Leveraging scalable computational materials packages and high-performance computing resources to simulate deformation and damage in polycrystalline metallic materials

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Invited talk at:
High-performance computing (HPC) community meeting
NASA Langley Research Center
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Saikumar “Sai” Yeratapally

Work Experience:
• Research engineer II at National Institute of Aerospace (NIA) (12/2019- current)
• Research engineer I at National Institute of Aerospace (NIA) (10/2017- 12/2019)
• Post-doctoral Research Associate at NIA (3/2016 – 10/2017)
• Research contractor at NASA Langley Research Center (3/2016 - current)

Education:
• Ph.D. in Aeronautics & Astronautics Engineering from Purdue University (12/2015)
• M.S. in Mechanical Engineering from Carnegie Mellon University (12/2010)
• B.E. (Honors) in Mech. Engineering from Birla Institute of Technology & Science (India) (8/2009)

Research Interests:
• Microstructure-performance linkage using crystal plasticity models
• Validation of crystal plasticity models
• Effect-of-defects in additively manufactured polycrystalline materials
• Materials informatics
Presentation outline

- **Background**
  - Polycrystalline materials
  - Strain localization
  - Fatigue crack initiation
  - Certification
  - Integrated computational materials engineering (ICME)
  - Materials genome initiative (MGI) and NASA Vision 2040

- **Crystal plasticity finite element (CPFE) simulations**

- **In-house scalable finite element solver, ScIFEN**
  - Overview
  - Scalability of ScIFEN compared to commercial solvers

- **Validation of CPFE formulation in ScIFEN**
  - Comparing ScIFEN’s predictions with high-energy X-ray diffraction measurements
  - Sources of discrepancy

- **Application of ScIFEN to investigate deformation in polycrystalline materials**
  - Nickel superalloys
  - Aluminum alloys
  - Additively manufactured Titanium alloys
Background: Polycrystalline materials

Echlin, Lenthe et al. (2020) ICME book chapter

Zhu et al. (2018) *Nature Communications*

Proudhon et al. (2018) *Materials*
Background: Strain accumulation

Microstructure of a nickel-base alloy

Strain maps obtained from experiments

Background: Fatigue crack initiation

- Fatigue crack initiation (FCI) in polycrystalline materials is primarily dependent on microstructure, inclusion/defect present in the material

*FCl at twin boundaries*

*FCl at inclusion*

- Linking defect/microstructure attributes to failure mechanisms and hence performance is essential for rapid qualification of materials
- High-fidelity micromechanical simulations provide a platform to quantitatively link defect/microstructure attributes to performance
- Validation of the high-fidelity simulations is important to be able to quantitatively understand the underpinning mechanisms of crack initiation

*Jiang et al. (2015)*

*Yeratapally et al. (2017)*
Background: Certification

Maher M (2014) DARPA Open Manufacturing strategy for accelerating metals additive manufacturing

Building Block Test Structure Required for Certification

<table>
<thead>
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<th>Size Scale</th>
<th>Analysis Validation</th>
<th>Components</th>
<th>Sub-components</th>
<th>Elements</th>
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<td>Cost ($M)</td>
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<td>2</td>
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</table>

Maher M (2014) DARPA Open Manufacturing strategy for accelerating metals additive manufacturing
Background: ICME

ICME: Integrated Computational Materials Engineering

http://www.dierk-raabe.com/multiscale-modeling/
The Materials Genome Initiative (MGI) seeks to uniquely and seamlessly integrate computation, experiment, and data to fuel the successful discovery of new materials and their more rapid deployment and incorporation into manufactured products.

-MGI white paper (2011)

NASA Vision 2040: “Accelerate model-based concurrent design, development, and deployment of materials and systems throughout the product lifecycle for affordable, producible aerospace applications.”

-Liu, Furrer et al. (2018)
NASA/CR—2018-219771
Polycrystalline materials
Strain localization
Fatigue crack initiation
Certification
ICME, MGI, NASA vision 2040
Crystal plasticity finite element (CPFE) simulations

➢ Link microstructure to heterogeneous accumulation of plastic strain/damage

➢ Provides complementary information that is not easy to obtain even from some high-fidelity experiments (for example evolution of sub-surface plastic strain)

Yeratapally et al. (2016) Acta Materialia
In-house scalable finite element solver, ScIFEN

ScIFEN¹: Scalable Implementation of Finite Elements by NASA

- ScIFEN is built on PETSc
- Leverages a suite of data structures and routines to achieve scalability.
- Utilizes open-source libraries like MOAB and HDF5 for parallel I/O operations.
- Scales well over thousands of processors, compared to commercial packages
- Includes phenomenological crystal plasticity (CP) models
- Interfaces with DREAM.3D¹¹, Gmsh¹² and SPPARKS¹³

Developers: Dr. James E. Warner, Dr. Geoffrey F. Bomarito
Dr. Jacob D. Hochhalter

