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Title: A Constitutive Modeling Framework for High Explosives

Author(s): Miller, Nathan Andrew
Brindley, Kyle Andrew

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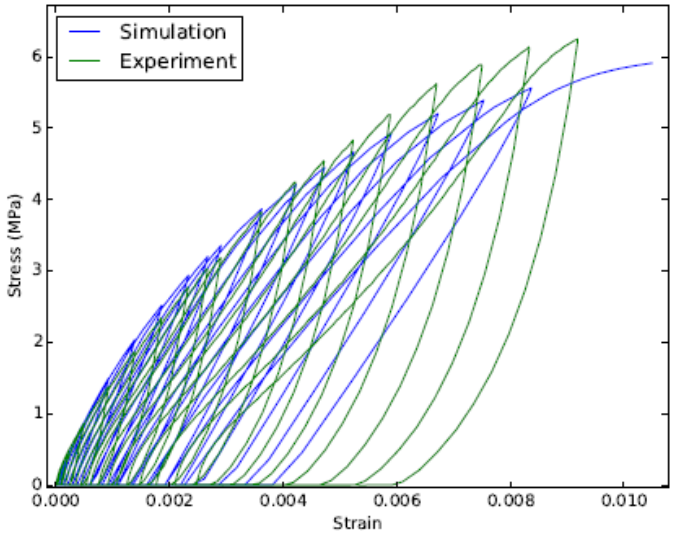
A Constitutive Modeling Framework for High Explosives

Nathan Miller – W-13
Kyle Brindley – W-13

Introduction

- Predictive capabilities on the response of the HE in a given system is frequently the major question in a given analysis
  - What is the HE doing and what is happening to the HE?
- Historically, W-13 used simple models to capture the behavior
  - Viscoelasticity
  - Drucker-Prager
- Recent efforts have dramatically improved our predictive capability
  - VPVD



Buechler et al., "A viscoelastic viscoplastic damage Model (VPVD)," *Internal LANL report*, ***2015***

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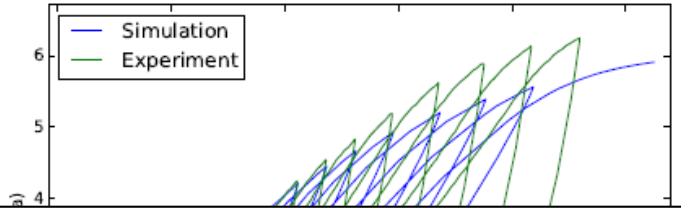

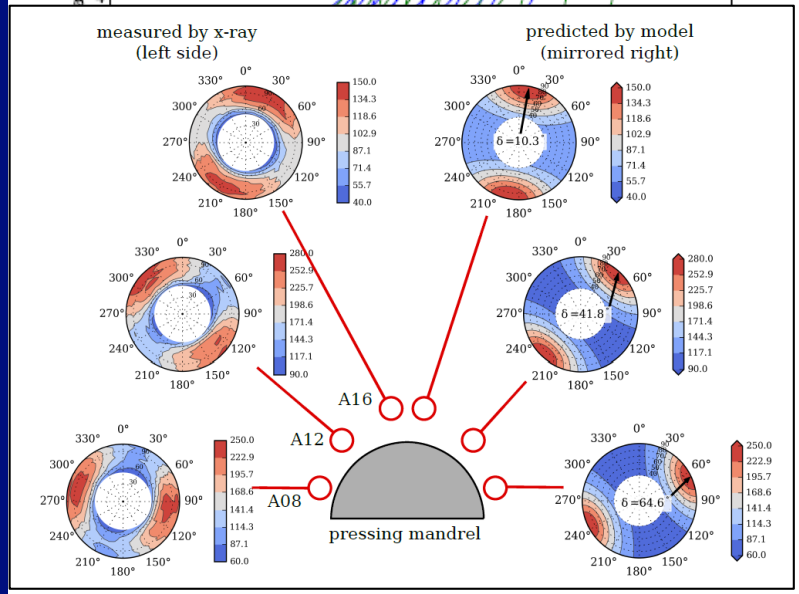

Buechler et al., "Modelling the effects of texture on thermal expansion in pressed PBX 9502 Components", *Proceedings of ICME*, **2016**

