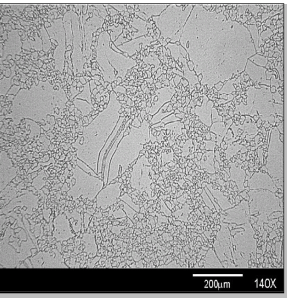
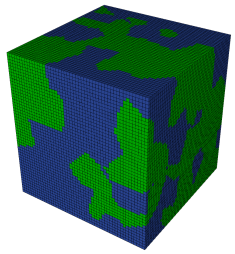
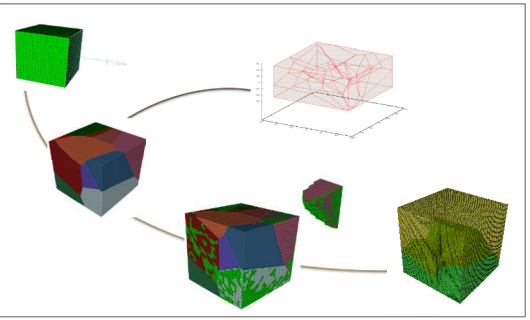
SAND2012-5859P







Effect of Partially Recrystallized Microstructures on Macroscopic Properties

Predicting Performance Margins Project

S. Pitts, A. Brown, J. Emery

Sandia National Laboratories

Exceptional service in the national interest

U.S. DEPARTMENT OF ENERGY

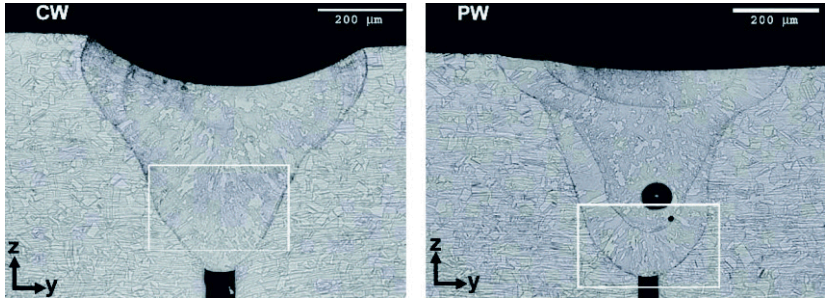
NNSA

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND NO. 2011-XXXXP

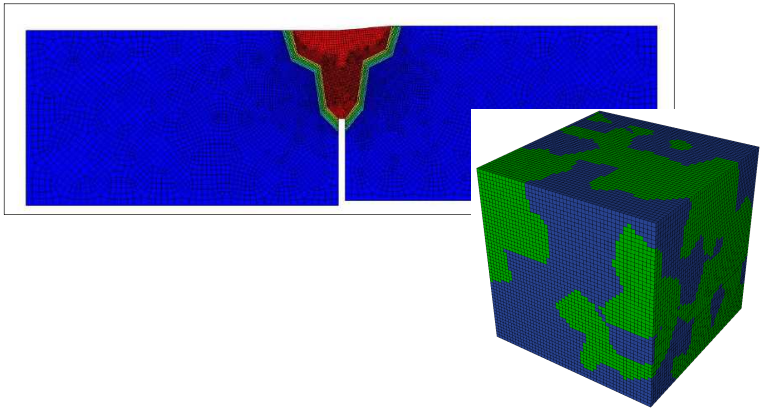
Predict Weld Response Confidently

Accurately predict influence of microstructure on macroscopic response with improved material models

