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Predicting Performance Margins (PPM): Linking the microscale to the macroscale

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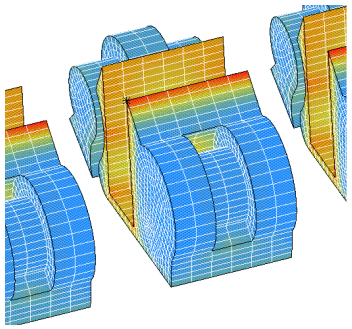
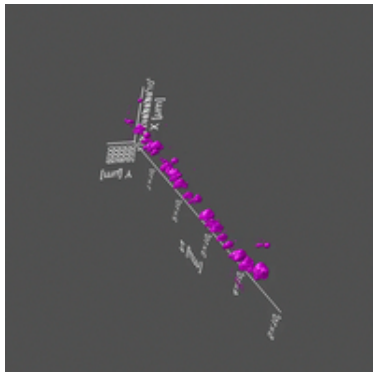
Current materials science gaps in support of the NW mission

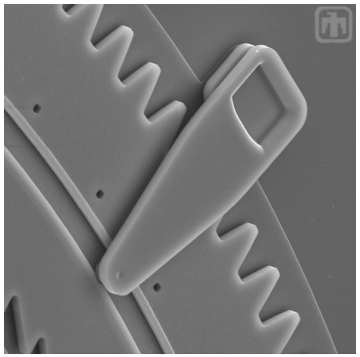
- **Component design for normal and abnormal environments**
  - The iterative, empirical design process is costly and slow.
  - New materials systems require designers to start over.



- **Engineering support for Sandia's Annual Review**
  - Current decisions rely on expert opinion.
  - Risk arises in predicting the as-yet-unobserved.



- **Shrinking component dimensions**
  - Our current statistical approach does not apply to miniaturized components.
  - All small parts are outliers.



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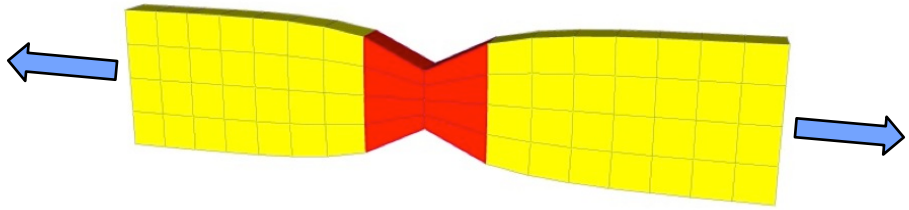
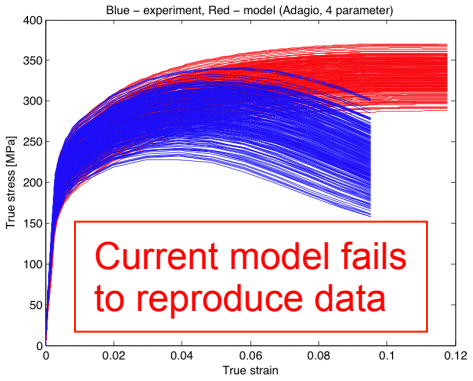
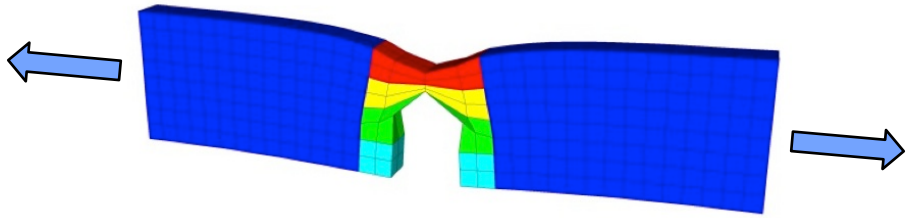
Bridging the materials science gap: Geometric variability in welds