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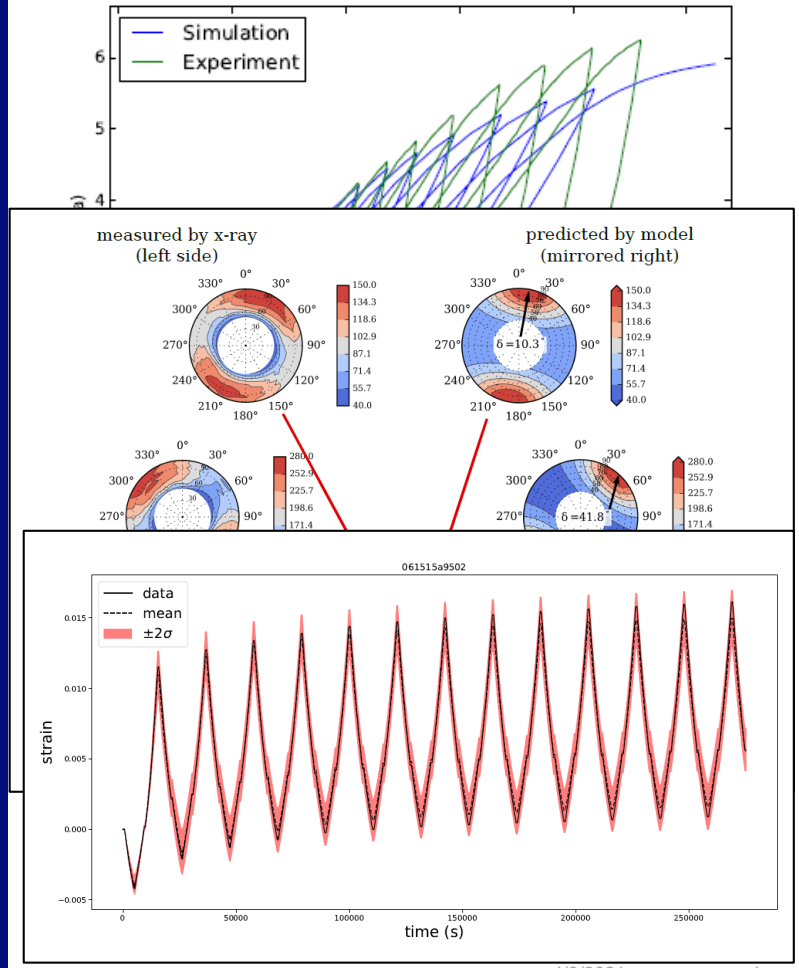
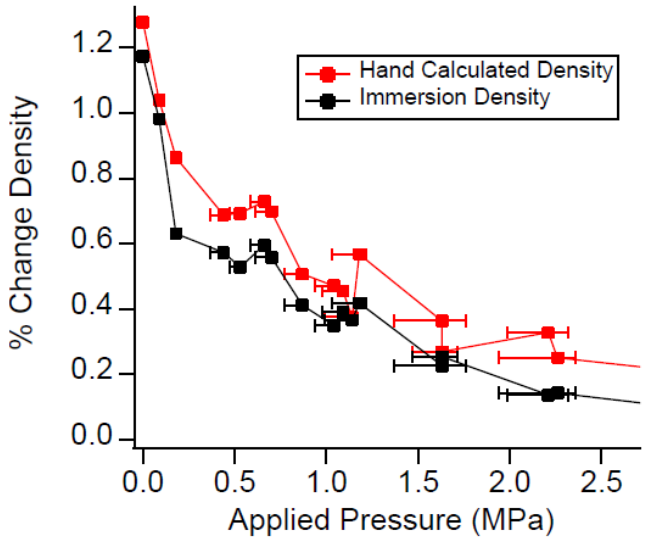
  - Phenomenological Ratchet Growth

Miller, "Towards Uncertainty Quantification of Material Models," Nuclear Weapons Engineering Analysis Conference, **2019**



Issues of Immediate Concern

- VPVD's codebase is fragmented into 9501 and 9502 versions
  - Miller merged them in ~2015 but they diverged again
- Calibration dataset was not version controlled
- The ratchet growth model can't capture pressure suppression of ratchet growth
  - Ratchet growth damaging effect missing too
- A fully coupled thermo-mechanical model is required



Woznick et al., "TATB ratchet growth and hydrostatically confined PBX 9502," *AIP Conference Proceedings*, **2020**

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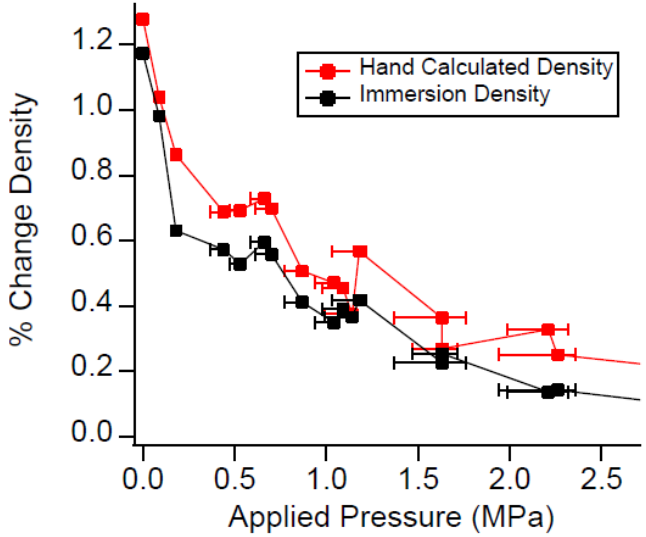
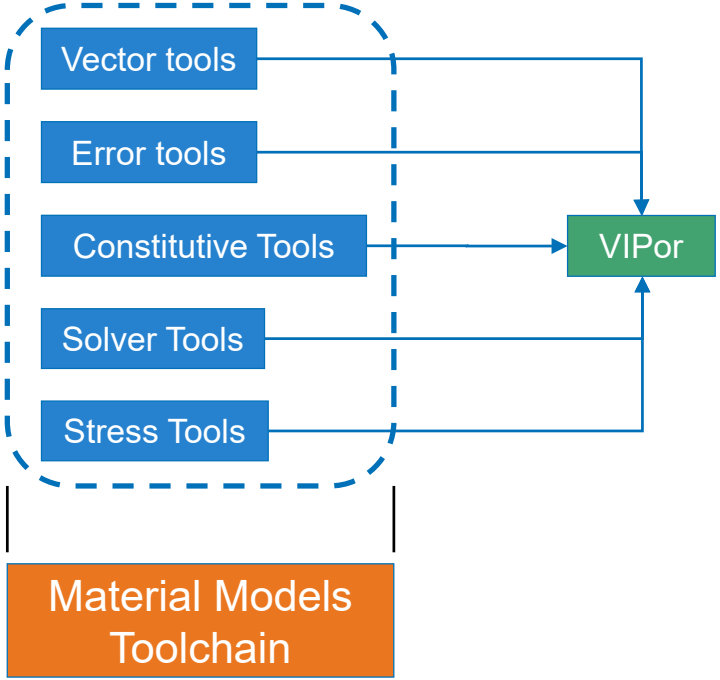


