# 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
November 4th, 2021

# Presenter biography

## 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)

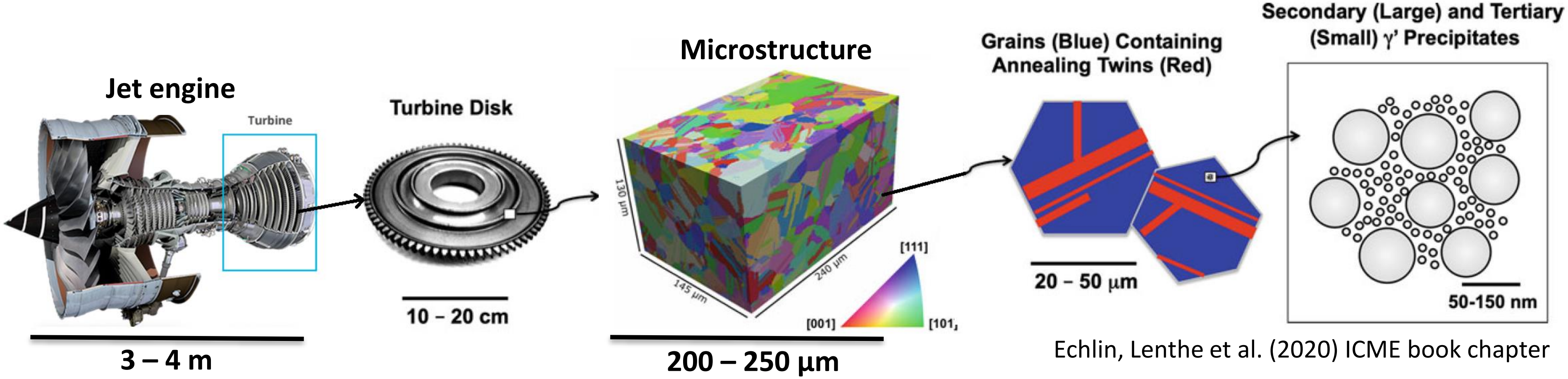
**Education**:
- Ph.D. in Aeronautics & Astronautics Engineering from Purdue University (12/2015)
- M.S. in Mechanical Engineering from Carnegie Mellon University (12/2010)
- B.E. (Honors) in Mech. Engineering from Birla Institute of Technology & Science (India) (8/2009)

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

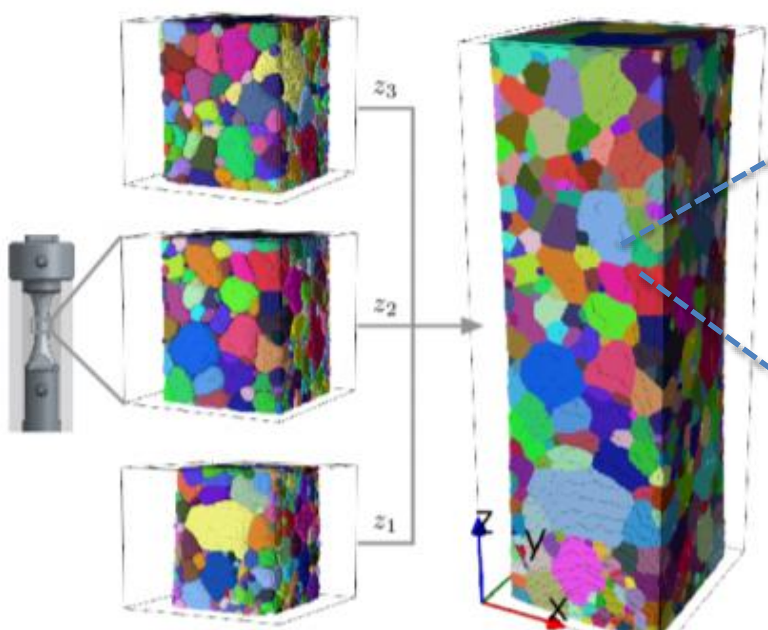
# Presentation outline

- 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

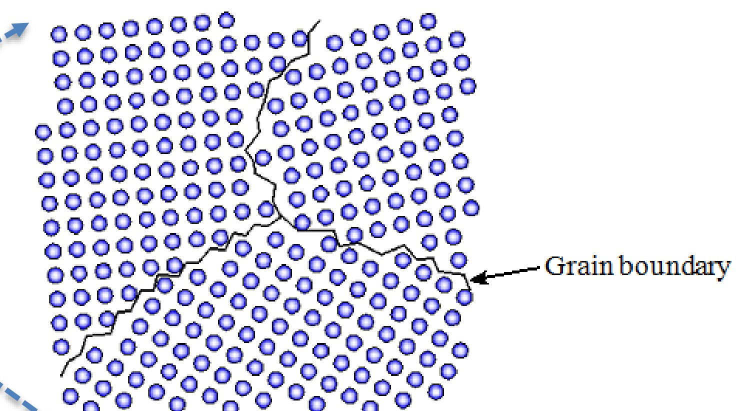
# Background: Polycrystalline materials




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




Proudhon et al. (2018) *Materials*

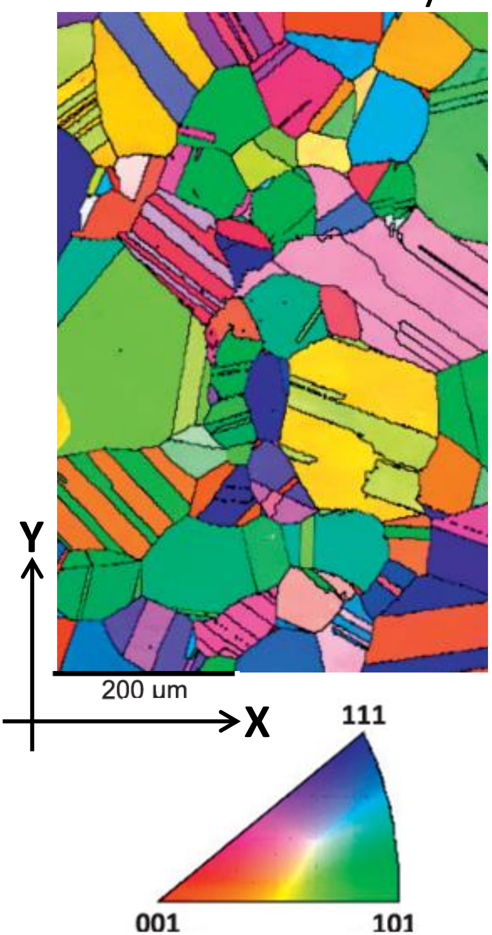


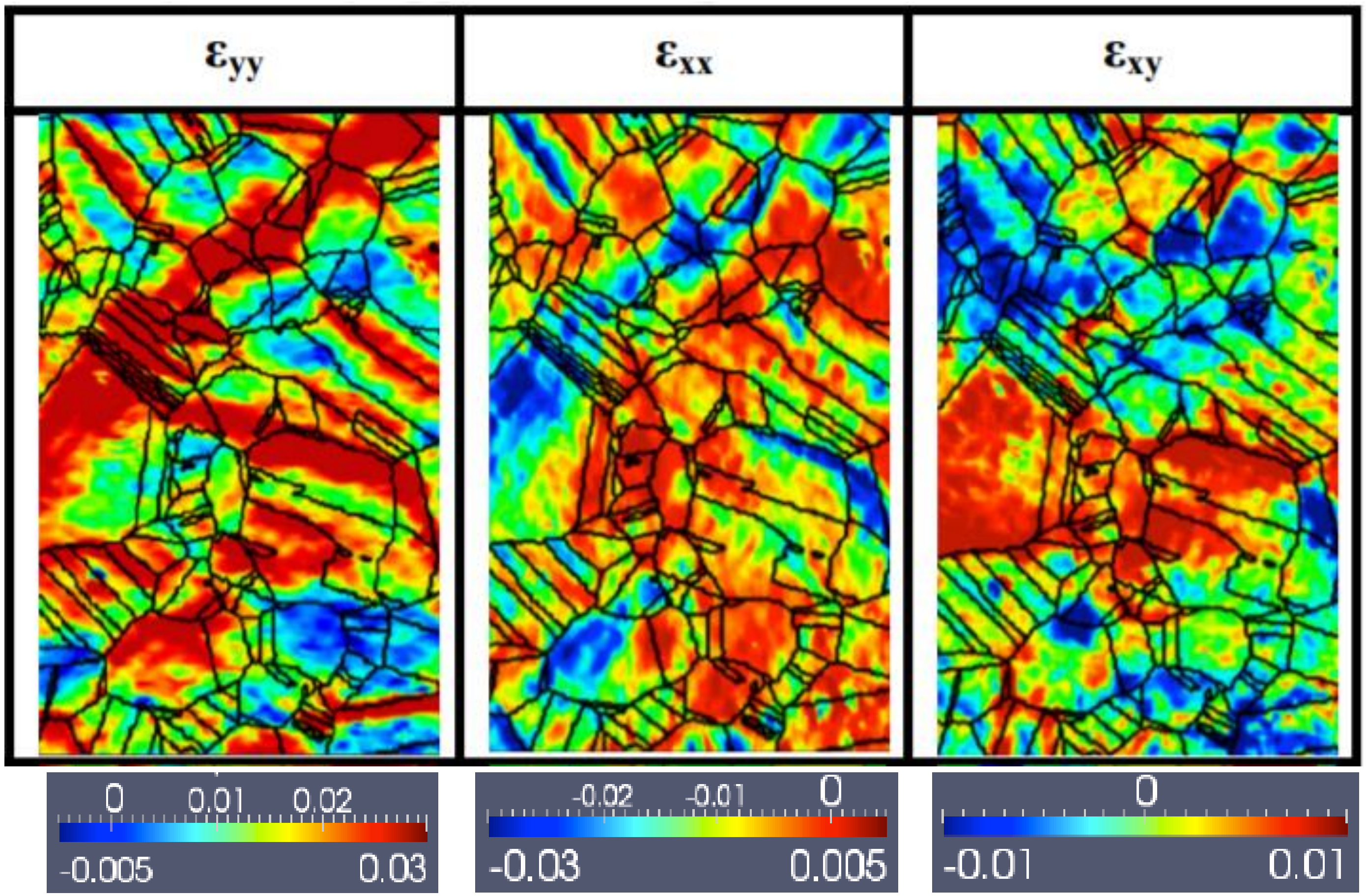

Zhu et al. (2018) *Nature Communications*

# Background: Strain accumulation

Strain maps obtained from experiments

**Microstructure** of a nickel-base alloy



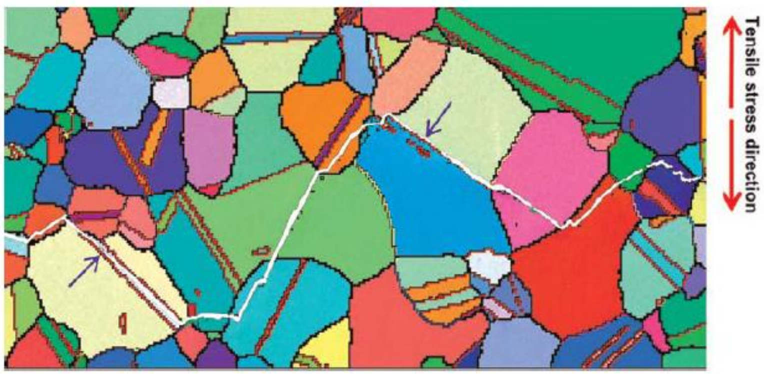




Sangid, Yeratapally, Rovinelli (2014) AIAA SciTech Proceedings

# Background: Fatigue crack initiation

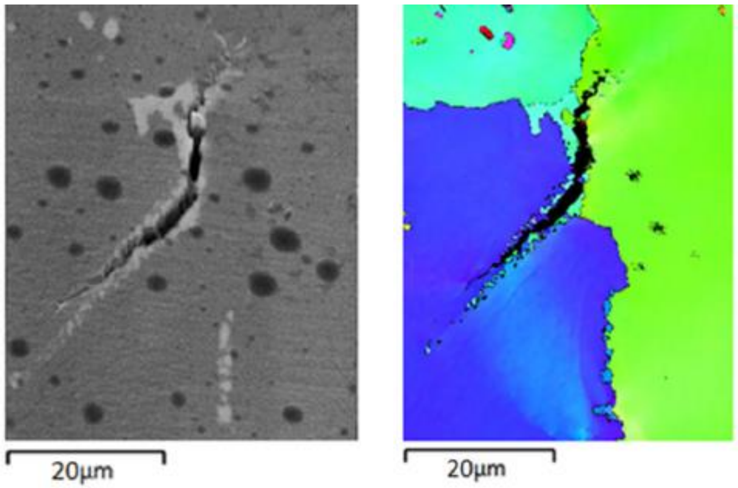
- Fatigue crack initiation (FCI) in polycrystalline materials is primarily dependent on microstructure, inclusion/defect present in the material