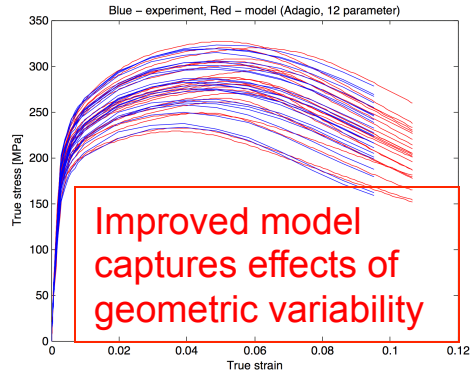
Current design approach (B61 LEP): Use a single-material model with 4 parameters; 8 elements per cross-section.



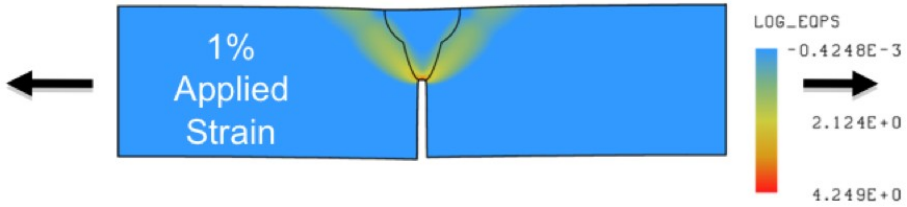


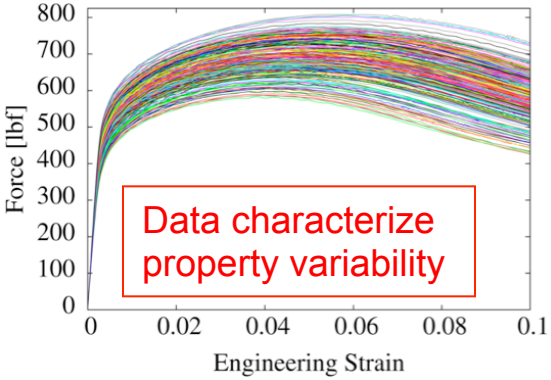
Bridging the gap: Homogenize to 3 material model with 12 parameters; 8 elements with notch per cross-section





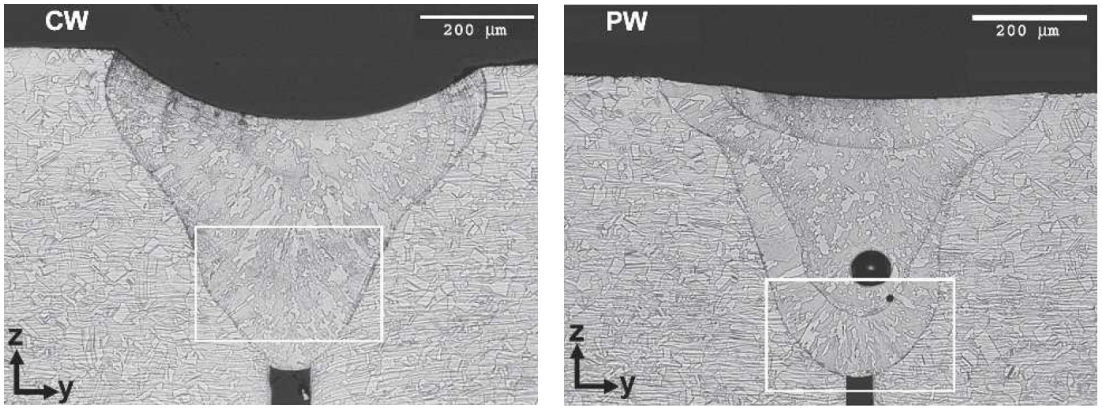
Materials science approach: Computational survey of weld geometries, varying weld depth, plate gap and offset



