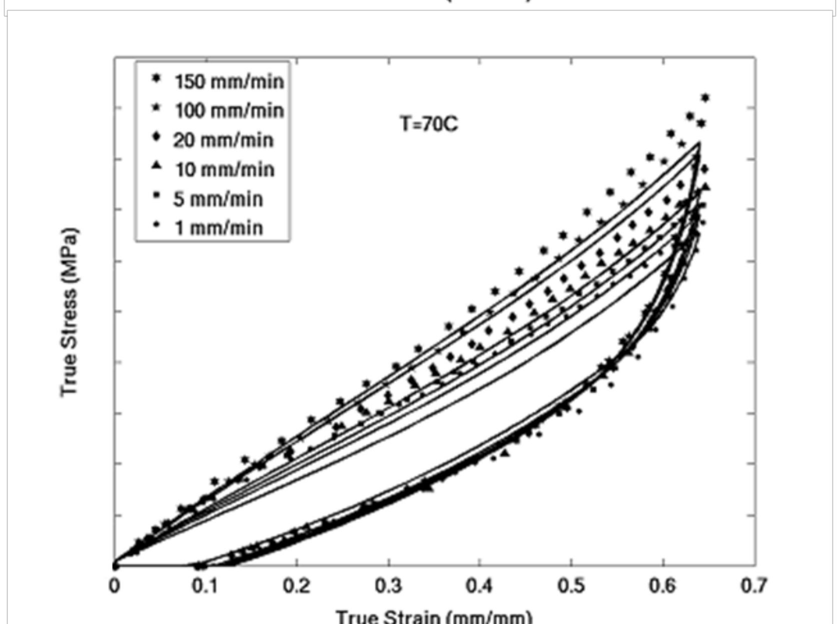
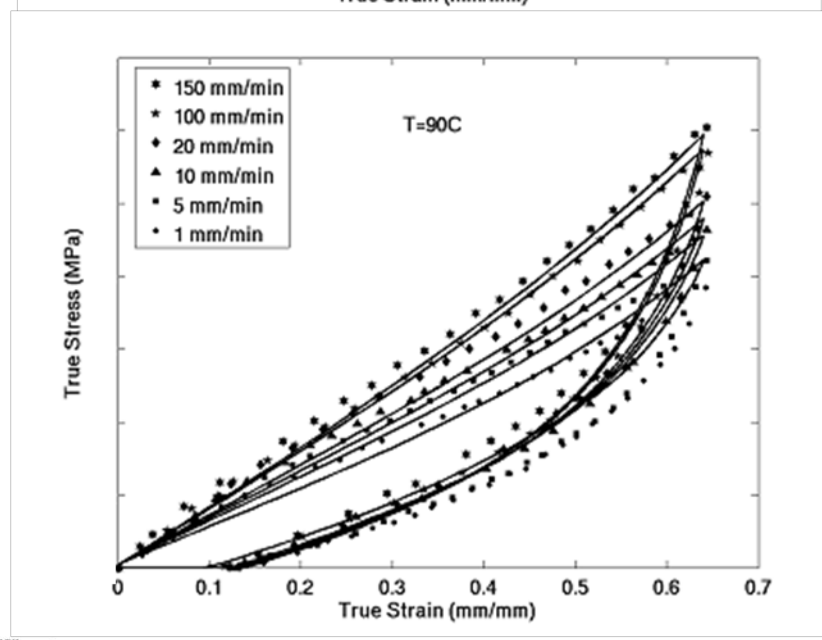
ISV Material Model prediciton (isothermal problems)