We seek a model developed in a rigorous development framework that can capture these behaviors

VIPor Overview

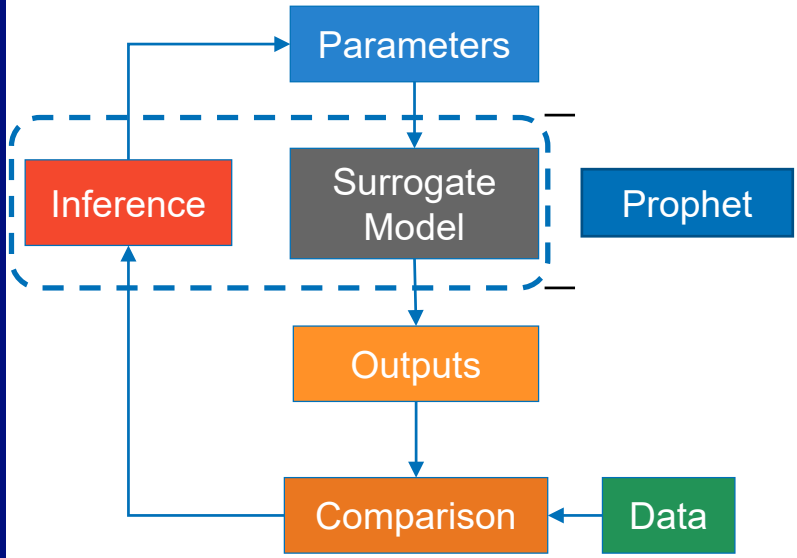
- V(iscous) I(sotropic) Por(osity) based model is the new W-13 HE framework
  - A generalization of VPVD to finite deformation
  - Handles thermal expansion within the subroutine
  - Developed within a software best-practices framework
    - Extensive testing
    - Continuous Integration
    - Version Control
    - Documentation
  - Coded in C/C++ for portability