*FCI at twin boundaries*




*Jiang et al. (2015)*

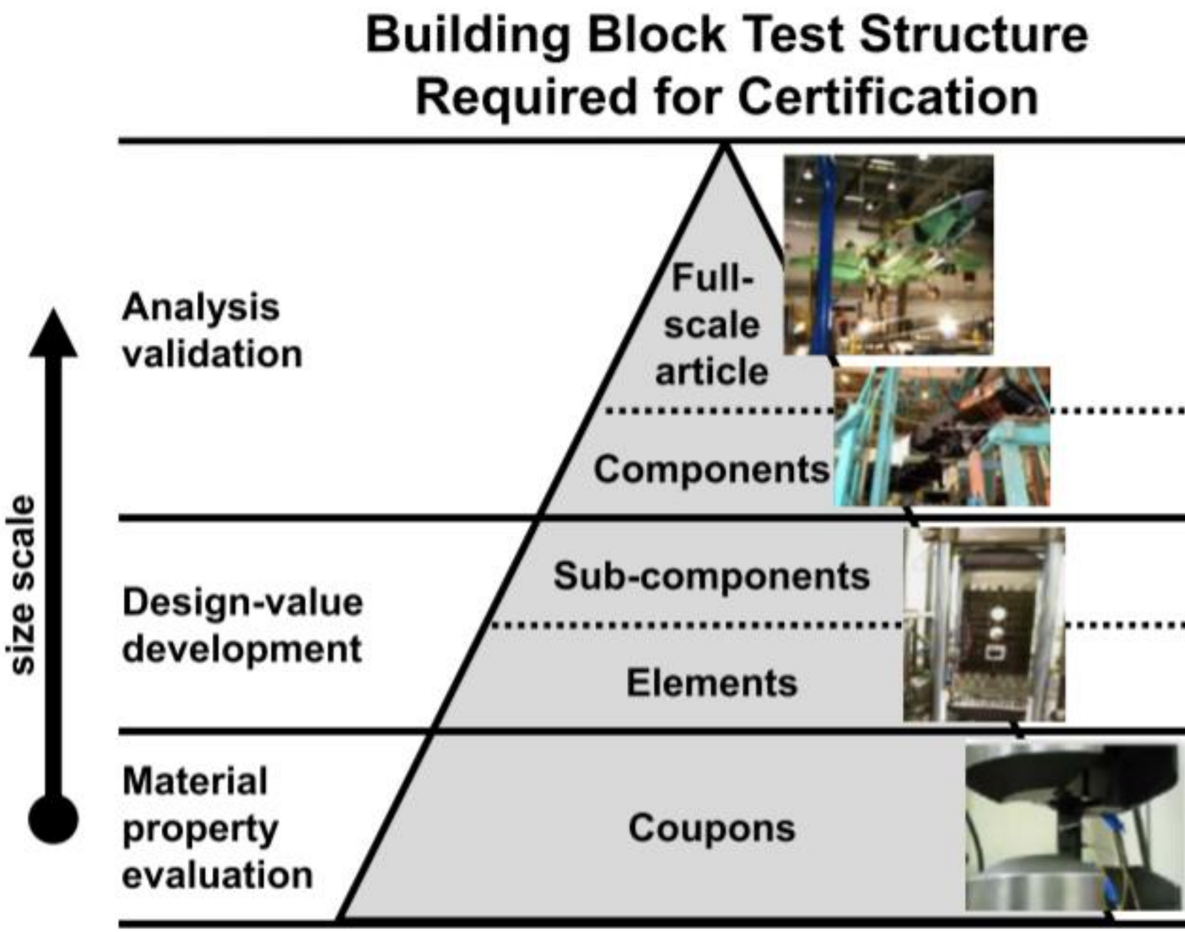
*FCI at inclusion*




*Yeratapally et al. (2017)*

- 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

# Background: Certification

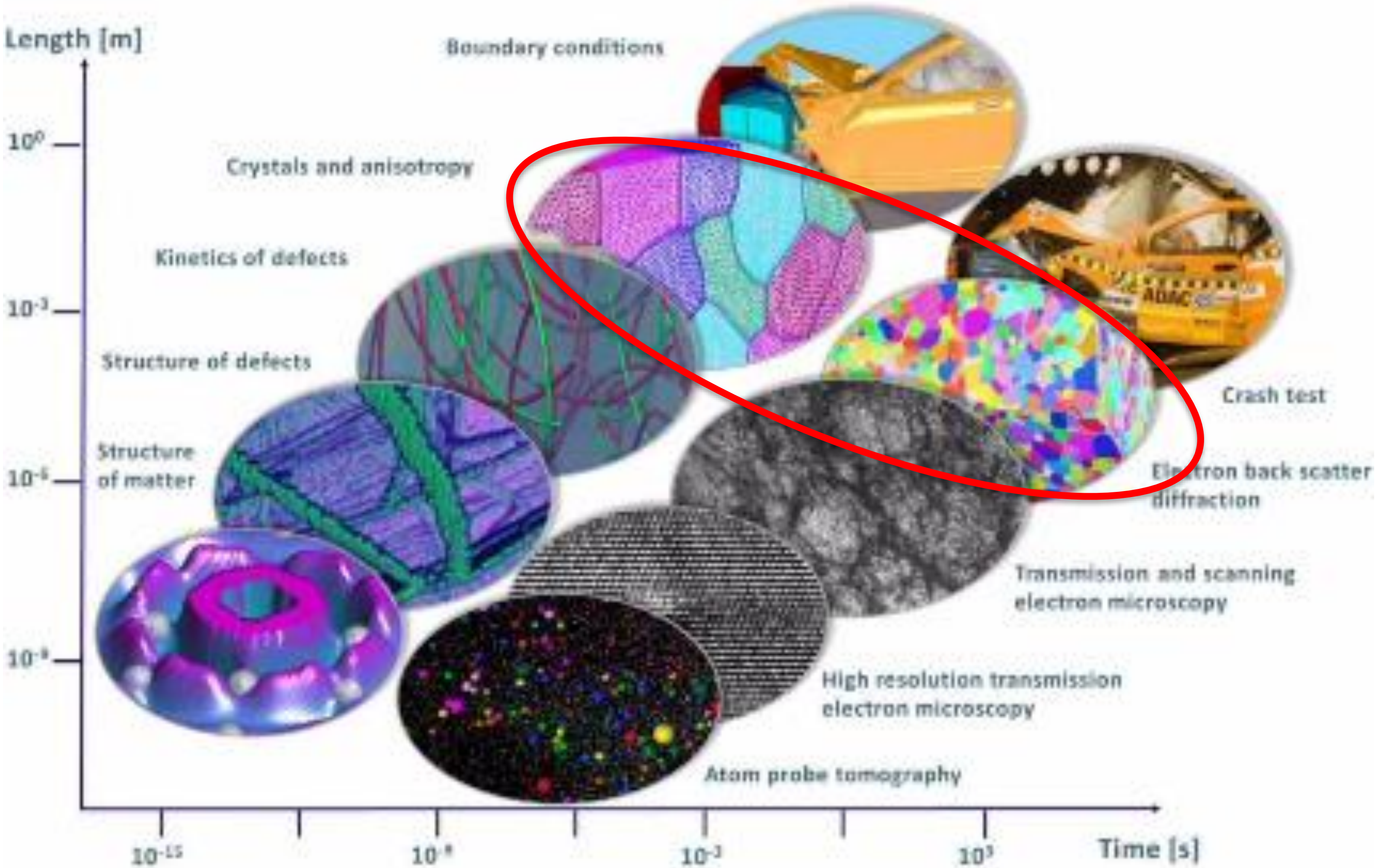



| | Specimen Count | Cost ($M) | Time (Yrs) |
|---|---|---|---|
| Full-scale article | 2-3 | 100-125 | 4 |
| Components | 10-30 | 10-20 | 3 |
| Sub-components | 25-50 | 10-35 | 3 |
| Elements | 2000-5000 | 10-35 | 3 |
| Coupons | 5000-100,000 | 8-15 | 2 |

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

# Background: ICME

**ICME: Integrated Computational Materials Engineering**

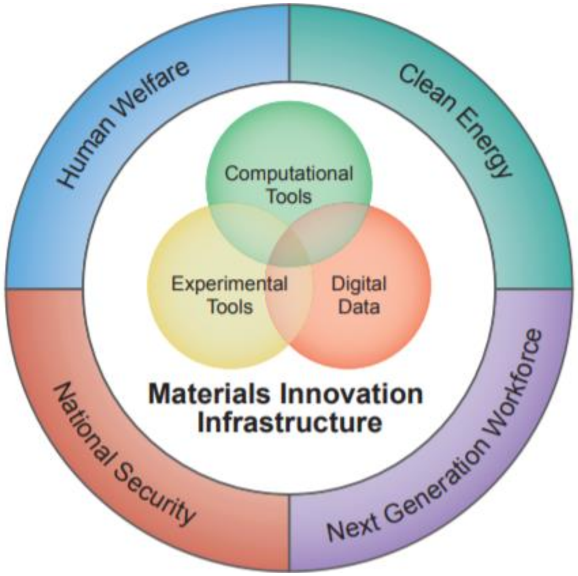



http://www.dierk-raabe.com/multiscale-modeling/

# Background: Materials genome initiative and Vision 2040

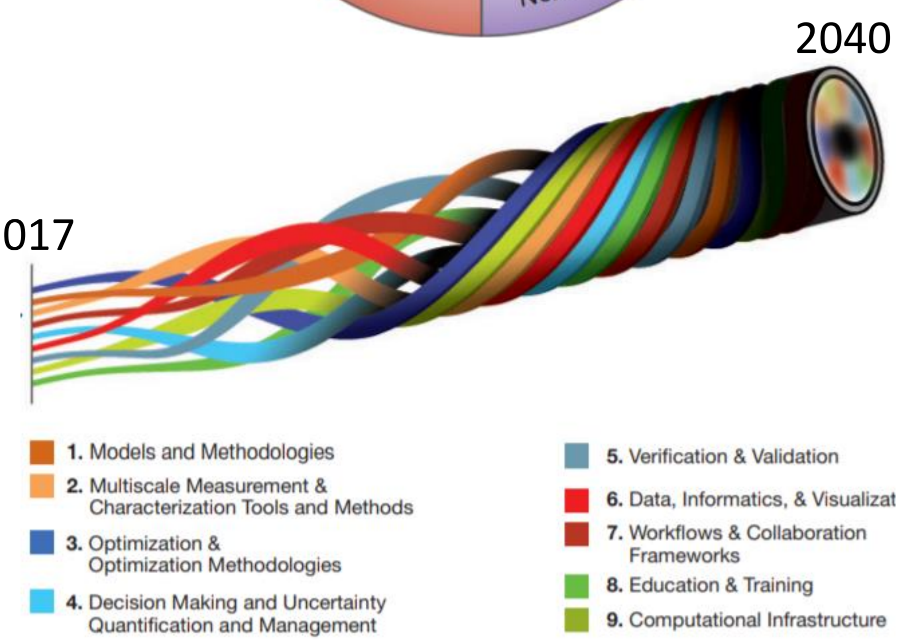
*The Materials Genome Initiative (MGI) seeks to uniquely and seamlessly integrate computation, experiment, and data to fuel the successful discovery of new materials and their more rapid deployment and incorporation into manufactured products.*

-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



# Background

Polycrystalline materials ✓

Strain localization ✓

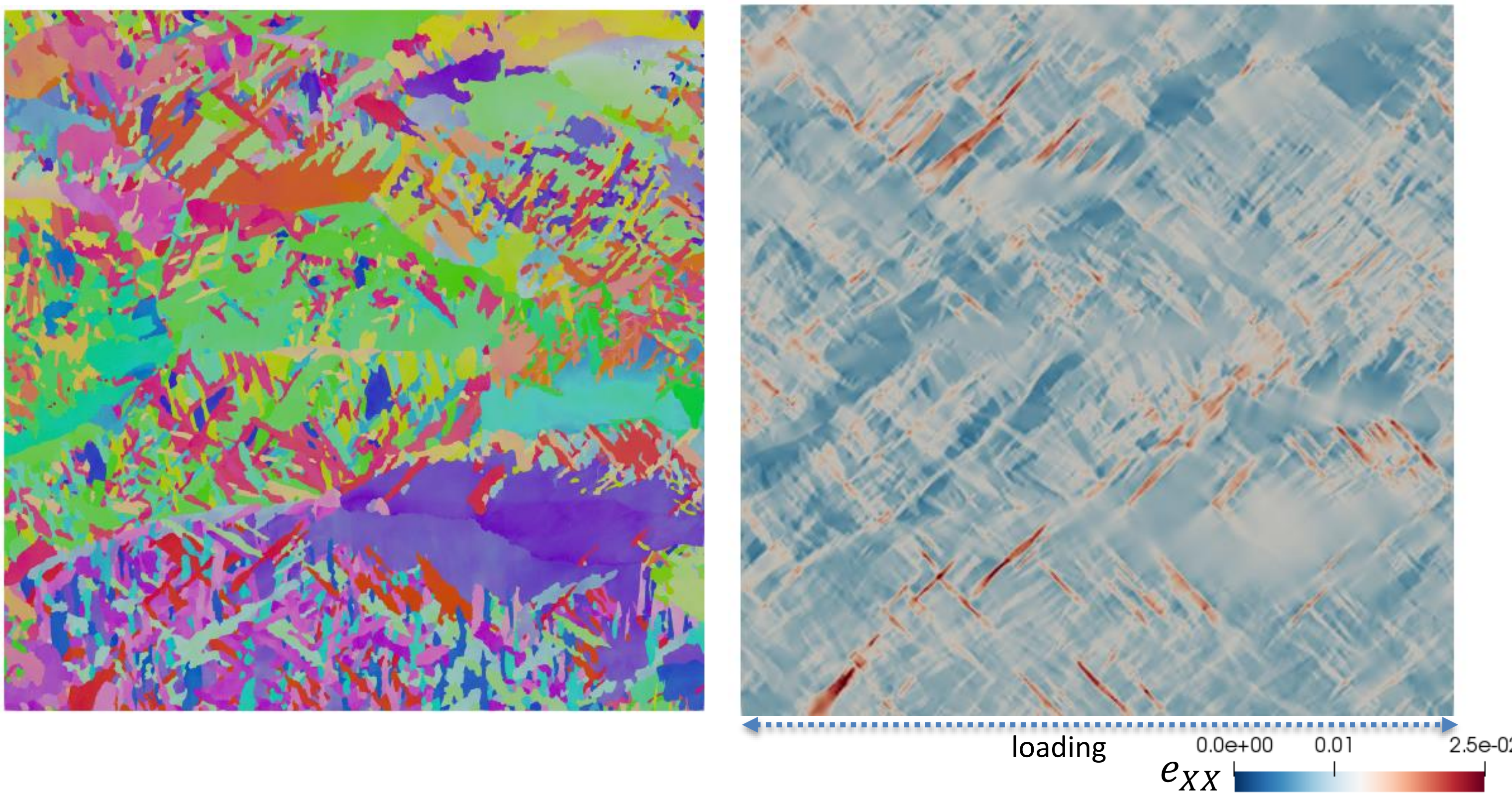
Fatigue crack initiation ✓

Certification ✓

ICME, MGI, NASA vision 2040 ✓

# Crystal plasticity finite element (CPFE) simulations

- Link microstructure to heterogeneous accumulation of plastic strain/damage

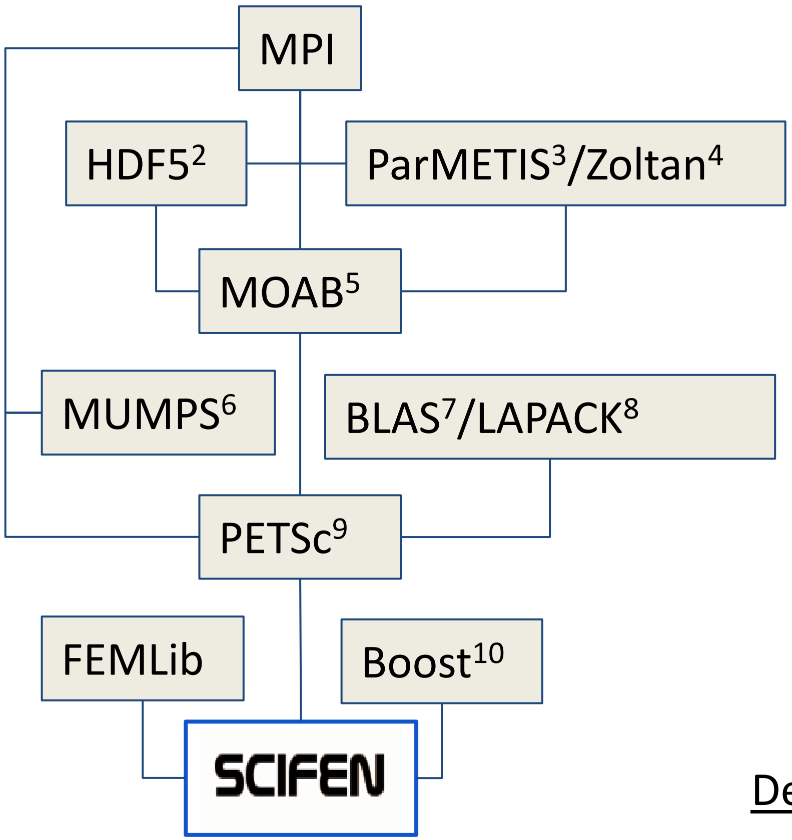



- Provides complementary information that is not easy to obtain even from some high-fidelity experiments (for example evolution of sub-surface plastic strain)