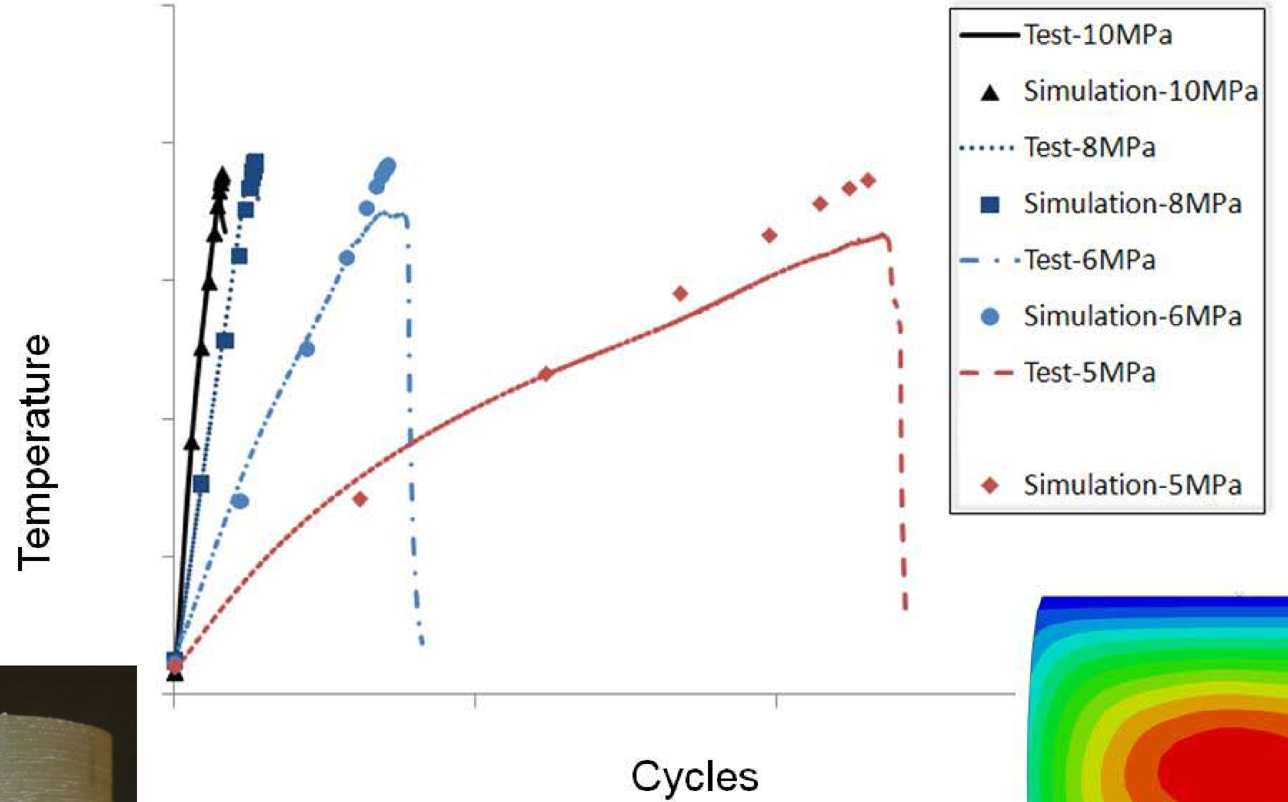


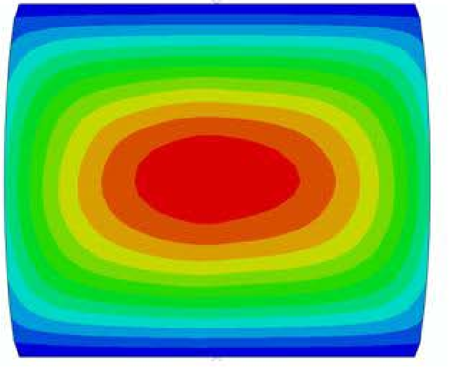




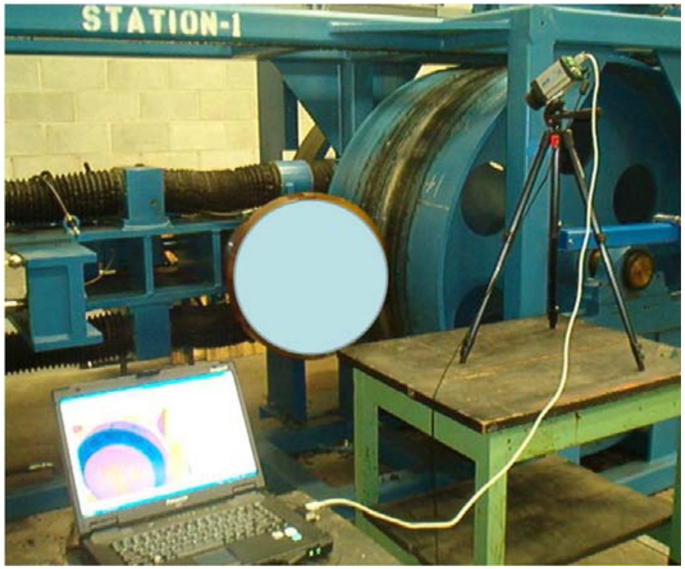


Thermal Fatigue Simulation at Medium Frequency for Various Stress Levels

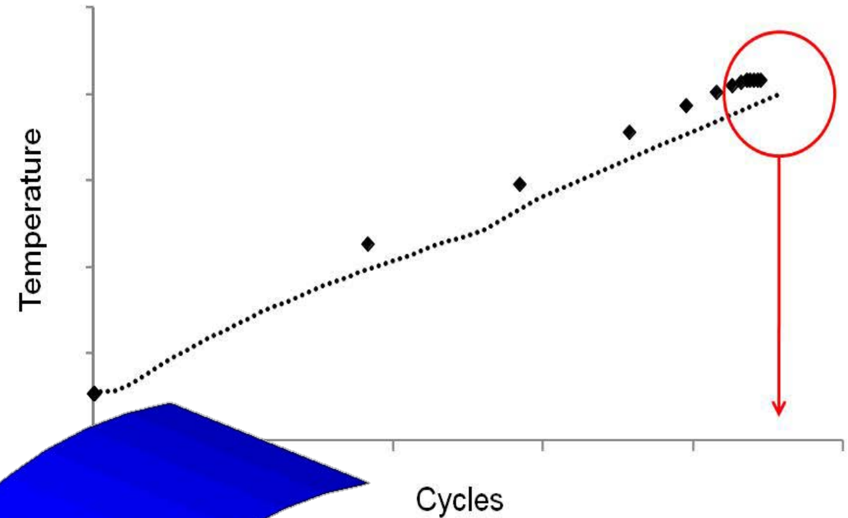


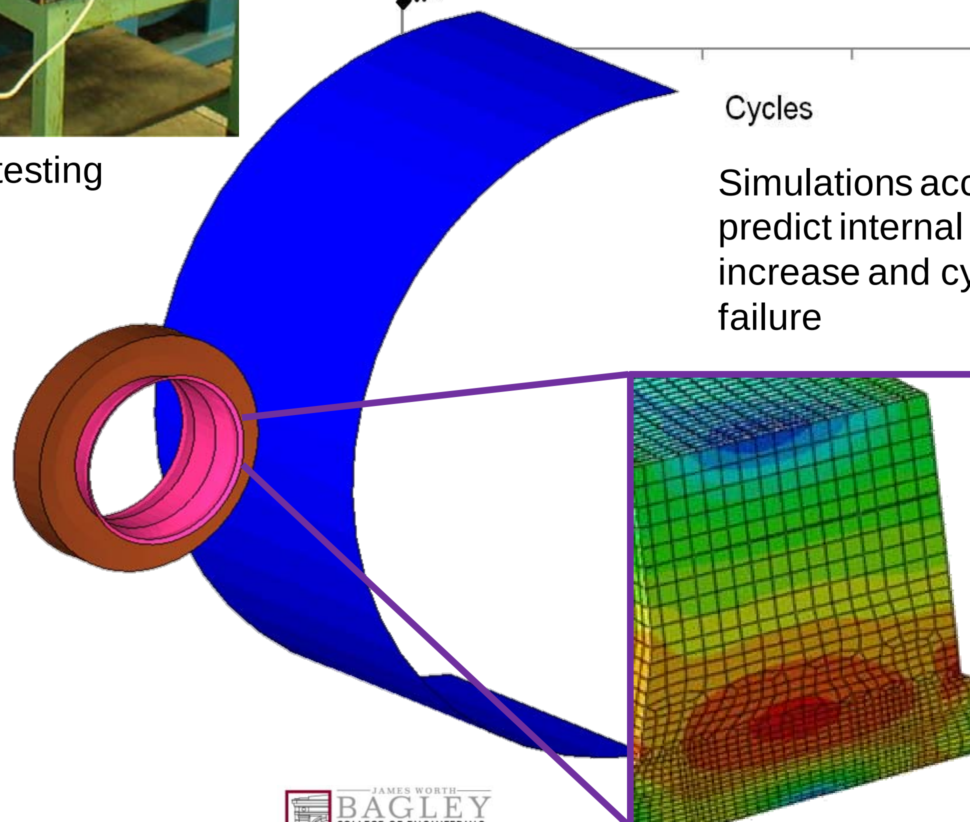


Component Life Prediction



Wheel dynamometer testing





Simulations accurately predict internal temperature increase and cycles to failure

Thermocouples embedded for internal measurements

Summary

1. Multidisciplinary Center

2. Lab equipment / Computational capability

3. Multiscale experiments

4. Multiscale modeling frameworks with ISV approach.

5. Application to Polyurethane insert component