VIPor and its supporting libraries



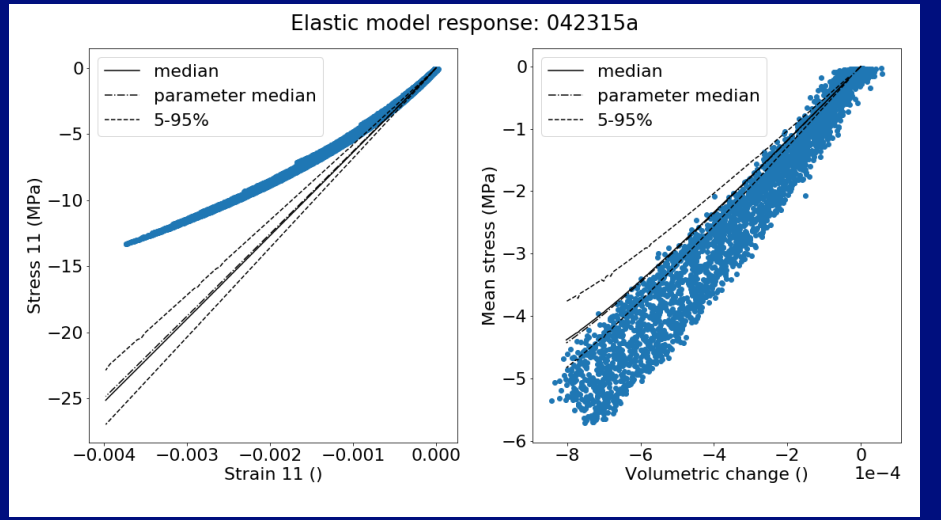
VIPor Calibration

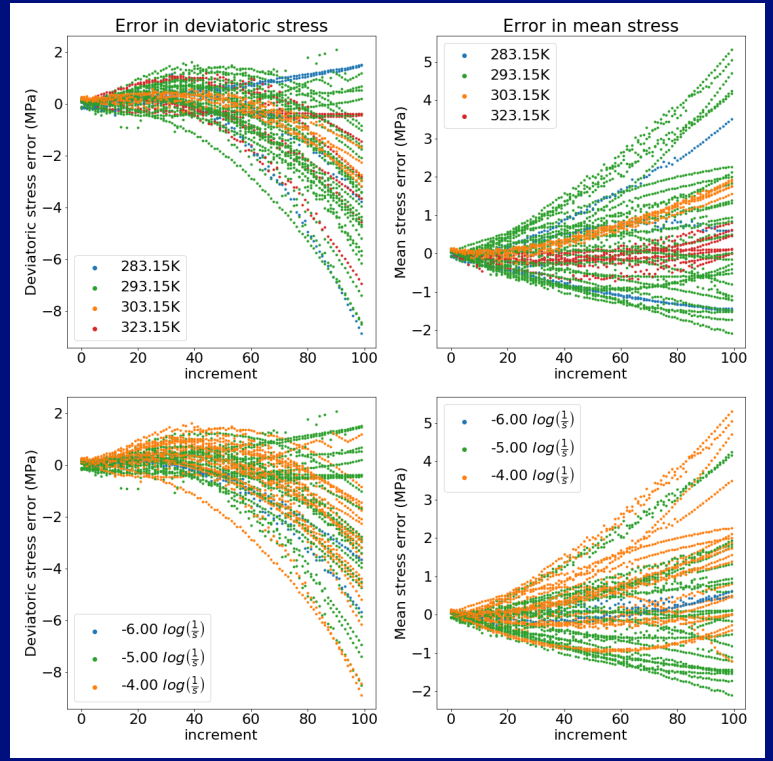
- Uncertainty Quantification
  - Using the uncertainty characterization process to quantify the uncertainties on our inputs
  - Bayesian inference code Prophet (dashed box) makes this easier
- Data exclusively obtained from version controlled Granta records
  - Allows for traceability of the data