*Yeratapally et al. (2016) Acta Materialia*

# *In-house* scalable finite element solver, ScIFEN

ScIFEN[1]: Scalable Implementation of Finite Elements by NASA



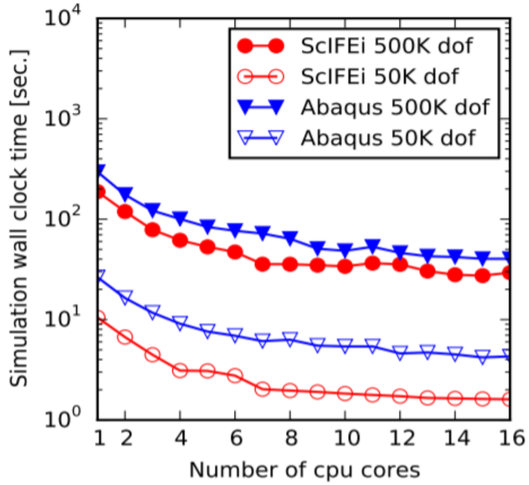

- ScIFEN is built on PETSc
- Leverages a suite of data structures and routines to achieve scalability.
- Utilizes open-source libraries like MOAB and HDF5 for parallel I/O operations.
- Scales well over thousands of processers, compared to commercial packages
- Includes phenomenological crystal plasticity (CP) models
- Interfaces with DREAM.3D[11], Gmsh[12] and SPPARKS[13]

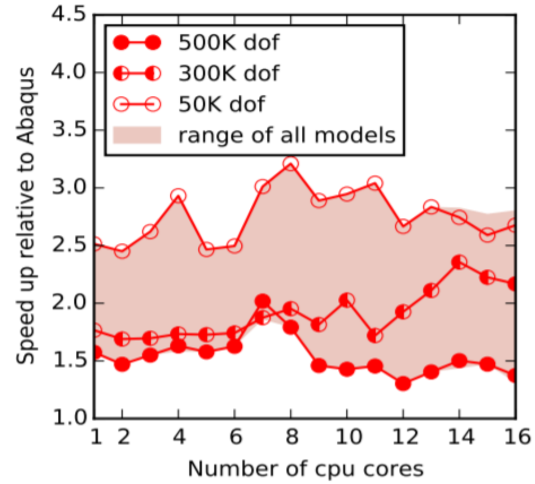
<u>Developers</u>: Dr. James E. Warner, Dr. Geoffrey F. Bomarito
Dr. Jacob D. Hochhalter

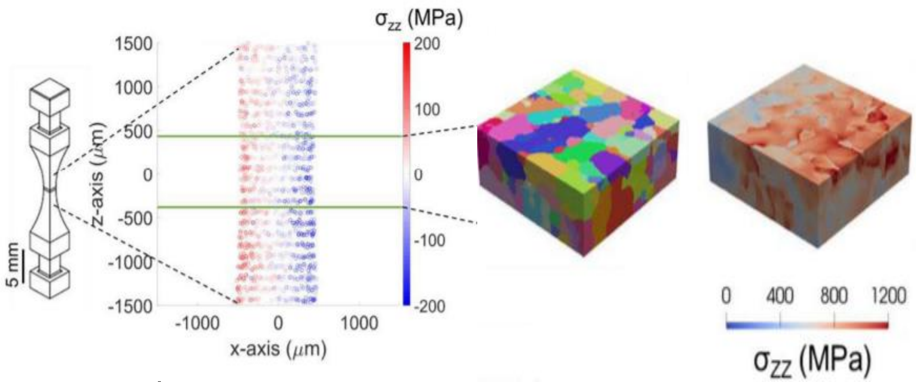
1. https://software.nasa.gov/software/LAR-18720-1
2. www.hdfgroup.com
3. http://glaros.dtc.umn.edu/gkhome/metis/parmetis/overview
4. http://www.cs.sandia.gov/zoltan/
5. http://sigma.mcs.anl.gov/moab-library/
6. http://mumps.enseeiht.fr/
7. www.netlib.org/blas/
8. www.netlib.org/lapack
9. www.mcs.anl.gov/petsc/
10. www.boost.org/
11. DREAM.3D http://dream3d.bluequartz.net/
12. Gmsh, https://gmsh.info/
13. SPPARKS, https://spparks.github.io/

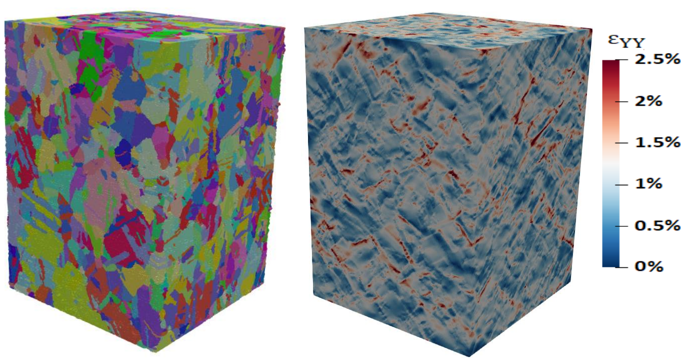
# Scalability of ScIFEN vs. Commercial FE solvers

Warner, Bomarito, Hochhalter
NASA/TM–2016-219180




FE solver: ABAQUS
Material: Inconel (nickel alloy)
Strain applied: 1%
CPUs: 320
Degrees of freedom (DoF): ~ 27 million
Simulation time: ~14 days

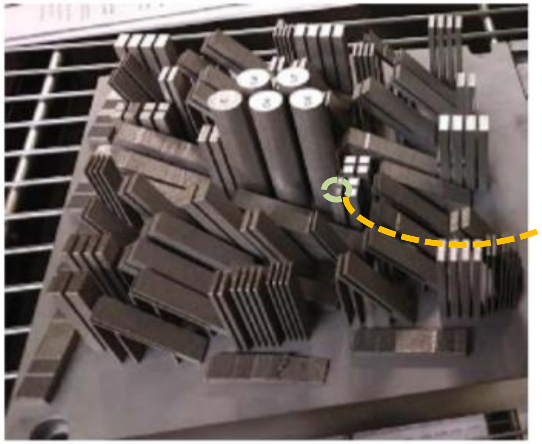
Source: Prithivirajan et al. (2021) Mater. & Design 197:109216

FE solver: ScIFEN
Material: Inconel (nickel alloy)
Strain applied: 1%
CPUs: 640
DoF: ~85.1 million
Simulation time: ~44 hours

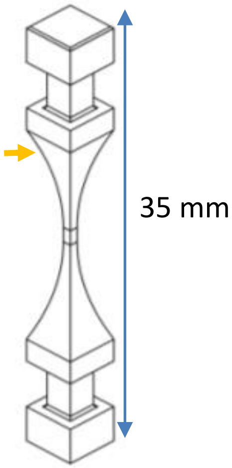
Source: Yeratapally et al. (2021) IMMI 10(2):196-217

# Additive manufacturing (AM) modeling challenge

*Final build*

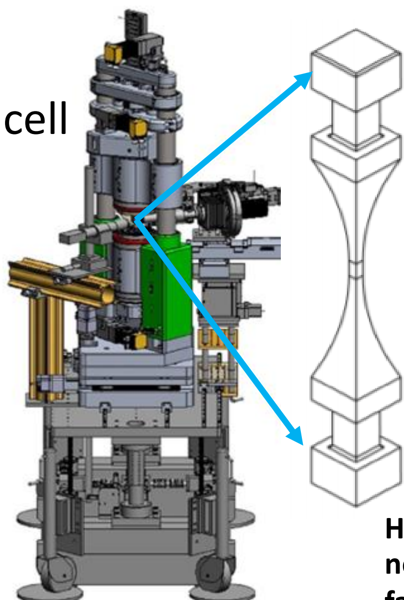


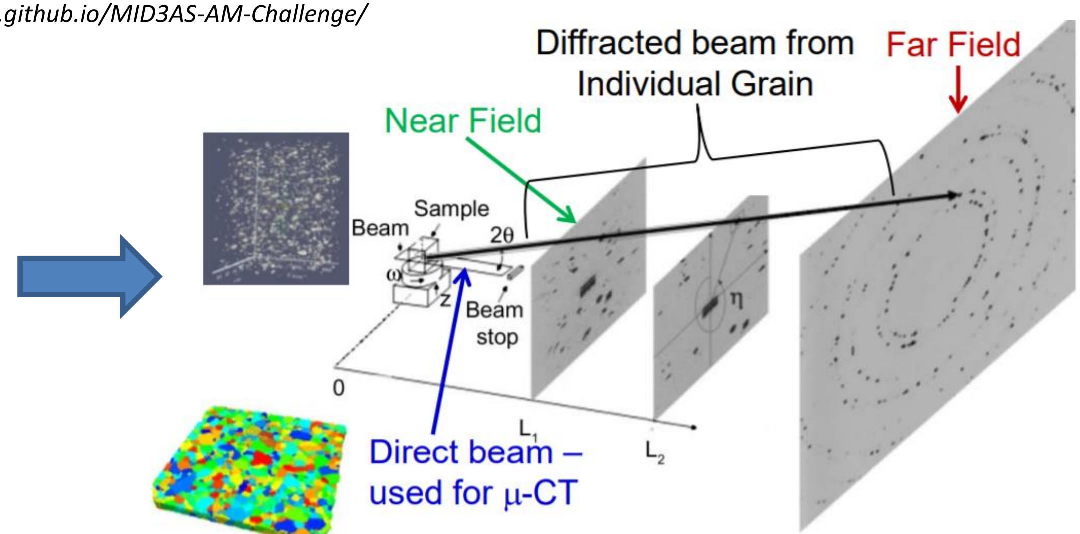
*Fully machined tensile coupon*




*<u>Source</u>: ARFL's AM modeling challenge series*
*https://materials-data-facility.github.io/MID3AS-AM-Challenge/*

Test cell



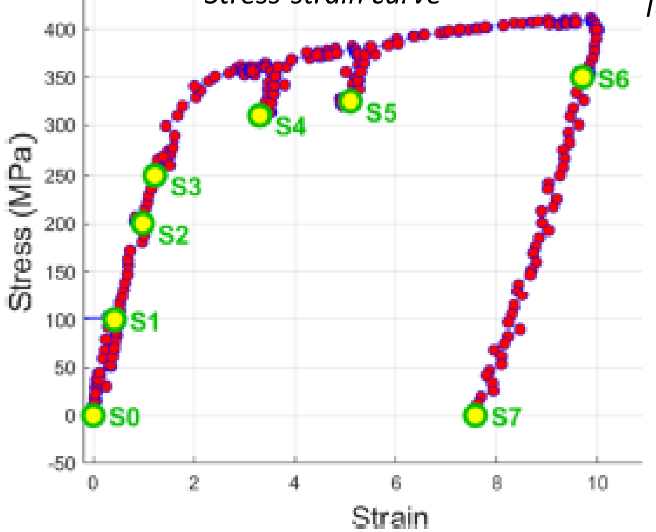



Poulson (2012) J. App. Crystallography 45

**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

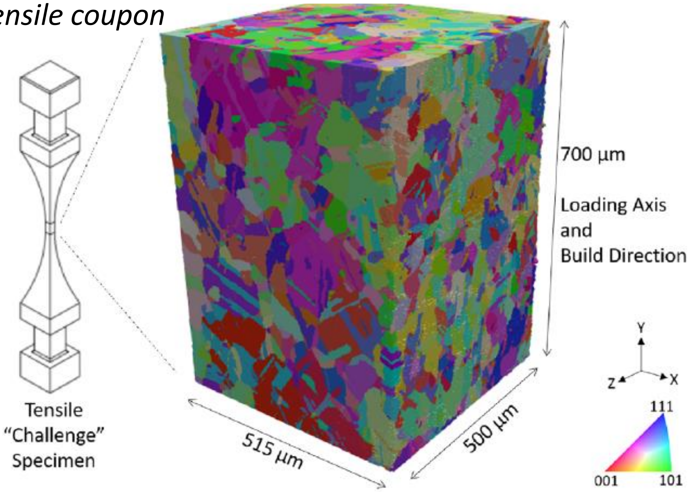
# AM modeling challenge: problem statement