- Scientific insight to engineering issues from a multidisciplinary effort



J. Puskar (2010)



Account for weld variability

- Local microstructure complex

"Continuum-Down" approach

- Establish a paradigm for variability modeling
- Captures geometric variation

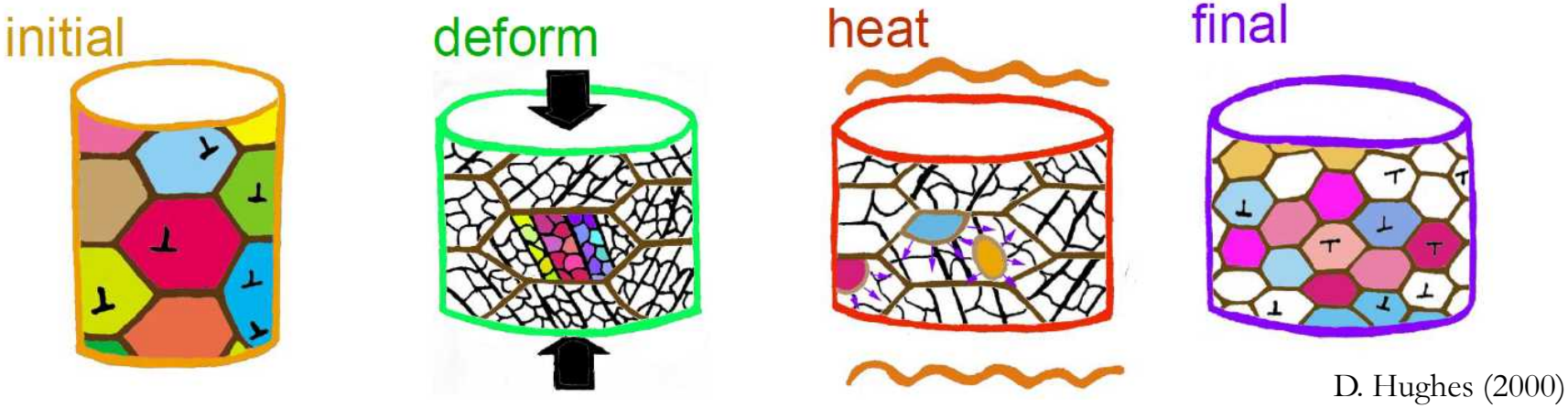
Extend approach to material property variation

- Grain structure, recrystallization

Recrystallization Lowers Strength

Recrystallization erases dislocation structure of worked material

Growth of dislocation free grains around larger worked grains



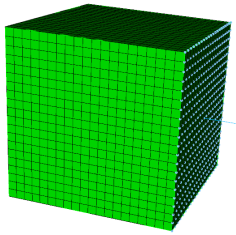
D. Hughes (2000)

Volume averaging of isotropic hardening in continuum model

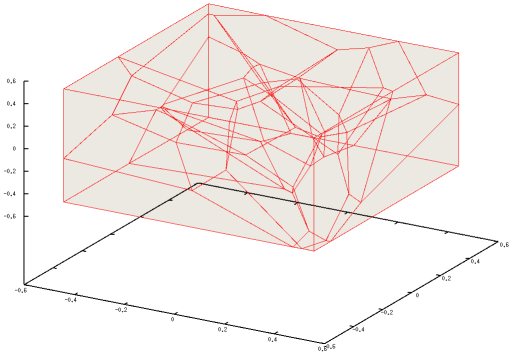
$$\bar{\kappa} = \sum_{i=0}^{n-1} \bar{\kappa}_{X_i - X_{i+1}} (X_i - X_{i+1}) + \bar{\kappa}_{X_n} X_n$$

Validity of continuum model near yield stress

Representative Volume Generation

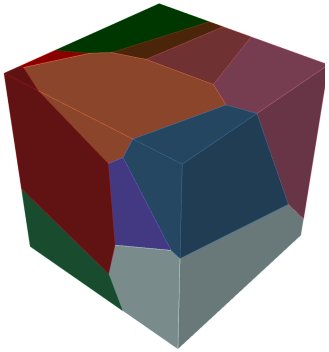


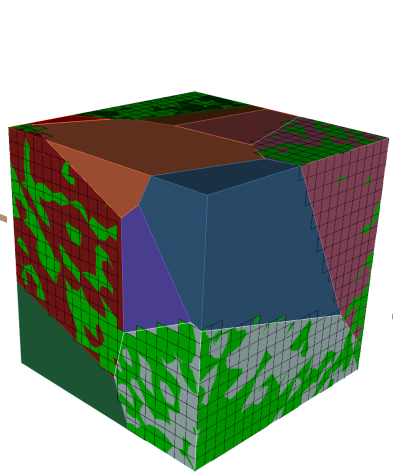
Original mesh and shape created in CUBIT



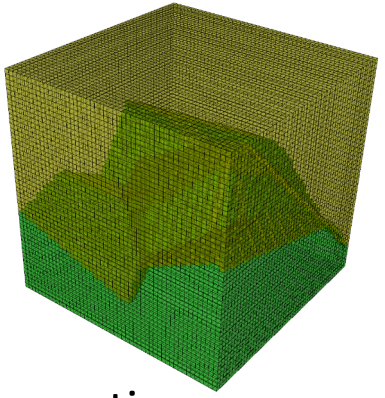
Generate Voronoi Tessellation input data