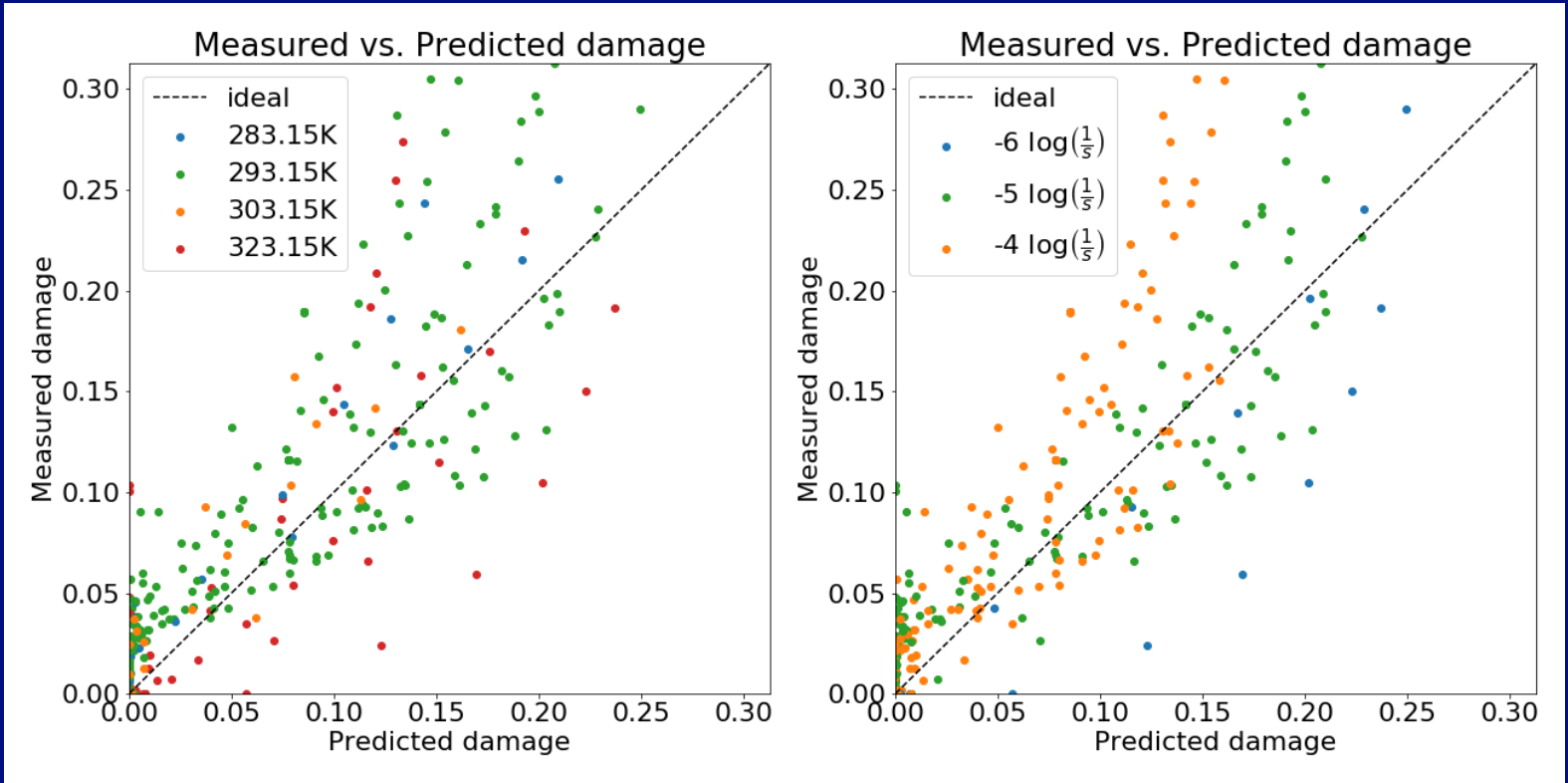
Bayesian inference toolchain

PBX 9502 Elasticity Calibration

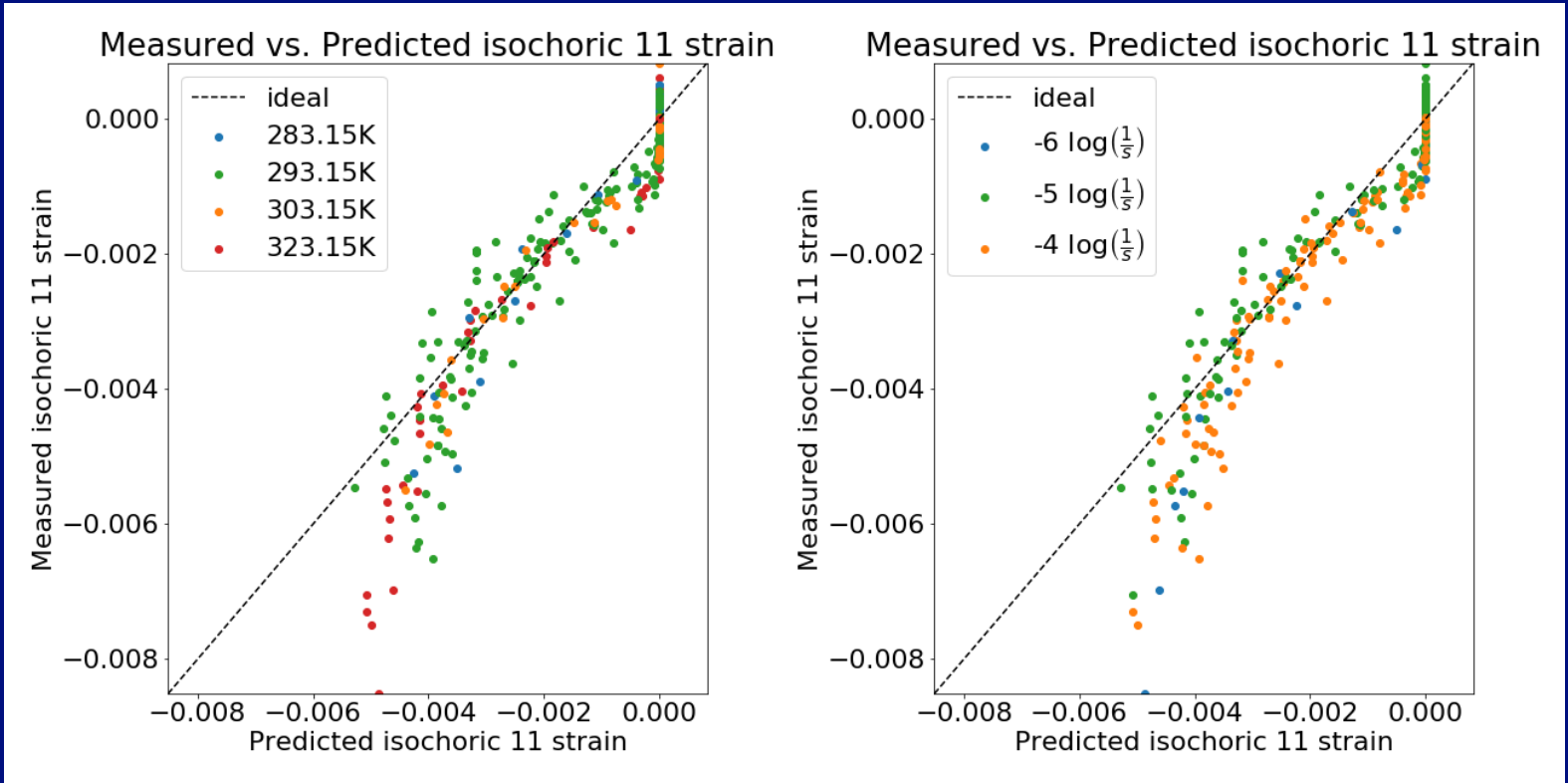




PBX 9502 Damage Calibration



PBX 9502 Irrecoverable Deformation Calibration