*Stress-strain curve*

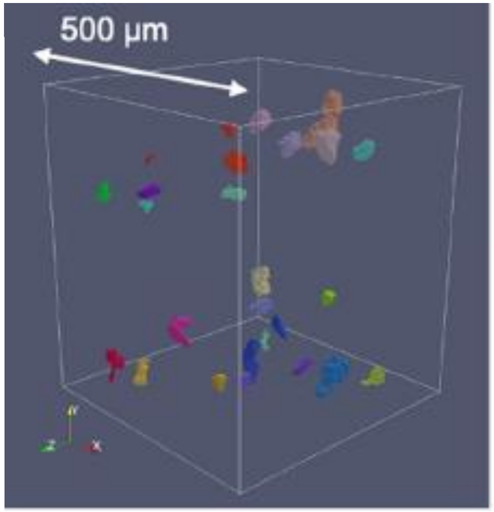



*Tensile coupon*

*Serial sectioned microstructure at gage section*




*28 "challenge" grains*

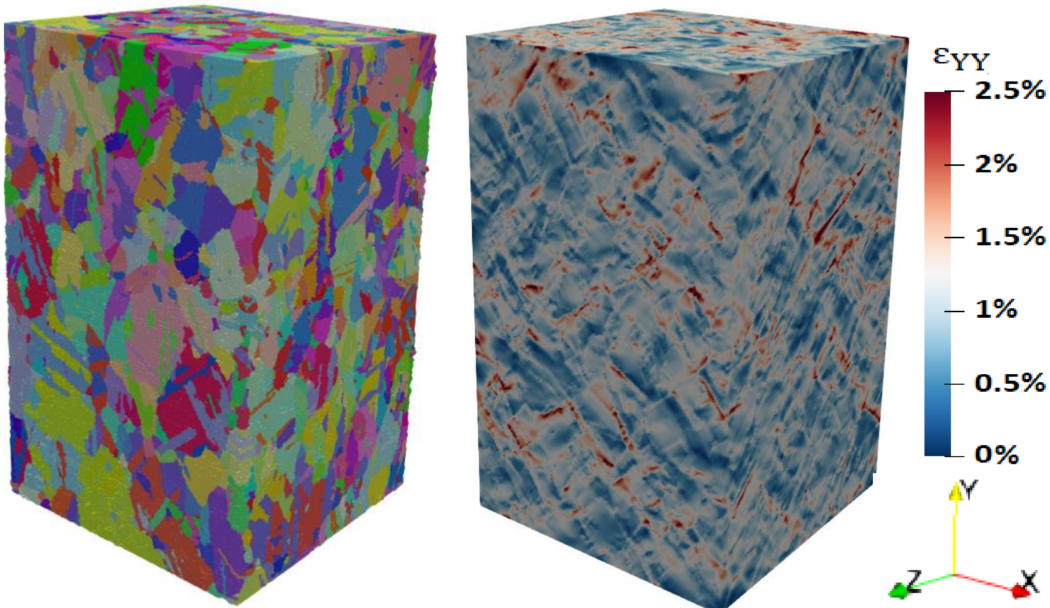


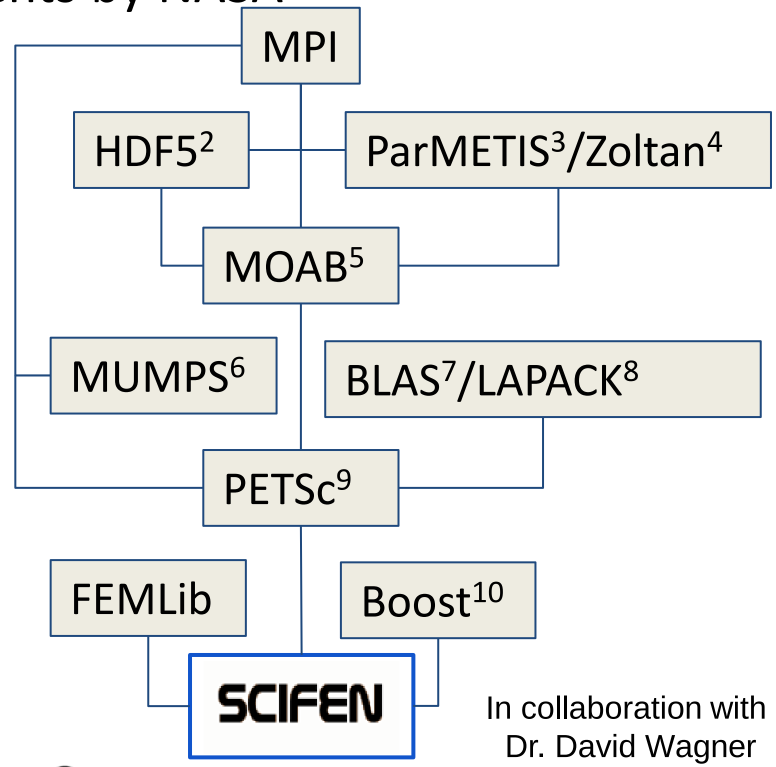

<u>**Challenge problem**</u>: Given the stress strain curve, serial-sectioned and reconstructed 3D microstructure, predict grain-average elastic strain tensor for 28 "challenge" grains at six different macroscopic load states, S1 through S6

*<u>Source</u>: ARFL's AM modeling challenge series*
*https://materials-data-facility.github.io/MID3AS-AM-Challenge/*

# CPFE simulations using ScIFEN

ScIFEN[1]: Scalable Implementation of Finite Elements by NASA

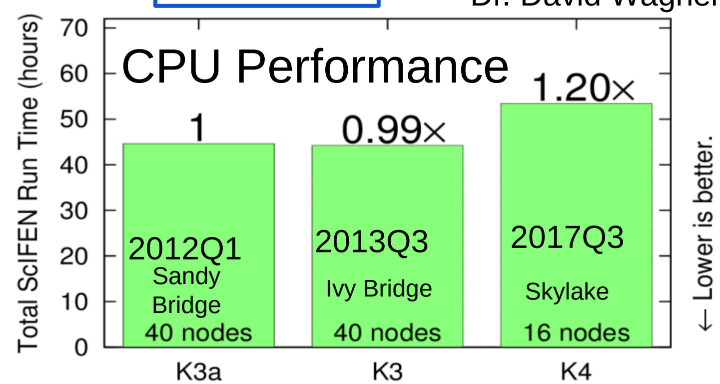



- 3D microstructure* of additively produced Inconel alloy
- Finite element mesh has ~85 million degrees of freedom
- Global strain applied in YY direction: 1%
- CP formulation: Strain-gradient based[11]
- Simulation time: ~44 hours on 640 processors on K-cluster

*AFRL AM modeling challenge: https://materials-data-facility.github.io/MID3AS-AM-Challenge/

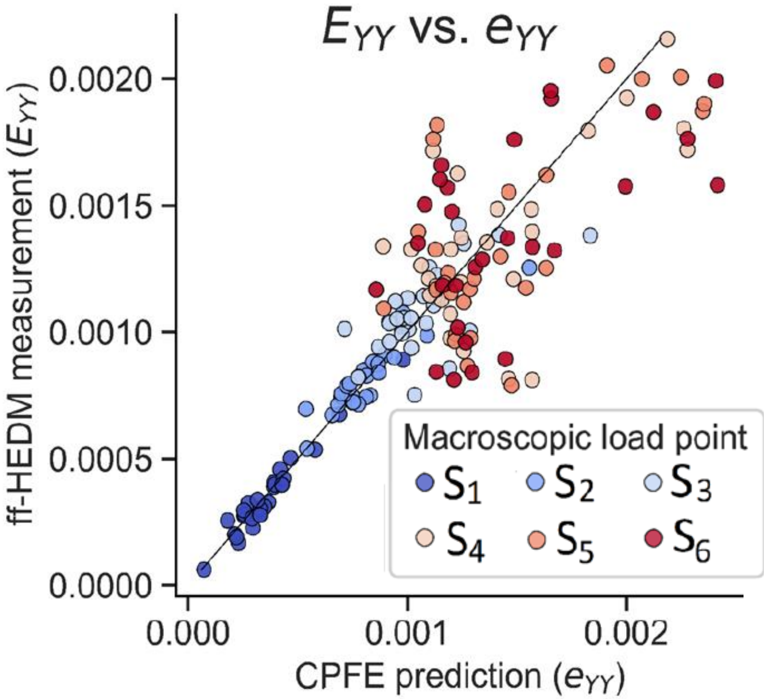
In collaboration with Dr. David Wagner

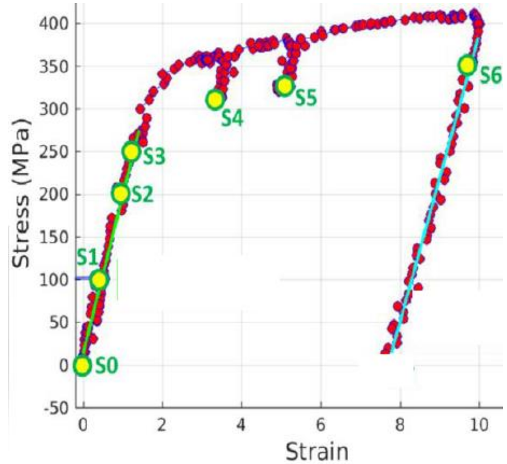


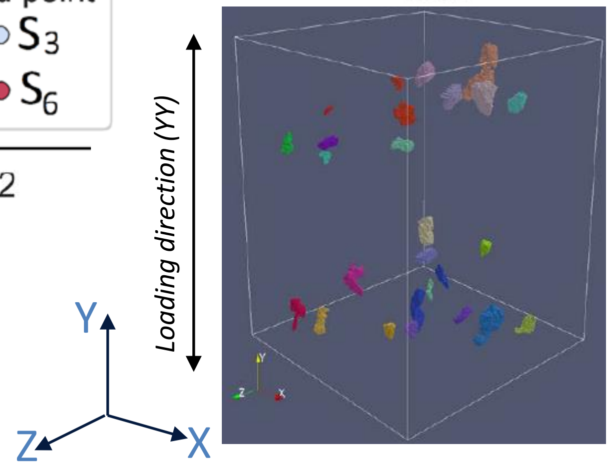

1. https://software.nasa.gov/software/LAR-18720-1
2. www.hdfgroup.com
3. http://glaros.dtc.umn.edu/gkhome/metis/parmetis/overview
4. http://www.cs.sandia.gov/zoltan/
5. http://sigma.mcs.anl.gov/moab-library/
6. http://mumps.enseeiht.fr/
7. www.netlib.org/blas/
8. www.netlib.org/lapack
9. www.mcs.anl.gov/petsc/
10. www.boost.org/
11. Acharya et al. (2000), JMPS 48

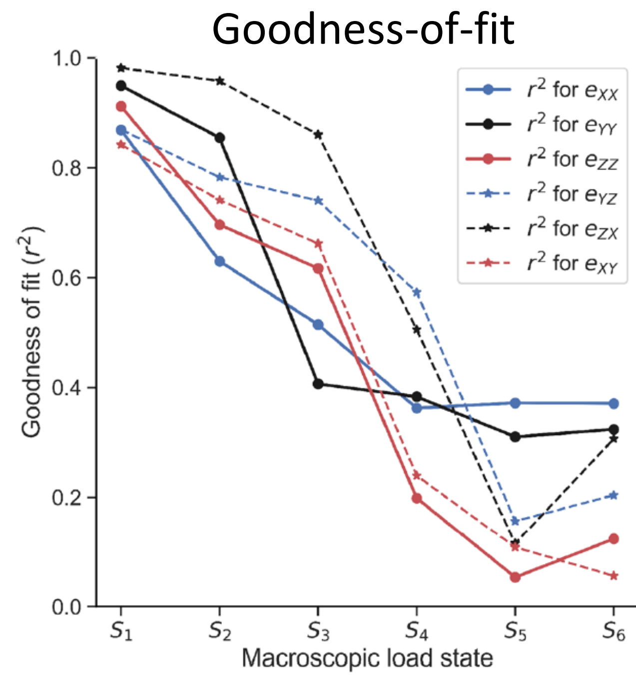
# ScIFEN's predictions vs. ff-HEDM measurements

CP predictions vs. ff-HEDM measurements



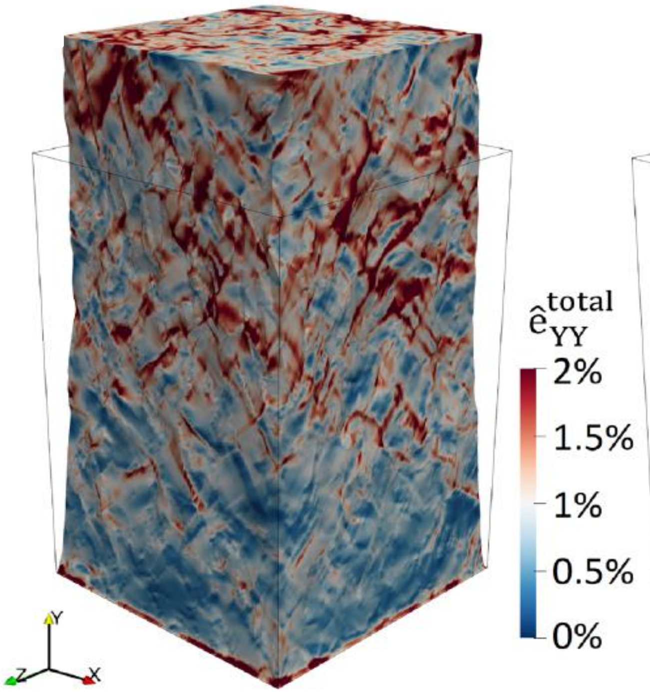




**<u>Observations:</u>**

- ➢ 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

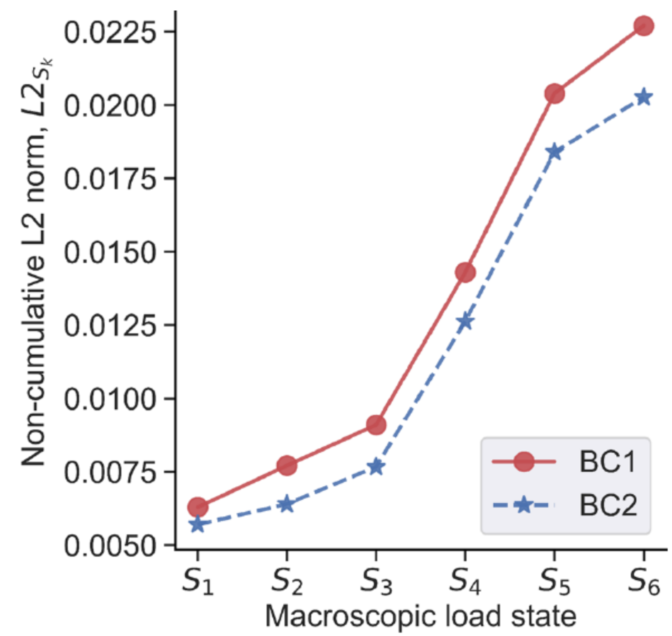
*Strain maps of total strain in YY direction, generated at global strain of 1%*