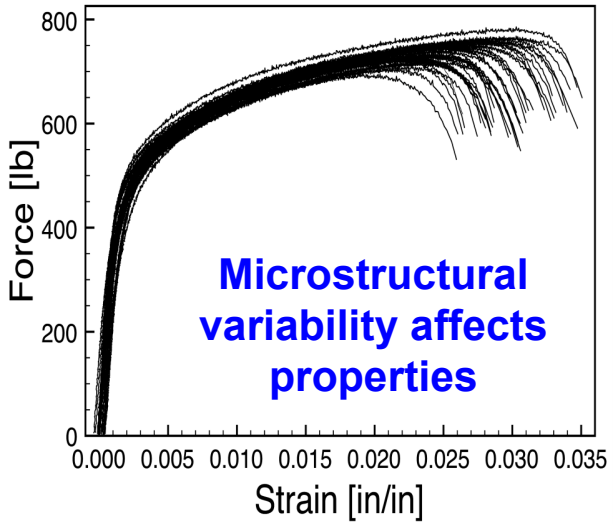


PPM Foundational Problem: Connecting microstructural variability to properties

- In a study of 40 nominally identical welds, we observed large variations in properties caused by local microscopic differences.
- Because of this variability, we must de-rate welds significantly to achieve reliability goals.



Microstructural details vary among weldments



- **PPM Project Goal:** Provide a science-based underpinning for design and analysis capabilities that links microscopic differences to property variability.

Paradigm shift, from the idealistic view that all parts are created equal to the realistic view that structure, properties, and performance are probabilistic.

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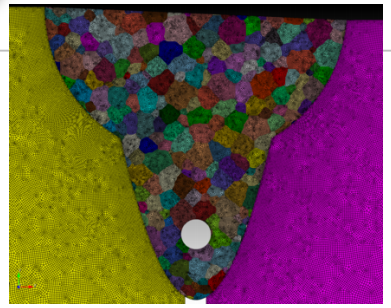
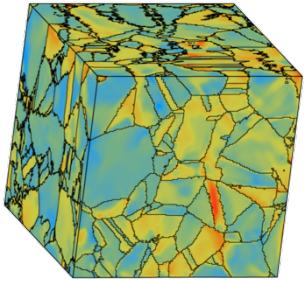
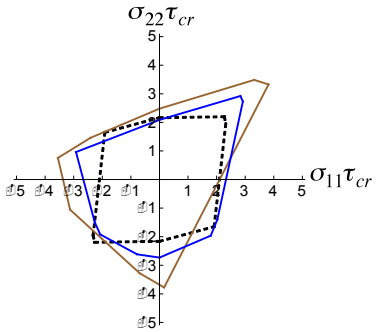
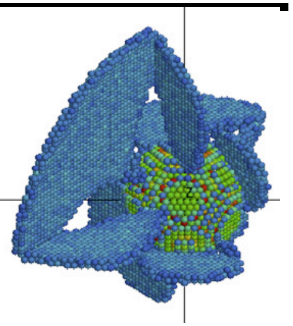
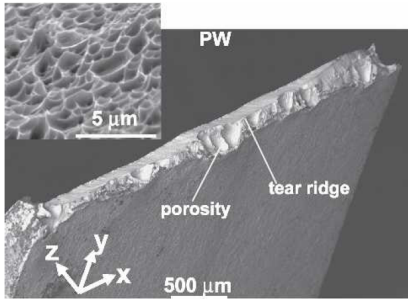
Extend modeling paradigm to capture the effects of microstructural variability