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1. https://software.nasa.gov/software/LAR-18720-1
2. www.hdfgroup.com
7. www.netlib.org/blas/
8. www.netlib.org/lapack
10. www.boost.org/
11. DREAM.3D http://dream3d.bluequartz.net/
Scalability of ScIFEN vs. Commercial FE solvers

FE solver: ABAQUS
Material: Inconel (nickel alloy)
Strain applied: 1%
CPUs: 320
Degrees of freedom (DoF): ~ 27 million
Simulation time: ~14 days
Source: Prithivirajan et al. (2021) Mater. & Design 197:109216

FE solver: ScIFEN
Material: Inconel (nickel alloy)
Strain applied: 1%
CPUs: 640
DoF: ~85.1 million
Simulation time: ~44 hours
Source: Yeratapally et al. (2021) IMMI 10(2):196-217
Additive manufacturing (AM) modeling challenge

**Final build**

![Final build image]

**Fully machined tensile coupon**

![Fully machined tensile coupon image]

Source: ARFL’s AM modeling challenge series

Test cell

![Test cell diagram]

**HEDM:** High energy X-ray diffraction microscopy

**near-field HEDM (nf-HEDM):** provides data to reconstruct individual grain morphologies

**far-field HEDM (ff-HEDM):** provides grain average orientations, elastic strains and centroids

AM modeling challenge: problem statement

**Challenge problem:** Given the stress strain curve, serial-sectioned and reconstructed 3D microstructure, predict grain-average elastic strain tensor for 28 “challenge” grains at six different macroscopic load states, S1 through S6

Source: ARFL’s AM modeling challenge series
CPFE simulations using ScIFEN

ScIFEN\(^1\): Scalable Implementation of Finite Elements by NASA

- 3D microstructure\(^*\) of additively produced Inconel alloy
- Finite element mesh has \(~85\) million degrees of freedom
- Global strain applied in YY direction: 1%
- CP formulation: Strain-gradient based\(^{11}\)
- Simulation time: \(~44\) hours on 640 processors on K-cluster


1. https://software.nasa.gov/software/LAR-18720-1
2. www.hdfgroup.com
7. www.netlib.org/blas/
8. www.netlib.org/lapack
10. www.boost.org/
11. Acharya et al. (2000), JMPS 48

CPU Performance

<table>
<thead>
<tr>
<th>Year</th>
<th>Sandy Bridge 40 nodes</th>
<th>Ivy Bridge 40 nodes</th>
<th>Skylake 16 nodes</th>
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<td>2012Q1</td>
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<td>0.99(\times)</td>
<td>1.20(\times)</td>
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<tr>
<td>2013Q3</td>
<td></td>
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<tr>
<td>2017Q3</td>
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</tbody>
</table>

In collaboration with Dr. David Wagner
ScIFEN’s predictions vs. ff-HEDM measurements

CP predictions vs. ff-HEDM measurements

Observations:
- There is a good agreement between CP predictions and ff-HEDM measurements in the elastic regime (S1-S3)
- Deviations start to develop in plastic regime (S4-S6)
Discrepancy 1: Boundary conditions

Strain maps of total strain in YY direction, generated at global strain of 1%

Non-cumulative L2 norm calculated at each macroscopic load state, $S_k$

**BC1**: Fully constrained bottom face

*Only one corner node on –Y face fully fixed and one edge fixed in X and Y directions*

**BC2**: Relaxed boundary conditions

$L2_{S_k} = \sum_{n=1}^{N} \sqrt{\sum_{i=1}^{6} \left( (E_{i})_{S_k}^{g_n} - (e_{i})_{S_k}^{g_n} \right)^2}$

(E) is ff-HEDM measurement; $(e_{i})_{S_k}^{g_n}$ is CP prediction; $S_k$ is macroscopic stress state; $g_n$ is grain ID; $N$ is # grains
Discrepancy 2: Missing physics (stress relaxation)

Far-field X-ray measurement of evolution of YY component of grain-average elastic strain in each of the 28 grains

CPFE prediction of evolution of YY component of grain-average elastic strain in each of the 28 grains

**Observation**: Phenomenological CP model used is unable to predict stress relaxation
Discrepancy 2: Missing physics (stress relaxation)

Setup of creep experiment at advanced photon source (APS)

- Stress relaxation during creep loading at 85% of the yield stress
- An intense slip band developed at the location of the corresponding grain that experienced stress relaxation


Journal: Integrating Materials and Manufacturing Innovation (IMMI)

Special Issue: Metal Additive Manufacturing Modeling Challenge Series 2020
Crack incubation in polycrystalline nickel alloy
Grain-particle interaction using CPFE simulations

Test specimen

Statistically equivalent 3D microstructure*

Opacity adjusted to show particles

FE mesh has:
- 33.3 million quad. tetrahedral elements
- 45.3 million nodes, hence 135 million DoF

Strain applied: 1.5%
CPUs: 1000
Simulation time: ~ 40 hours.