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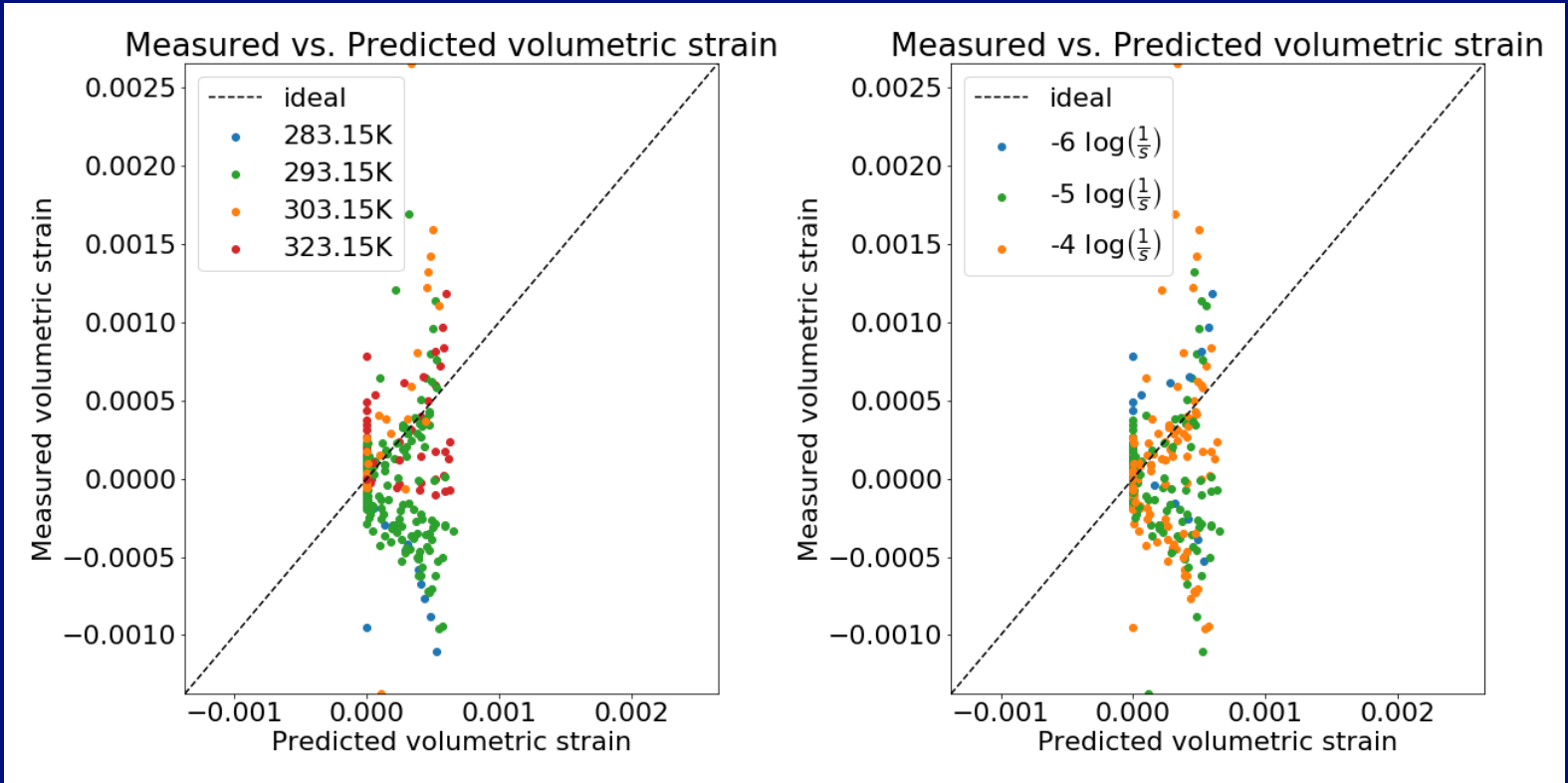

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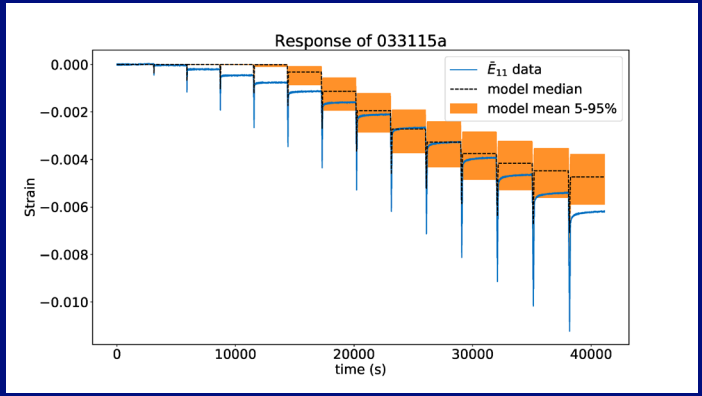