C. Rycroft. Chaos 19 (2009) 041111



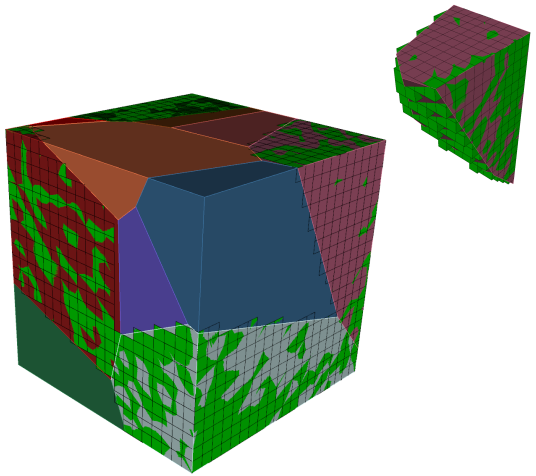


Retain robust hex elements in geometry



Assign material properties

Microstructure Incorporated



Voronoi tessellation structure

- Voronoi cells well accepted grain model
- Python script generates background Voronoi cell structure, hex cell assignment

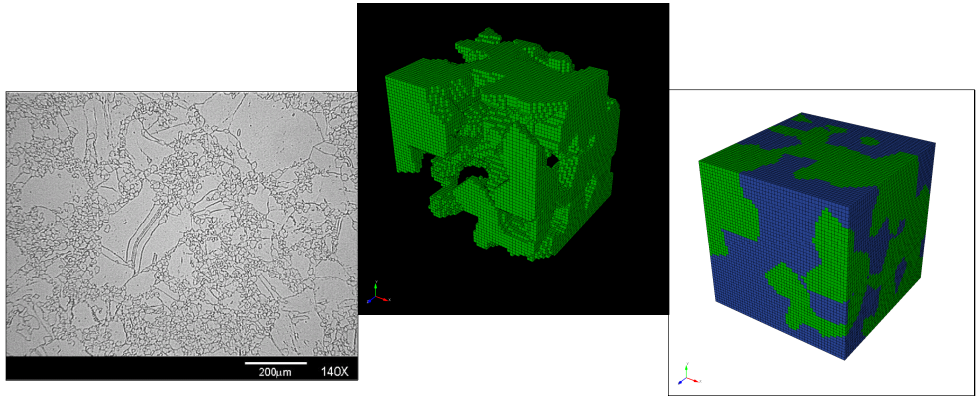
Sort elements into grains, location based

- Hex elements necessary for robustness

J. Emery, M. Veilleux, J. Bishop, C. Battaile

Recrystallized material properties assigned to smallest grains

- Volume fraction controlled
- Python script sorts cells



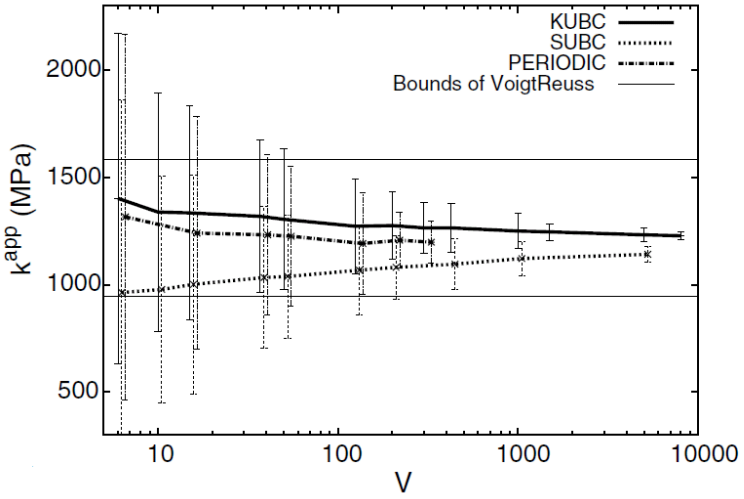
Future Realizations of RVE

Use smaller RVE volumes

- Compensate by averaging over many realizations

Effective properties bounded

- Periodic converges quickest



Heut. J. Mech. Phys. Solids 38 (1990) 813-841

Calculate required realizations

- Compute mean, variance of RVE series apparent properties
- Find size from desired precision

$$2D_z(V) = 2D_z\sqrt{\left({A_3}/{V}\right)^{\alpha}}$$

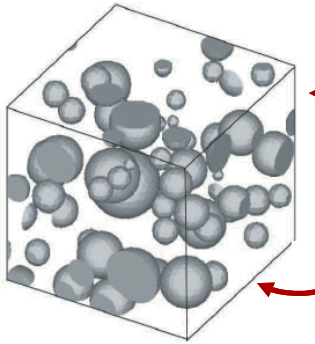
Kanit et.al. Int. J. Solids Struct. 40 (2003) 3647-3679