**BC1**: Fully constrained bottom face

**BC2**: Relaxed boundary conditions
*(Only one corner node on –Y face fully fixed and one edge fixed in X and Y directions)*

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

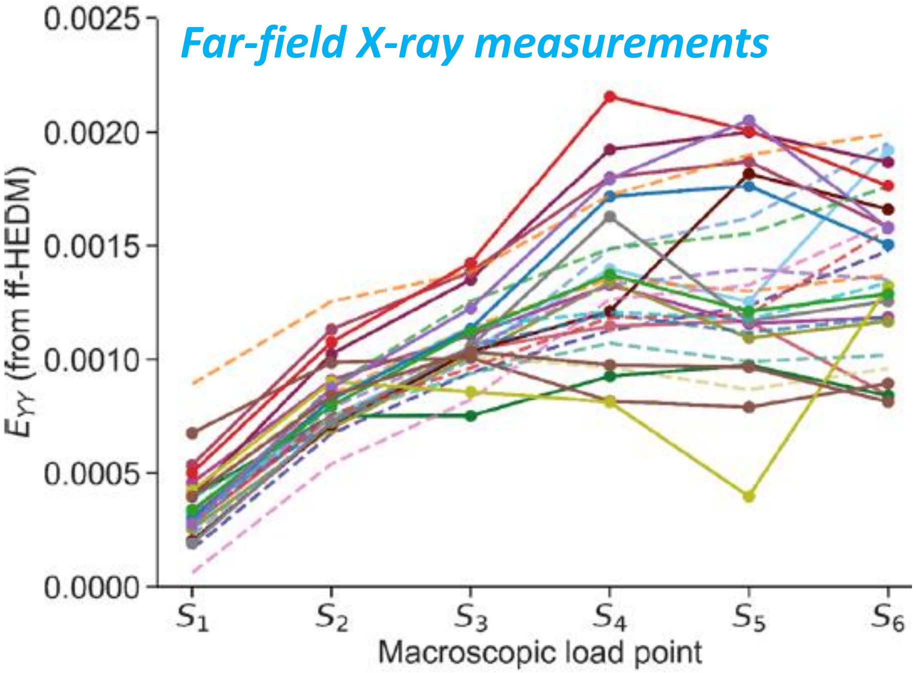



$$L2_{S_k} = \sum_{n=1}^{N} \sqrt{\sum_{i=1}^{6} \left( \left(E_i\right)_{S_k}^{g_n} - \left(e_i\right)_{S_k}^{g_n} \right)^2}$$

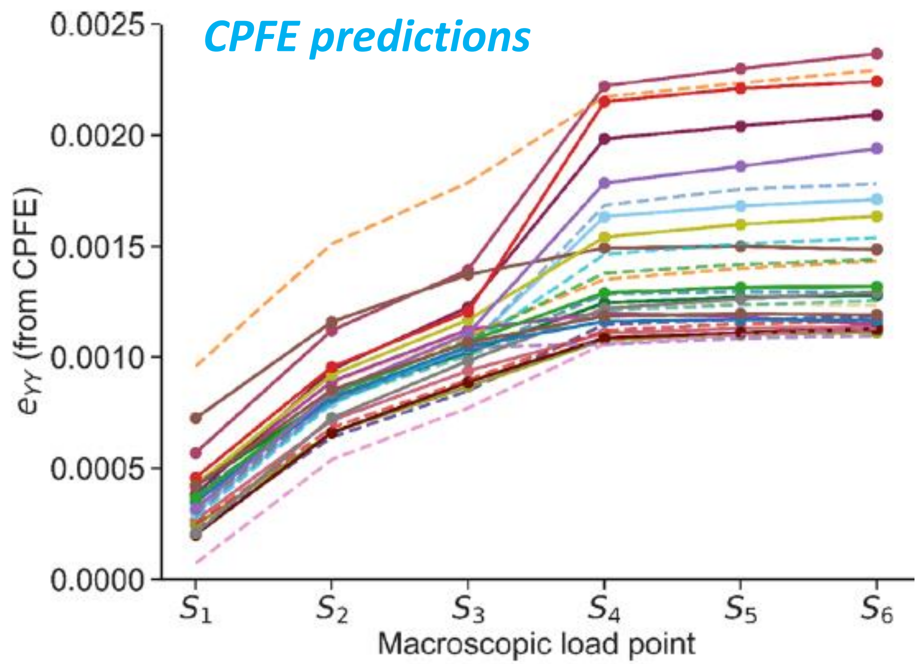
***$(E_i)_{S_k}^{g_n}$ is ff-HEDM measurement;*** ***$(e_i)_{S_k}^{g_n}$ is CP prediction;*** ***$S_k$ is macroscopic stress state;*** ***$g_n$ is grain ID;*** ***N is # grains***

# 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*

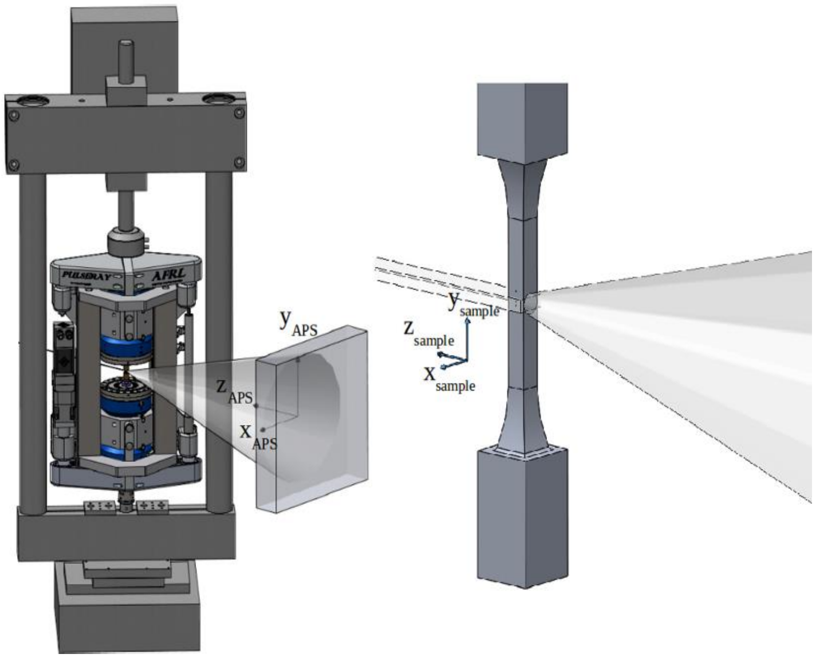



*CPFE prediction of evolution of YY component of grain-average elastic strain in each of the 28 grains*

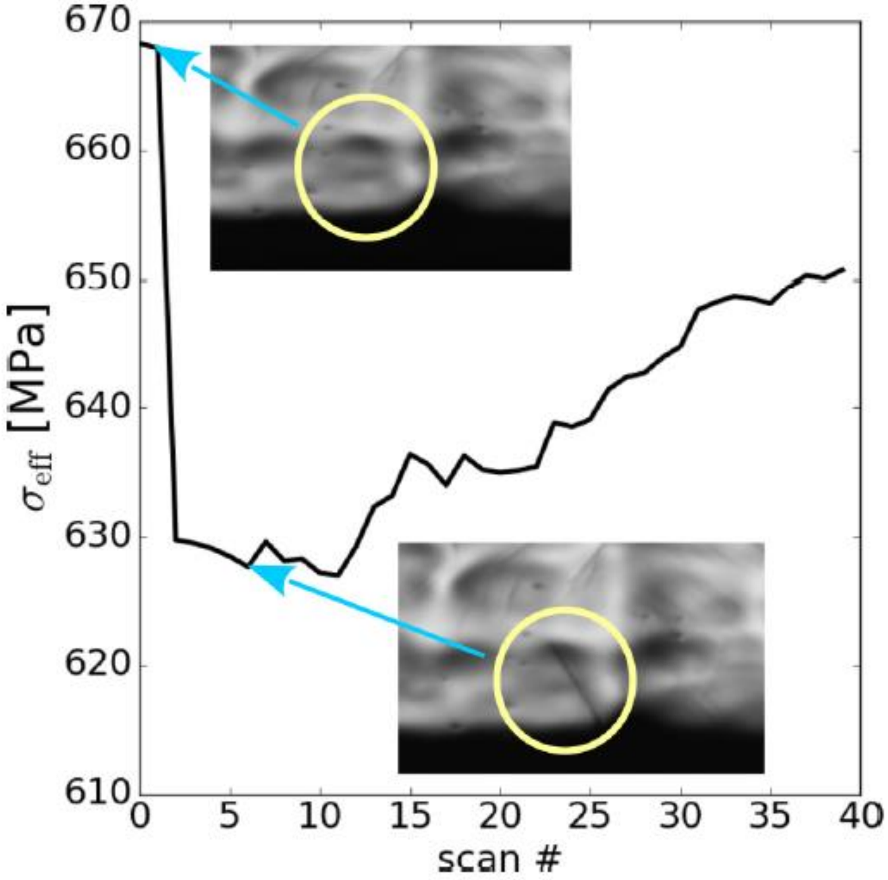



**Observation**: Phenomenological CP model used is unable to predict stress relaxation

# 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*

Source: Beaudoin et al. Physical Review B. 96, 174116 (2017)

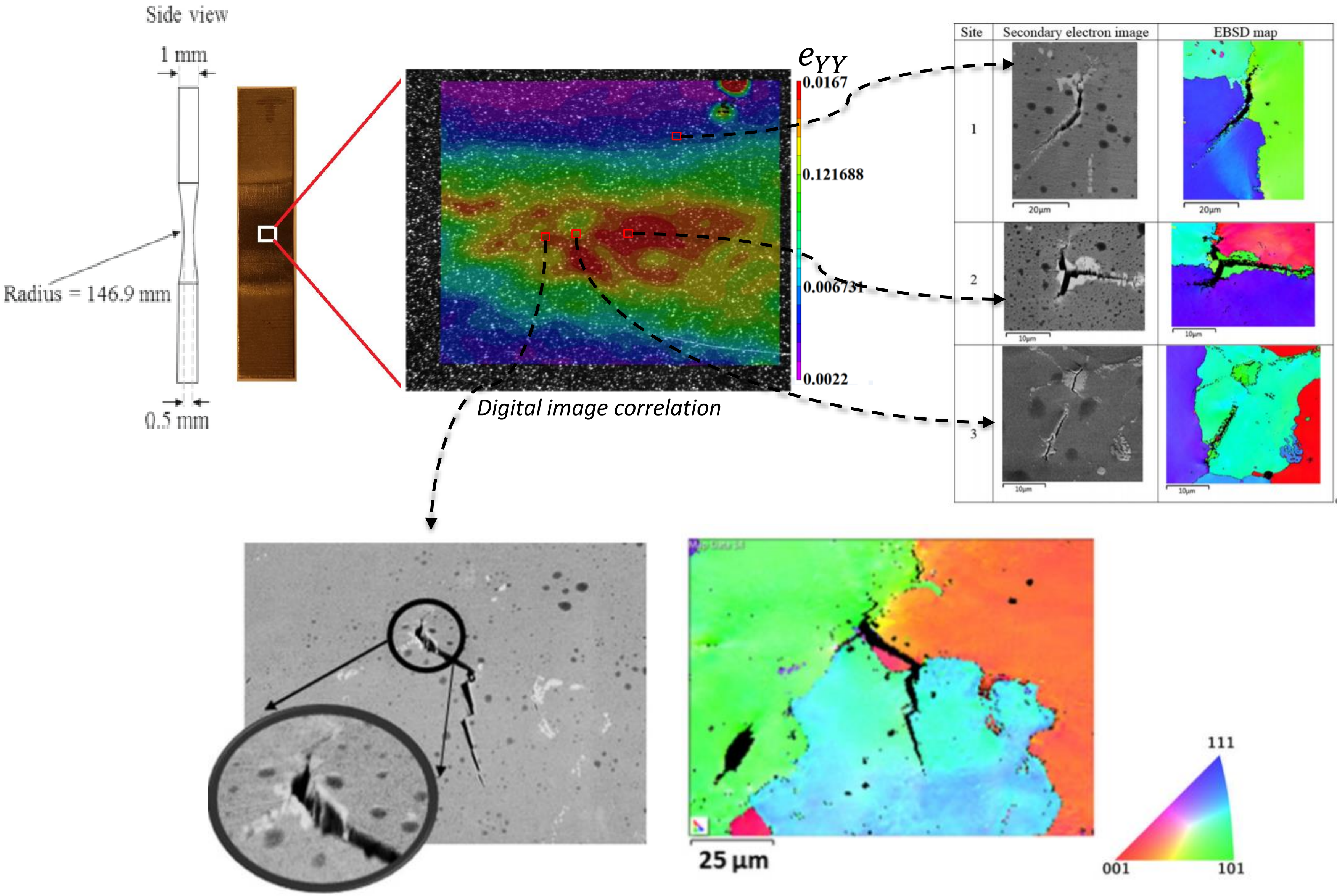
# For more detailed discussion

**Saikumar R. Yeratapally**, Albert R. Cerrone, Edward H. Glaessgen, "*Discrepancy between crystal plasticity simulations and far-field high energy X-Ray diffraction microscopy measurements*" Integrating Materials and Manufacturing Innovation 2021; 10(2):196-217. DOI: 10.1007/s40192-021-00216-5