Stress state of just particles

FE problem solved using ScIFEN

* Created using DREAM.3D (http://mai.bluequartz.net/)
Factors influencing stress-state of particles

- Particles aligned with load axis experience high stresses.
- Particles with large free-surface areas are subjected to higher stresses.
For more detailed discussion

Scatter in fatigue performance

Polycrystalline U720 alloy


American airlines Boeing 767, 2006


Boeing 767-223, 2002

Air safety investigation report 200205780


Accounting for fatigue scatter due to microstructure

**Statistically representative microstructures**

**Heterogeneous stress field**

Predicted scatter in fatigue
Fatigue crack growth in AA7075-T651 alloy

Crack incubation ($N_{inc}$) occurs very early in life and is subject to microstructure-sensitive variation.

Multiscale simulation to compute the life of the structure consumed by incubation, nucleation and propagation of microstructurally-small cracks ($N_{MSC}$).

Traditional continuum fracture mechanics, FRANC3D, to compute the life of the structure consumed by growth of microstructurally-large cracks ($N_{MLC}$).

$$N_{total} = N_{inc} + N_{MSC} + N_{MLC}$$
Digital twin feasibility study: Non-deterministic estimation of fatigue life

Simulate variability in microstructure

- 100 microstructure instantiations created using DREAM.3D

Yeratapally, Leser et al. (2020) Engineering fracture mechanics

November 4th, 2021

HPC community meeting at NASA LaRC

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Digital twin feasibility study: Non-deterministic estimation of fatigue life

Simulate variability in microstructure

Philips XL-30, ESEM

Test specimen

Al 7075 microstructure

Sintay, Rollet, 2010

Microstructurally-small fatigue crack growth (MSFCG) data (from model)

Paris law

\[
\frac{da}{dN} = C(\Delta K)^m
\]

Probability density

Probability density

Details of one of the 100 simulations

- # Elements: 18 million Quadratic Tet elements
- # Nodes: ~25 million nodes
- # DoF: ~75 million
- Strain applied: 0.6% in XX direction (elastic regime)
- # cycles: 10
- Total run time: ~5 hrs on 400 procs
- FE solver: ScIFEN
The expected value of predicted fatigue life had an absolute percent error of 9.5% when compared to a tested specimen.

Linear elastic fracture mechanics technique was used to model fatigue crack growth in a homogeneous material while maintaining and propagating the uncertainty quantified at the micro-scale to the final prediction.

Not all sources of uncertainty were quantified and propagated in this case study, the methods used are intended to be scalable to more realistic applications.
For more detailed discussion

Laser powder-bed fusion: An additive manufacturing (AM) technique that uses a high-power density laser to melt and fuse metallic powders together into a 3D component.
Effect-of-defects on performance of additive materials

AM process simulation SPPARKS\textsuperscript{1}

Use Output from SPPARKS and generate .stl files of grains using DREAM.3D\textsuperscript{2}

DREAM.3D\textsuperscript{2}/Gmsh\textsuperscript{3}

Use ScIFEN\textsuperscript{4} to solve for heterogeneous stress/strain fields

Cut section views of 3D microstructure

\[\varepsilon_{yy} = 0.075, \quad 0.06, \quad 0.04, \quad 0.02, \quad 0.00 \]

\[\varepsilon_{zz} = 3\% , \quad 2\% , \quad 1\% \]

[2] dream3d.bluequartz.net

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For more detailed discussion

Summary

• Discussed why computational materials models are required to realize and achieve the goals of MGI and NASA Vision 2040
• Use of crystal plasticity finite element (CPFE) simulations
• *In-house* finite element (FE) solver, ScIFEN
  ➢ Scalability of ScIFEN compared to commercial FE solvers
• Validation of CPFE formulation in ScIFEN
  ➢ Compared predictions with high energy X-ray diffraction microscopy measurements
  ➢ Identified model discrepancies
• *Application of ScIFEN to understand deformation, crack initiation and growth in polycrystalline alloys*
  ➢ Particle cracking in nickel alloy
  ➢ Short crack growth in aluminum alloy
  ➢ Effect-of-process specific defects in additively produced Titanium
Acknowledgements

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  ➢ Transformational Tools and Technologies (TTT) project (FY 19 thru FY22)
  ➢ Internal Research and Development (IRAD) projects (FY19, FY20)
  ➢ Convergent Aeronautics Solutions (CAS): Digital Twin project (FY 16, FY17)

• A huge thanks to everyone who collaborated in the work discussed
  ➢ Drs. Patrick Leser, Jacob Hochhalter, Christapher Lang, James Warner, Geoffrey Bomarito, David Wagner, John Newman, Timothy Ruggles, Edward Glaessgen, Albert Cerrone
Thank you!