Apparent homogenized material properties are calculated by averaging the results of many RVE simulations

Preliminary Homogenization Efforts

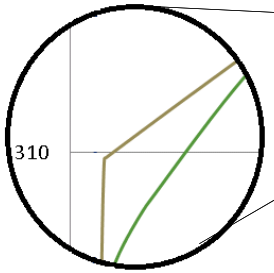
Mechanically periodic boundaries with non-periodic structure

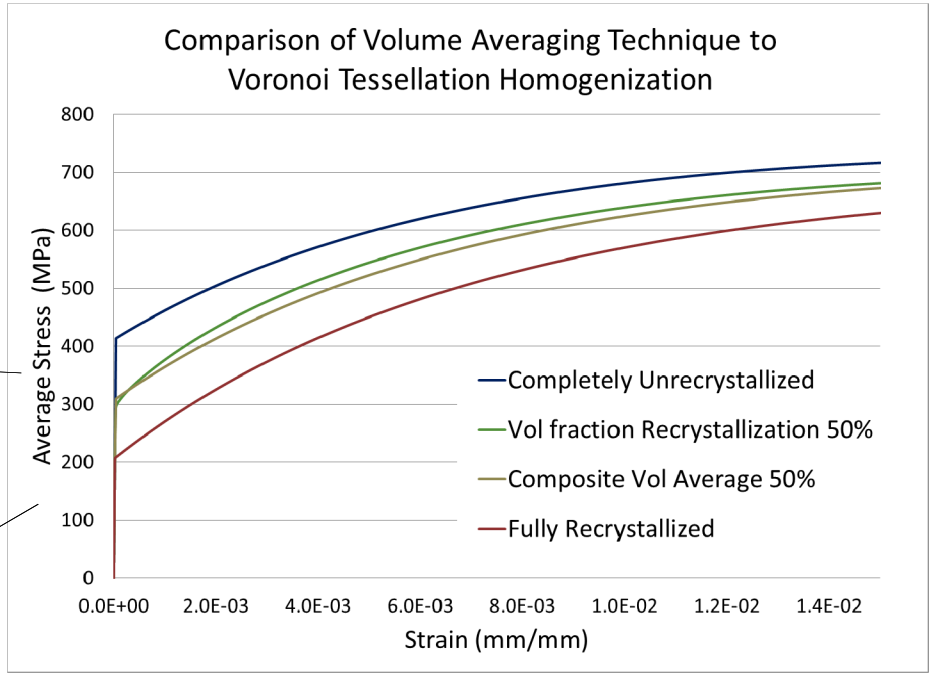
Multiple point constraints allow sides to move while remaining planar



Surfaces constrained to remain parallel to load direction

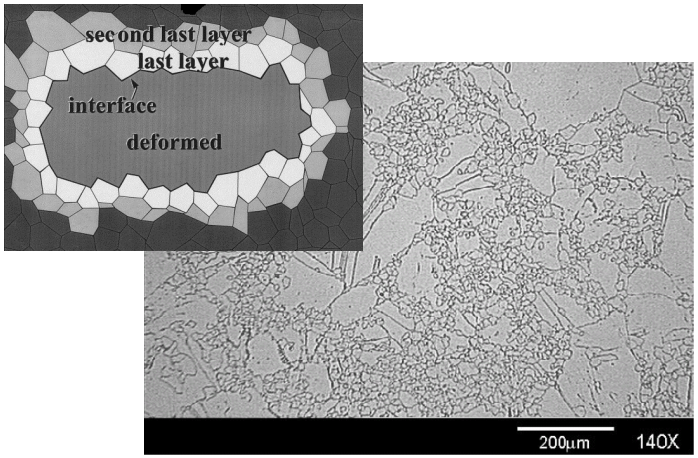
H. Shen and C. Brinson.
J. Mech. Mat. Struct. (2006)
1179-1204





Volume averaging does not fully predict homogenized response

Accurately Reflect Microstructure



Develop python scripting tool

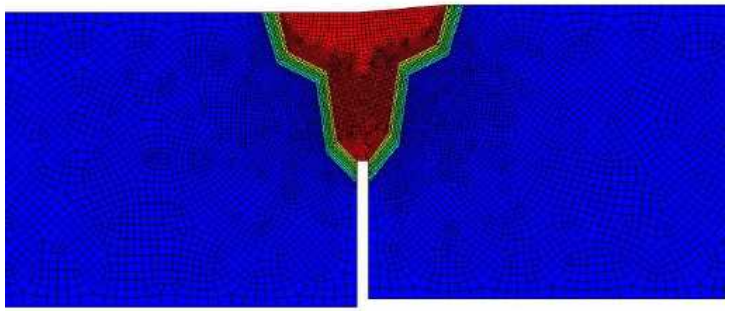
- Identify interfaces among grains
- Interface elements assigned recrystallized material properties
- Volume fraction dictates thickness