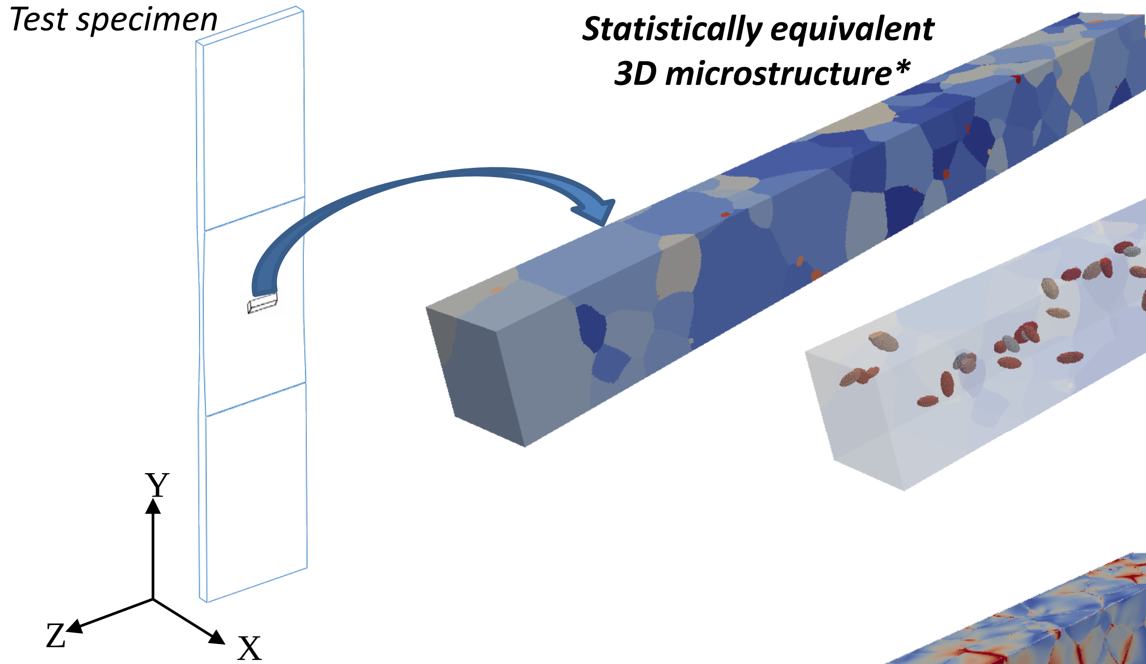
Journal: Integrating Materials and Manufacturing Innovation (IMMI)

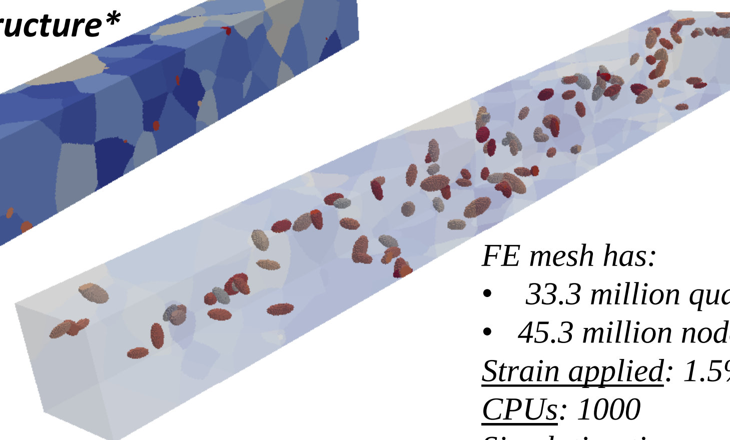
Special Issue: Metal Additive Manufacturing Modeling Challenge Series 2020

# Crack incubation in polycrystalline nickel alloy



# Grain-particle interaction using CPFE simulations



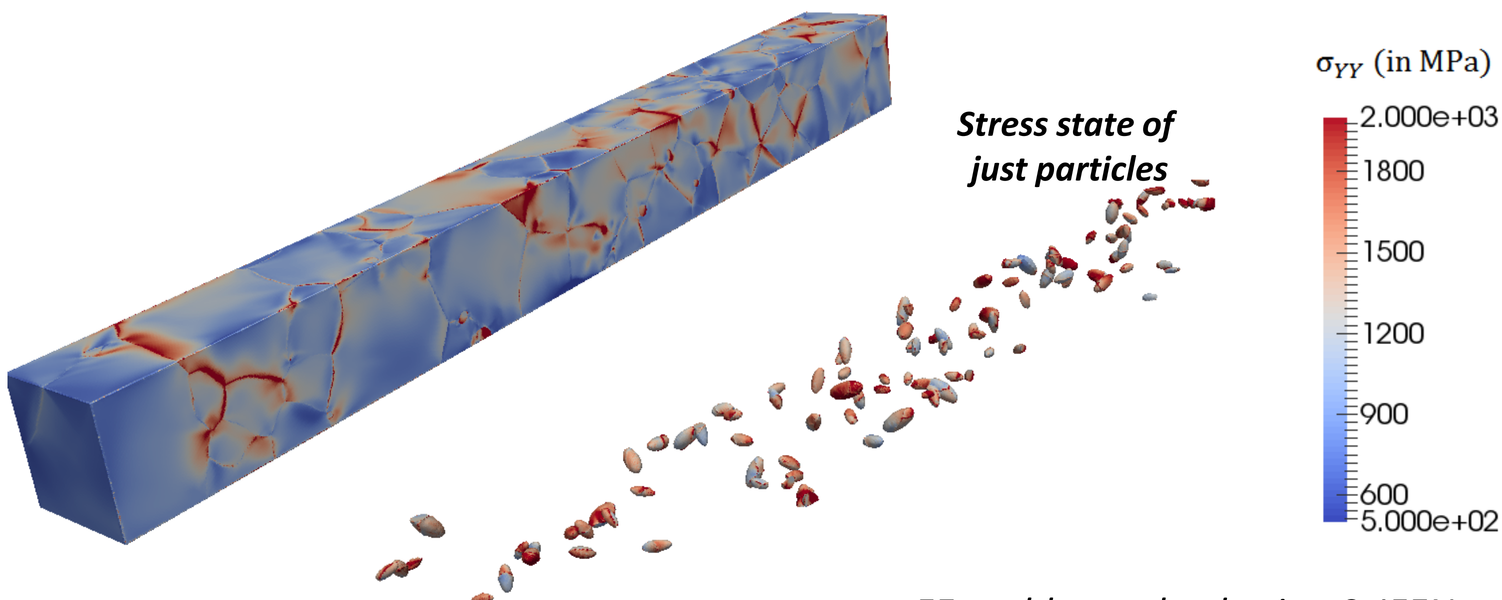

*FE mesh has:*

- *33.3 million quad. tetrahedral elements*
- *45.3 million nodes, hence* ***135 million DoF***

*Strain applied: 1.5%*

*CPUs: 1000*

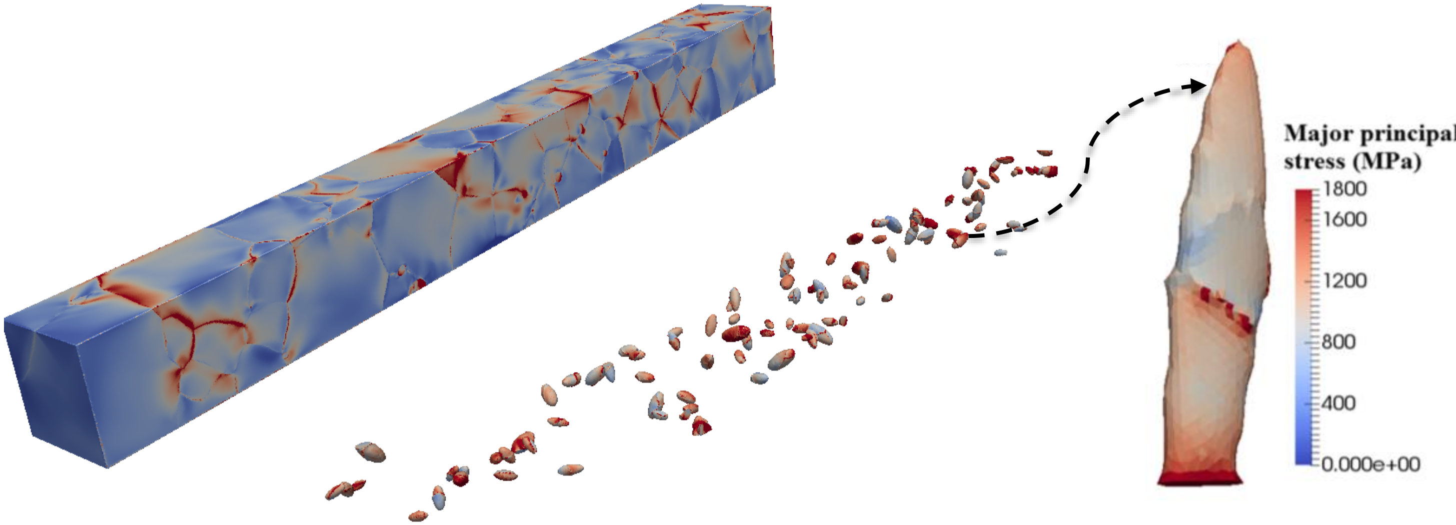
*Simulation time: ~ 40 hours.*

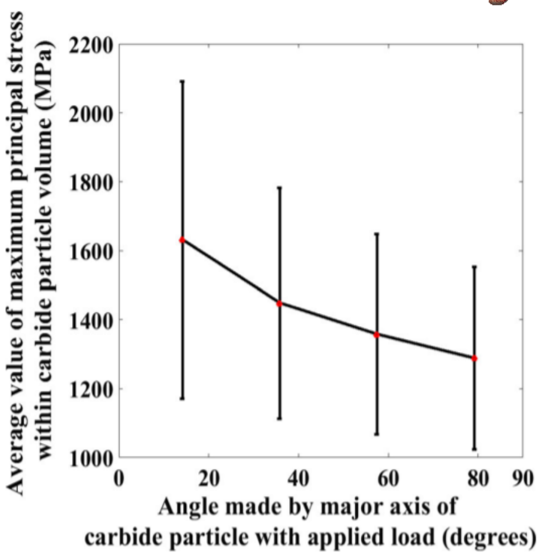


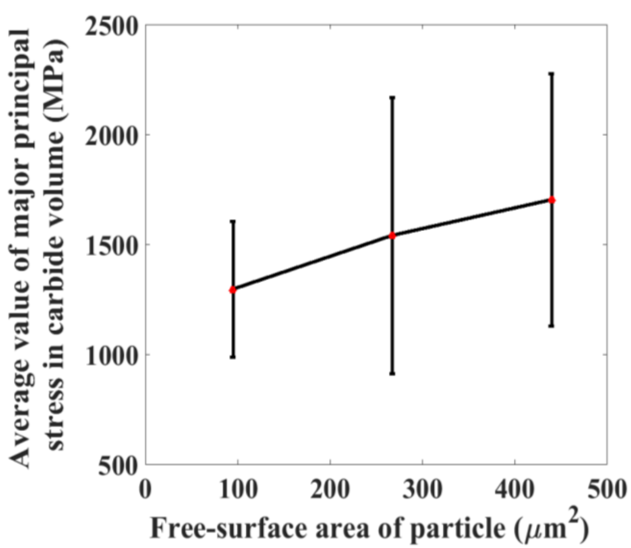

FE problem solved using ScIFEN

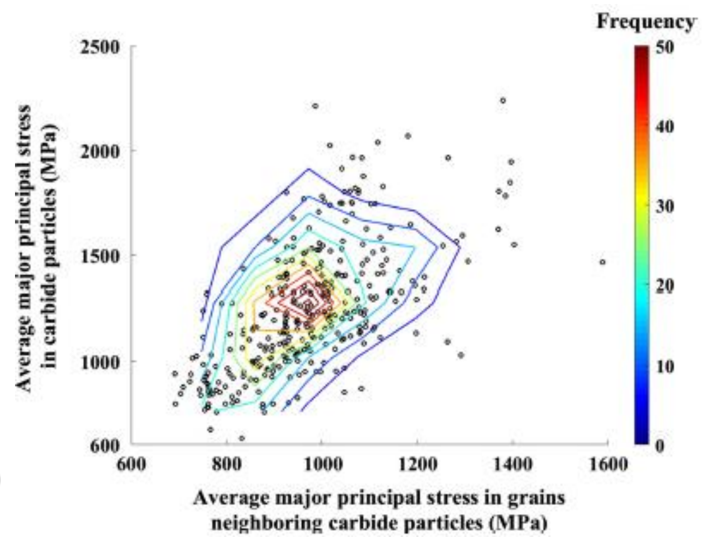
* Created using DREAM.3D (http://mai.bluequartz.net/)

# Factors influencing stress-state of particles



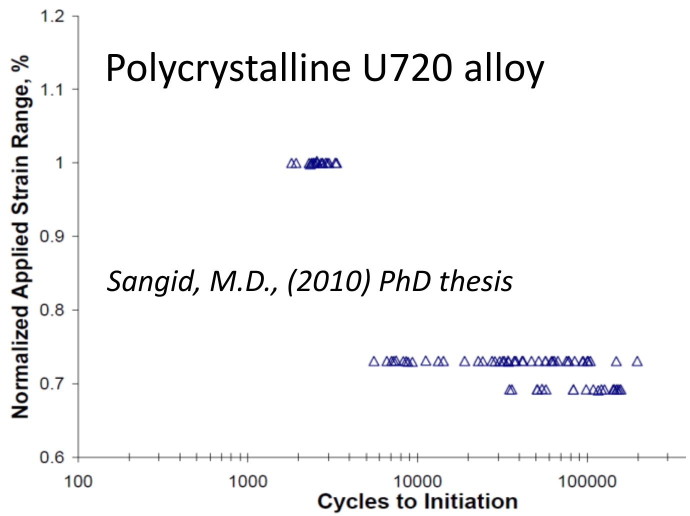



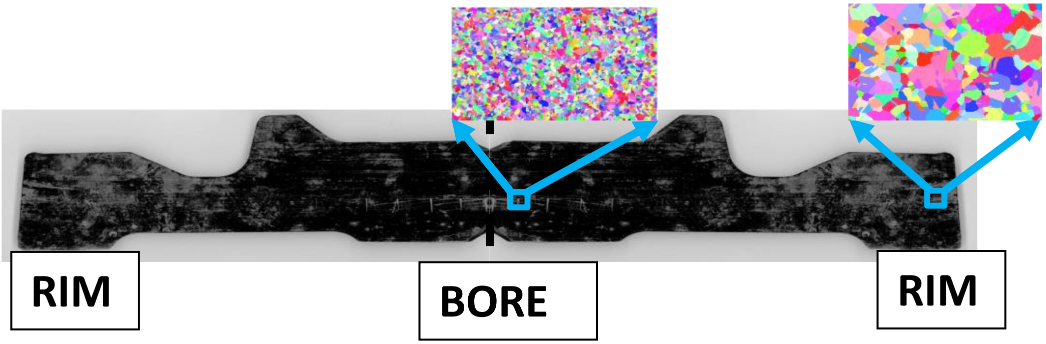

- ➢ Particles aligned with load axis experience high stresses.
- ➢ Particles with large free-surface areas are subjected to higher stresses.