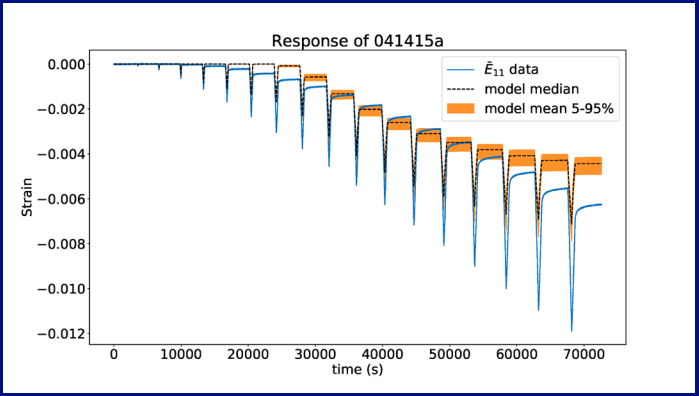

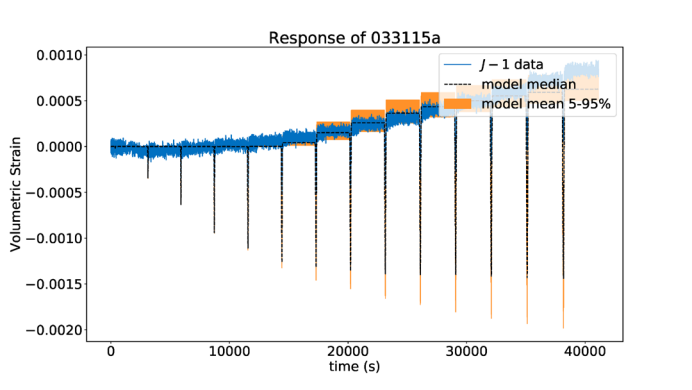

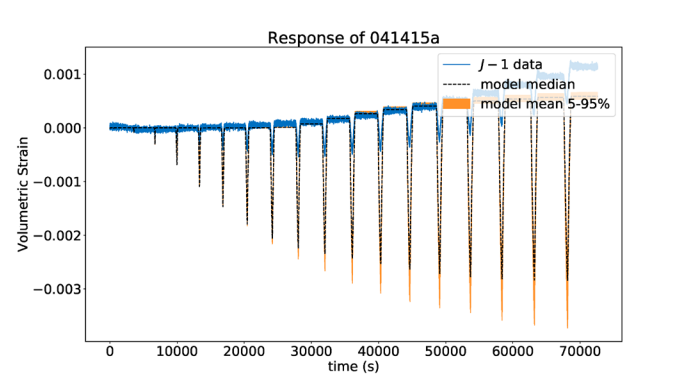

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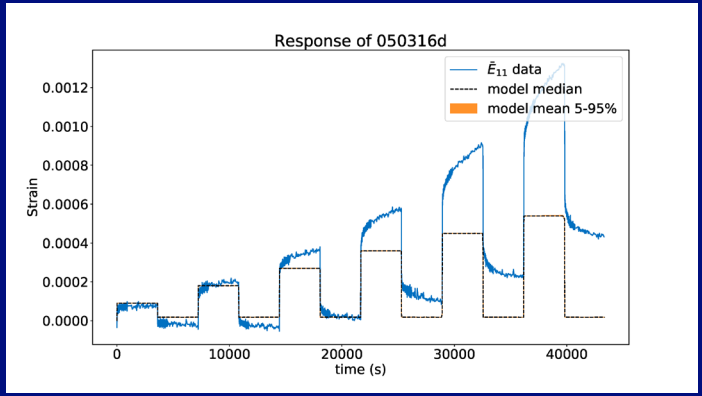
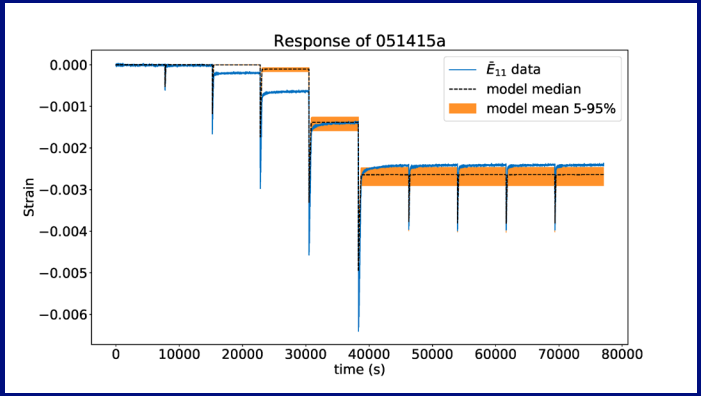
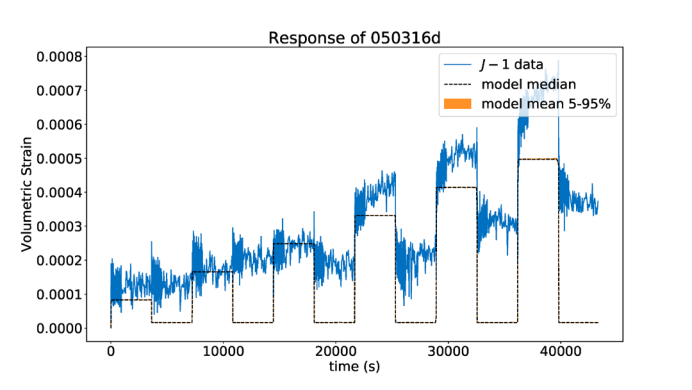
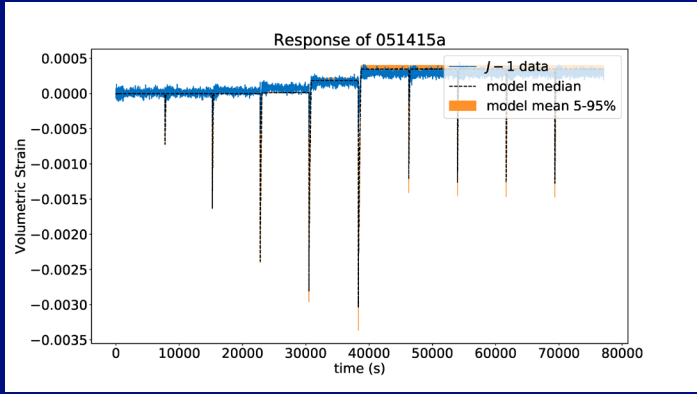
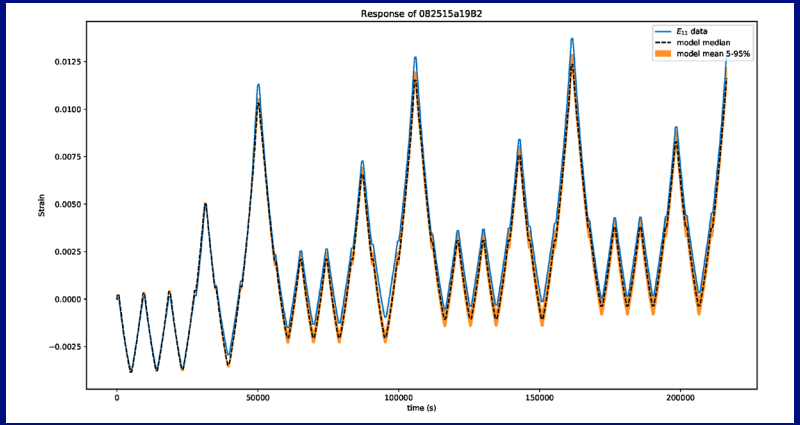