Microstructure informs RVE geometry

E. Barker (2011), Ponge and Gottstein (1998) Acta. Mat.

Weld Heat Affected Zone (HAZ)

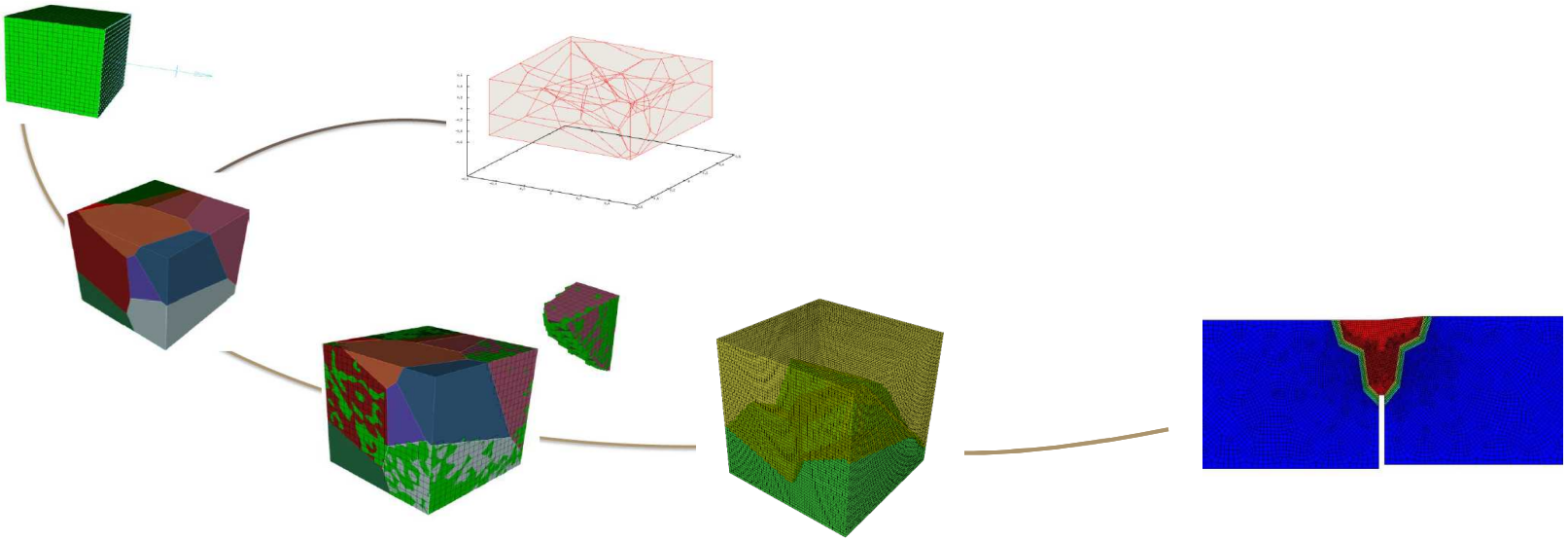
- Model partially recrystallized microstructures in the HAZ
- Effect of variability on macroscale weld response

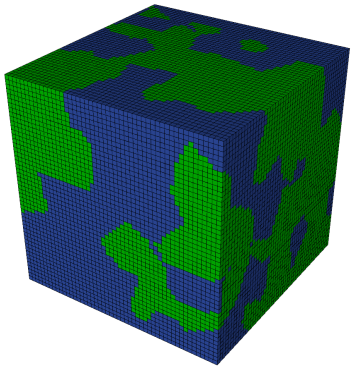


L. Diebler (2012)

Summary

- Validity of continuum recrystallization model examined
- RVE geometry informed by actual microstructure
- Python scripting tools developed
- Target application for Heat Affected Zone (HAZ) model





ACKNOWLEDGEMENTS

Arthur Brown, John Emery, Joe Bishop, Mike Vielleux

Erin Barker, Pacific Northwest National Laboratory

Stephanie Pitts

Washington State University, Computational Mechanics and Materials

Nuclear Energy University Programs Fellow

pitts.stephanie@gmail.com