# For more detailed discussion

**Saikumar R. Yeratapally**, Jacob D. Hochhalter, Timothy J. Ruggles, Michael D. Sangid "*Investigation of fatigue crack incubation and growth in cast MAR-M247 subjected to low cycle fatigue at room temperature*" International Journal of Fracture 2017; 208:79-96

# Scatter in fatigue performance




*Connor, Rae, Mitchell, Hardy, Lemsky; Dual microstructure heat treated discs: microstructural characterization, 7th Int. Charles Parsons Turbine Conference 2007.*

*B. Lin et al. MSE A 527 (2010) 3581–3587.*

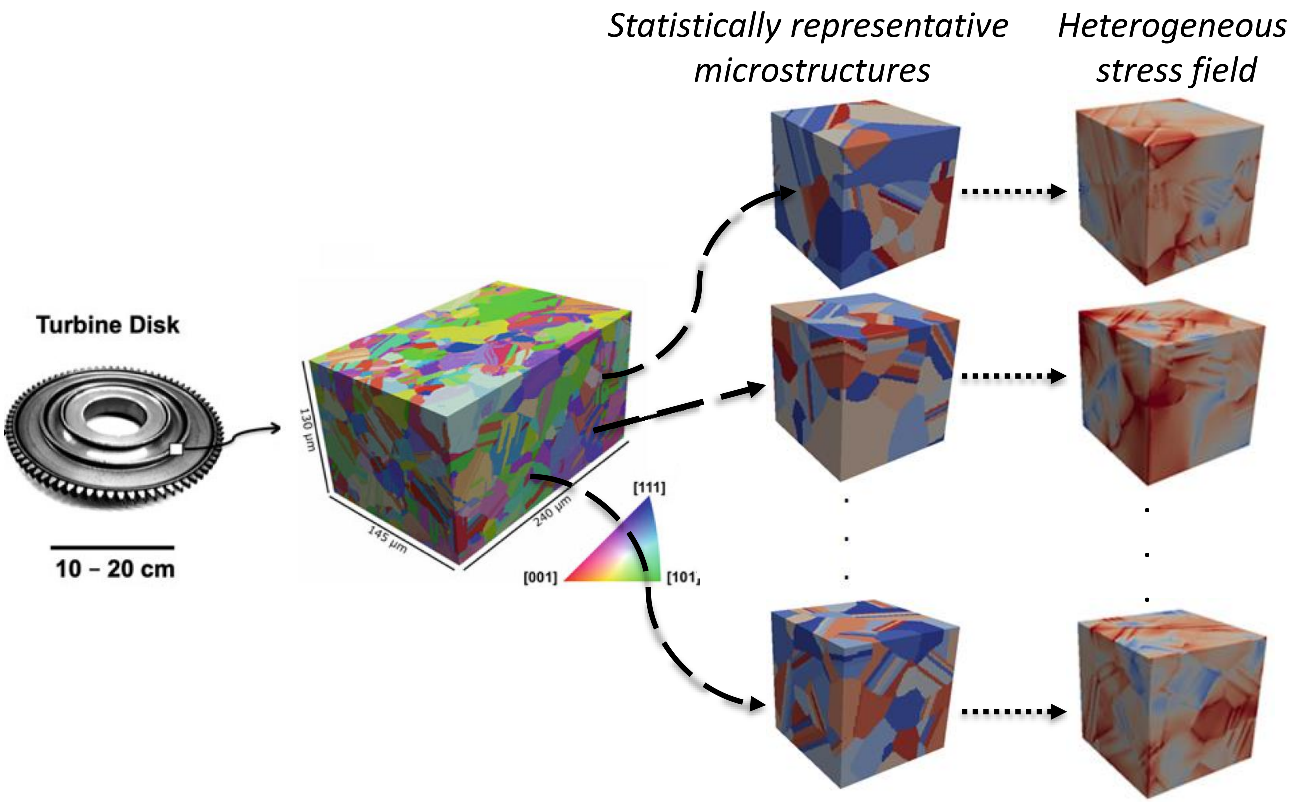
*American airlines Boeing 767, 2006*

*J. Escobar. (2008) Aircraft Maintenance Technology Society.*

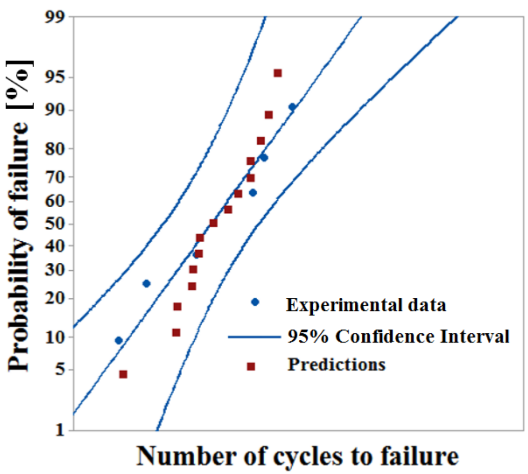
*Boeing 767-223, 2002*

*Air safety investigation report 200205780*

# Accounting for fatigue scatter due to microstructure

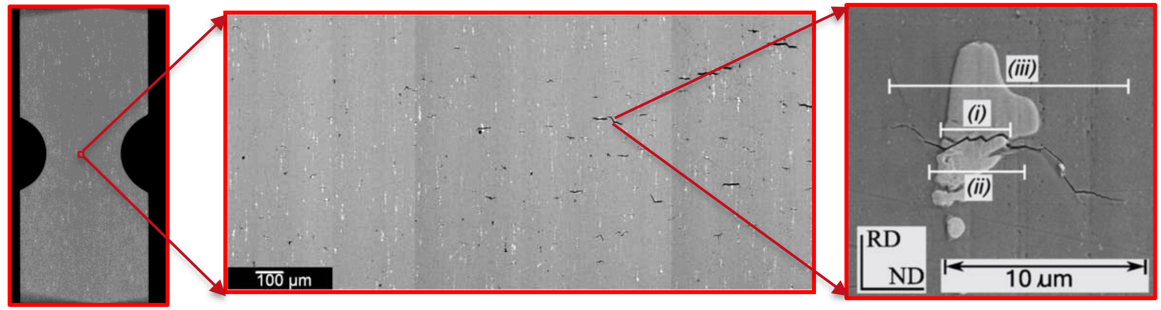



*Predicted scatter in fatigue*

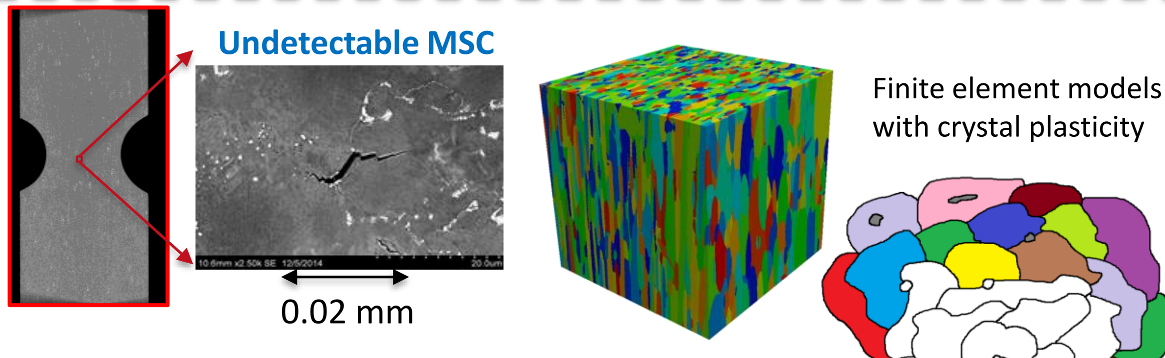


# Fatigue crack growth in AA7075-T651 alloy

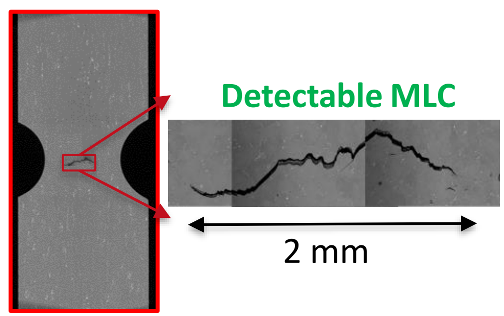
Crack incubation ($N_{inc}$) occurs very early in life and is subject to microstructure-sensitive variation

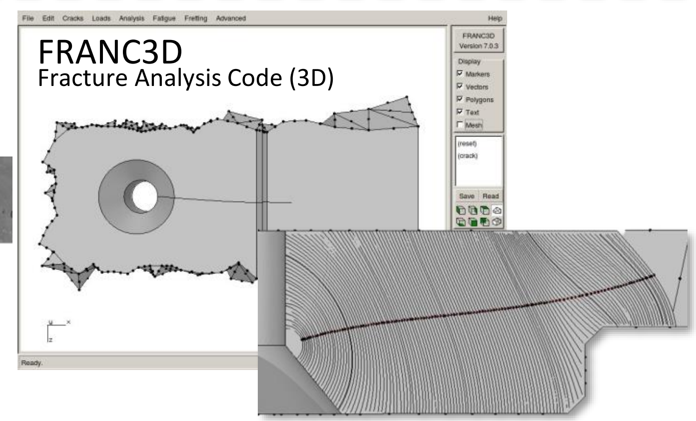



Multiscale simulation to compute the life of the structure consumed by incubation, nucleation and propagation of microstructurally-small cracks ($N_{MSC}$)



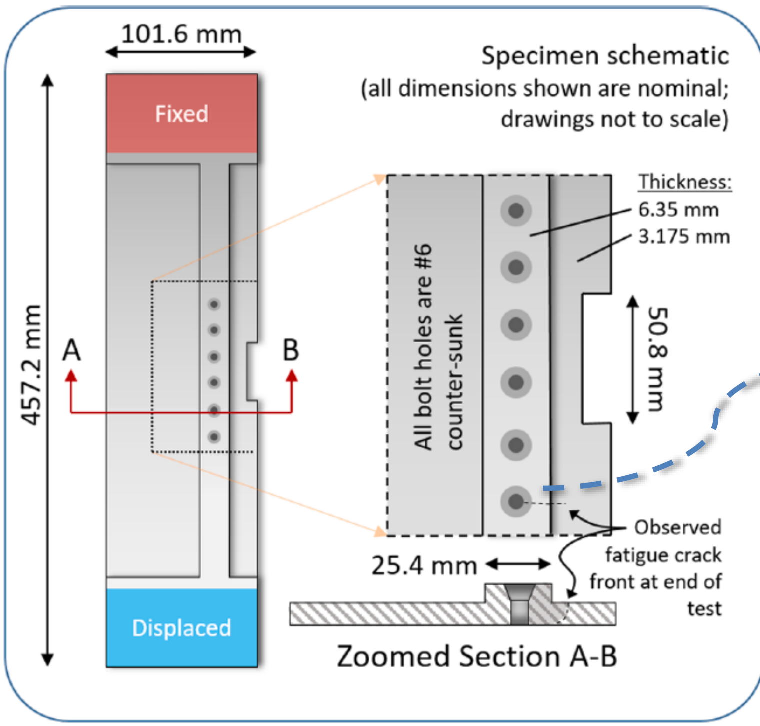

Traditional continuum fracture mechanics, FRANC3D, to compute the life of the structure consumed by growth of microstructurally-large cracks ($\mathbf{N_{MLC}}$)




$$N_{total} = N_{inc} + N_{MSC} + N_{MLC}$$

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

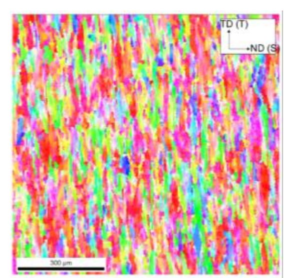



*Yeratapally, Leser et al. (2020) Engineering fracture mechanics*

*Philips XL-30, ESEM*

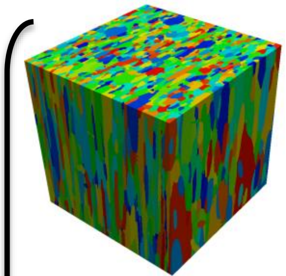
*Test specimen*

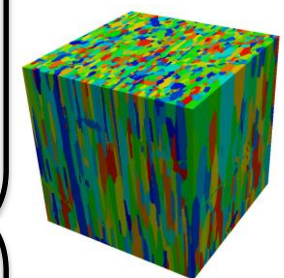
*Al 7075 microstructure*



*Sintay (PhD thesis), 2010*

Simulate variability in microstructure





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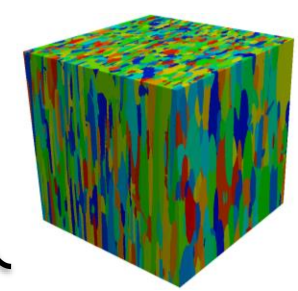
100 microstructure instantiations created using DREAM.3D