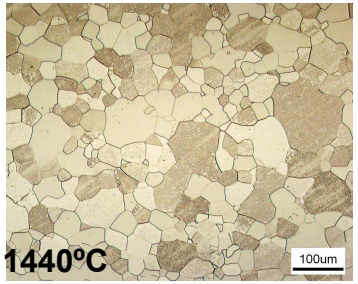


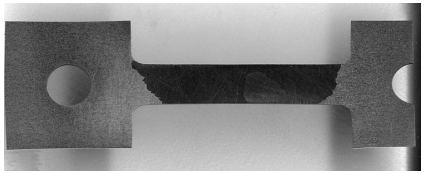


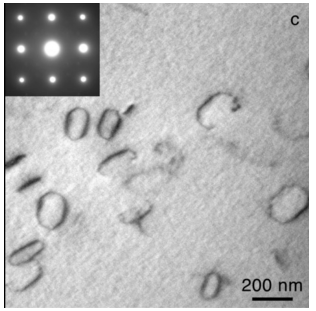












Material performance

Microstructural effects

Single crystal behavior

Atomic scale phenomena

10^0 m
10^6 s

10^{-3} m
10^3 s

10^{-6} m
10^0 s

10^{-9} m
10^{-9} s

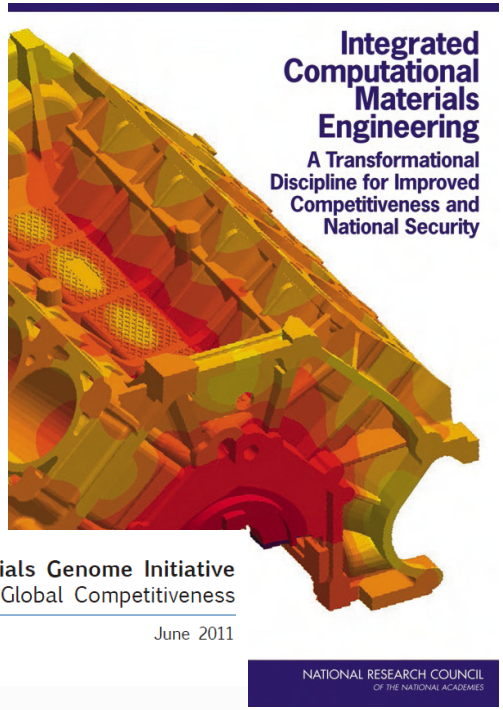
Task 3 | **Task 2** | **Task 1**

PPM adopts ICME best practices to achieve project goals

- The National Academies developed a set of recommendations for successful Integrated Computational Materials Engineering (ICME) programs, which we follow in this project.

- The Office of Science and Technology Policy (OSTP) Materials Genome Initiative seeks to build efforts in this area, with $100M in the White House FY12 budget.

- **The PPM project positions Sandia as a leader in this evolving field.**



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PPM provides broad impact over the long term

- **Customer impact:** Provide science-based models and data to support engineering judgments in future AARs, LEPs, and the Nuclear Weapons campaigns.

- **Materials Science Base:** Sustain and grow the MS&T science base with a view to future NW challenges and needs.

- **Career Development:** Support the scientific growth of early- and mid-career staff members by providing a sustained opportunity to pursue scientific answers to engineering questions.

- **Prototype Best Practices:** Model successful strategies for subsequent materials science projects supporting the NW mission.

  Failure in brittle materials, aging of soft materials, materials in extreme environments, etc.

Project team structure enables collaboration, scientific advances, and impact

Task 1: Nanoscale framework for crack initiation and growth in Ta and Ta alloys

[J Zimmerman, C Weinberger]

Task 2: Microscale effects of defect fields in Ta and Ta alloys

[B Boyce]

Task 3: Connecting microstructural variability to performance margins in structural metals

[C Battaile]

Technical Advisory Council

[S Foiles, D Medlin, J Michael, N Moody, D Reedy, C Robino]

Customer Advisory Council

[B Paulsen (chair), D Balch, E Fang, S Harris, M Hedemann, T Mattsson, J McLaughlin, B Oetken, S Whalen]

External Collaborators

[LLNL, LANL, UT Austin, Michigan State University, Georgia Tech, Caltech, Carnegie Mellon, Cornell, etc.]

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