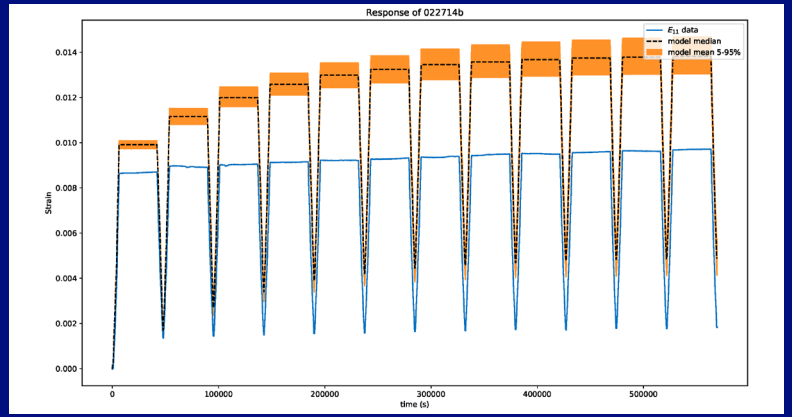


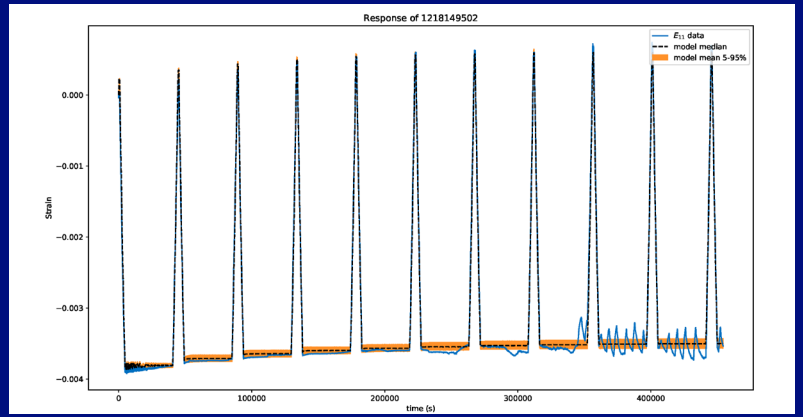




PBX 9502 Irrecoverable Thermal Deformation Calibration







Conclusions

- The VIPor modeling framework offers an enhanced ability to simulate fully coupled thermo-mechanical analyses
- The application of UQ to a constitutive model of this complexity is a first for W-13
- The development of the constitutive model using software best practices and continuous integration is a first for W-13
- The model form of VIPor should be improved for increased fidelity in irrecoverable deformation prediction for tensile and low stress cycles
- Calibration of the pressure-dependent irrecoverable thermal deformation has been delayed due to changing priorities
- Future efforts are desired to incorporate efficient microstructural models for enhanced predictive capability