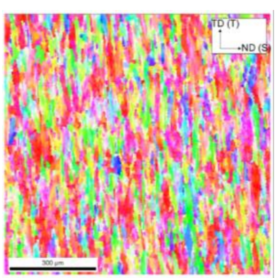


# Digital twin feasibility study: Non-deterministic estimation of fatigue life

*Philips XL-30, ESEM*

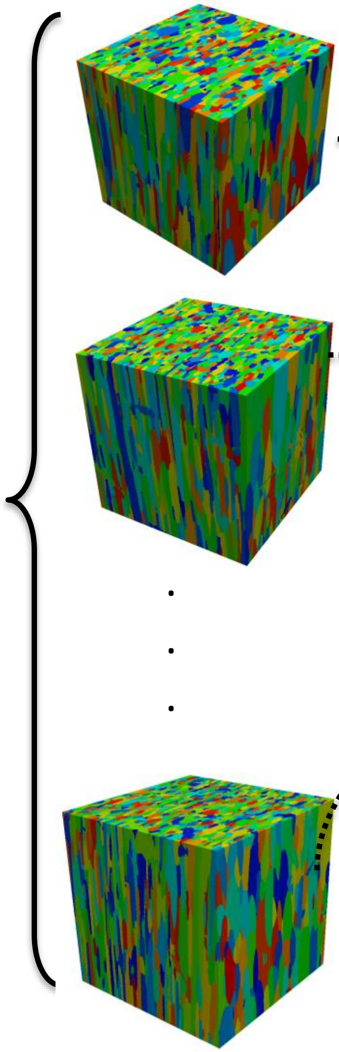
*Test specimen*

*Al 7075 microstructure*

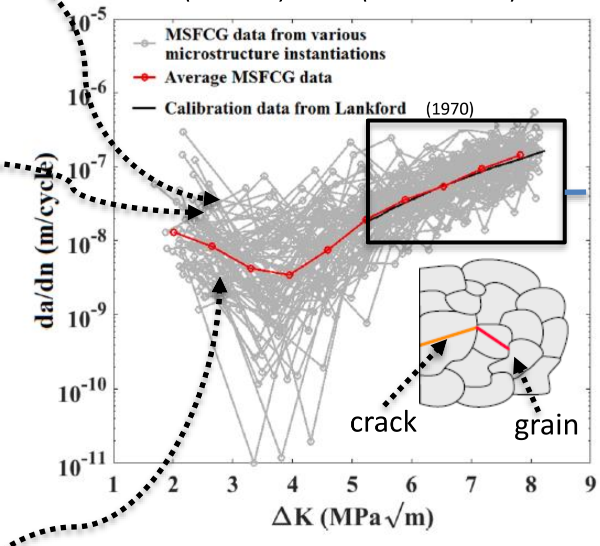



*Sintay, Rollet, 2010*

Simulate variability in microstructure

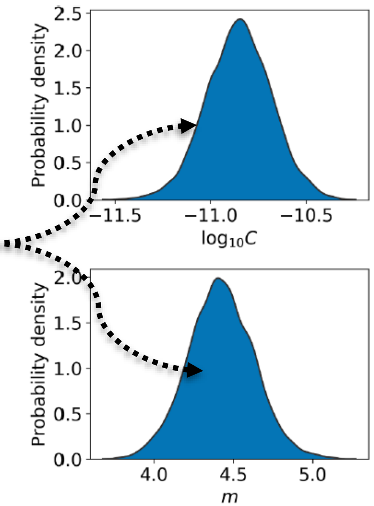


Microstructurally-small fatigue crack growth (MSFCG) data (from model)




Paris law

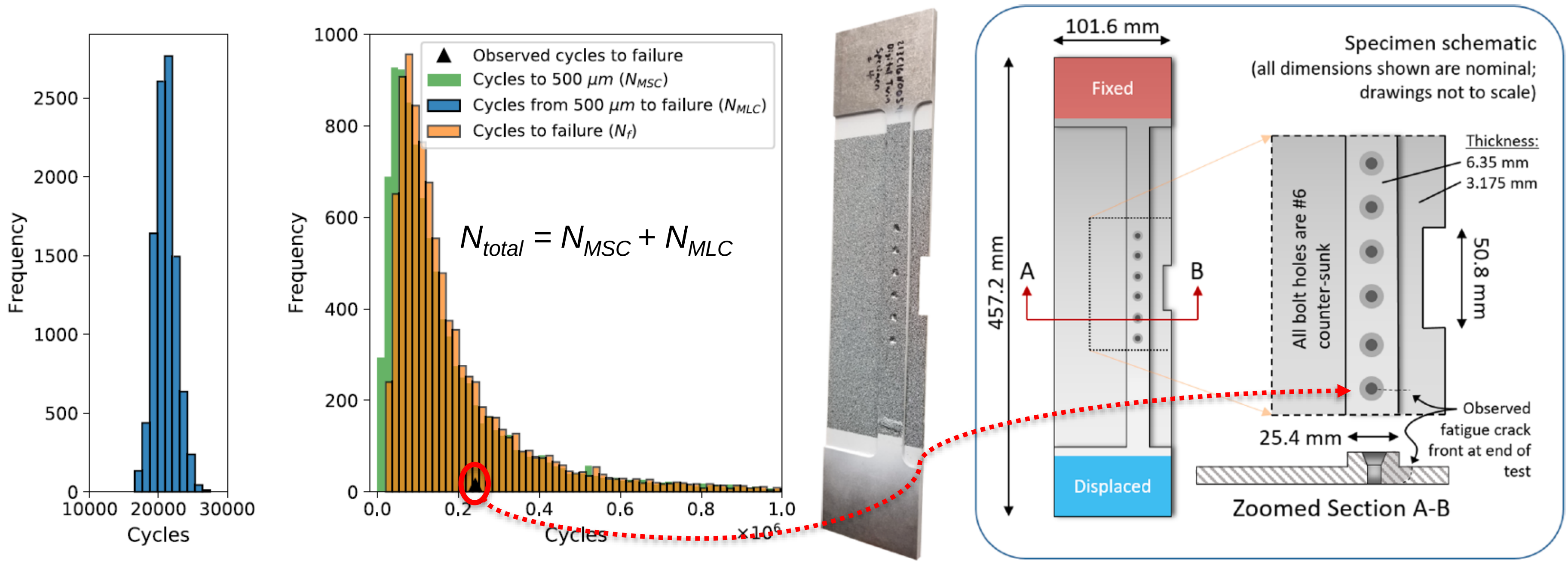
$$\frac{da}{dN} = C(\Delta K)^m$$




**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

# Digital twin feasibility study: Comparing with experiment




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

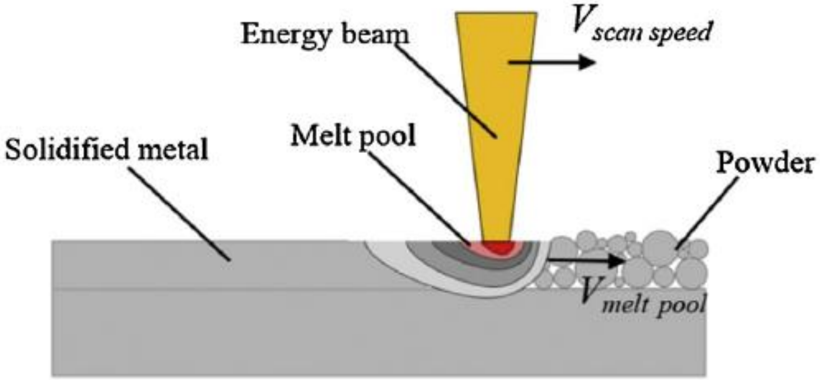
- The expected value of predicted fatigue life had an absolute percent error of 9.5% when compared to a tested specimen.
- Linear elastic fracture mechanics technique was used to model fatigue crack growth in a homogeneous material while maintaining and propagating the uncertainty quantified at the micro-scale 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

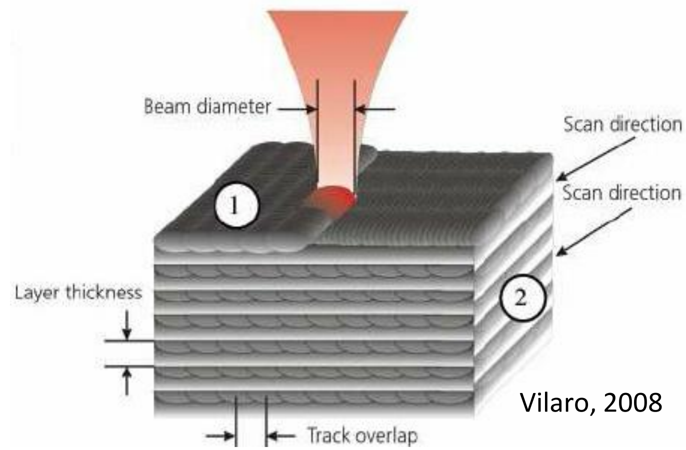
**Saikumar R. Yeratapally**, Patrick E. Leser, Jacob D. Hochhalter, William P. Leser, Timothy J. Ruggles, "*A digital twin feasibility study (Part I): Non-deterministic predictions of fatigue life in aluminum alloy 7075-T651 using a microstructure-based multi-scale model*" Engineering Fracture Mechanics 2020; 228:106888

# Effect-of-defects on performance of additive materials

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

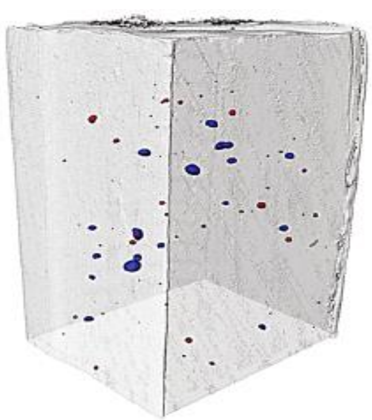



H. Gong et al. / Additive Manufacturing 1–4 (2014) 87–98



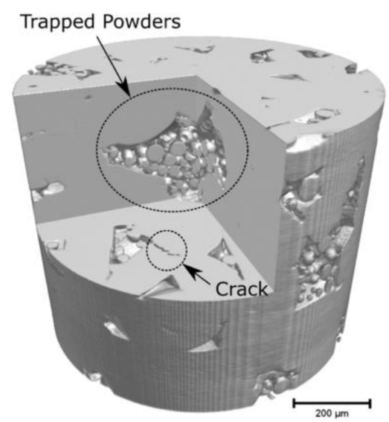

Vilaro, 2008

### *Keyhole porosity*



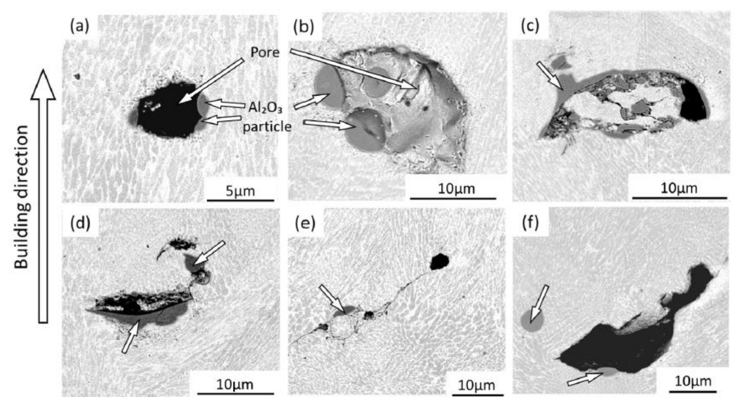
*Cunningham, R. et al. JOM, Vol. 69, No. 3, 2017*

### *Lack of fusion (LoF) porosity*



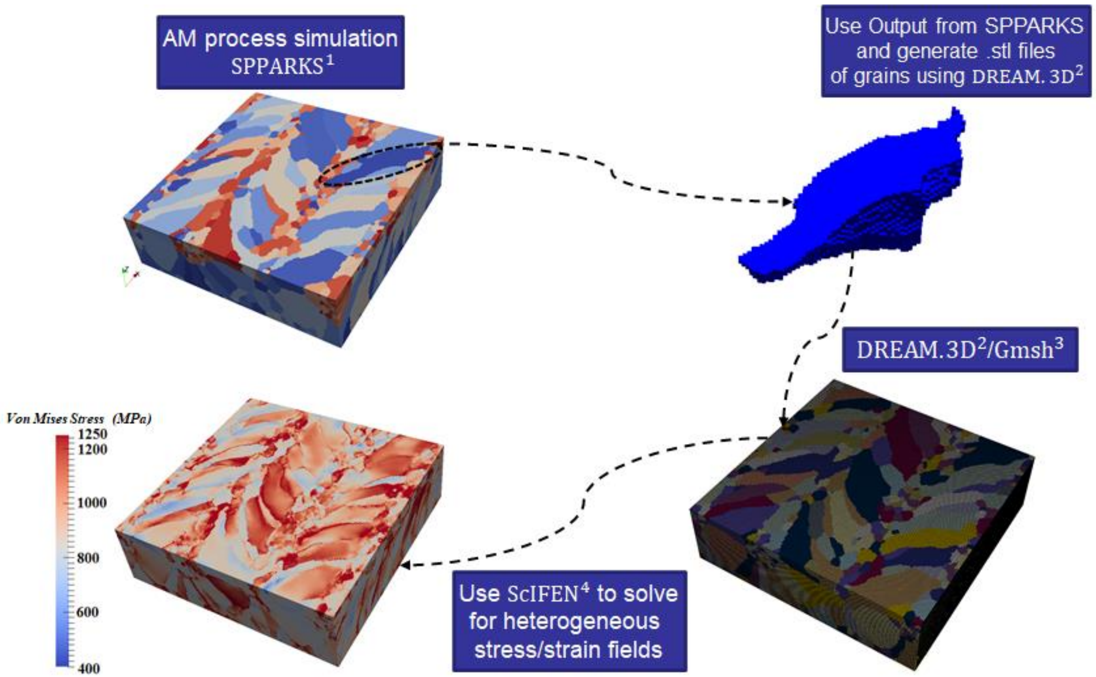

*Kim, Moylan, et al., Addit Manuf (2017)*

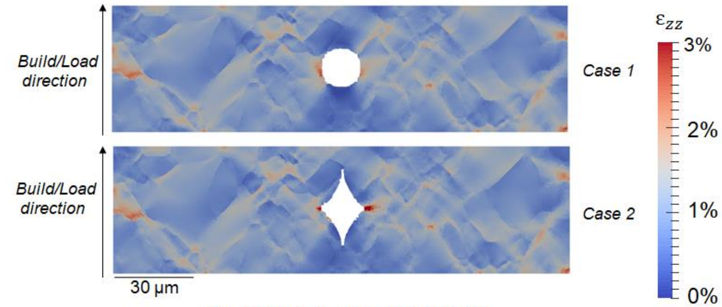
### *Oxide induced porosity*




*Tang et al. Int. J. Fatigue, Vol. 94, 2017, pp. 192-201*

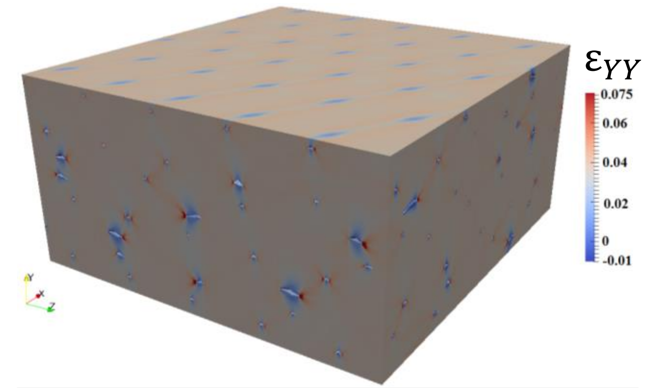
# Effect-of-defects on performance of additive materials

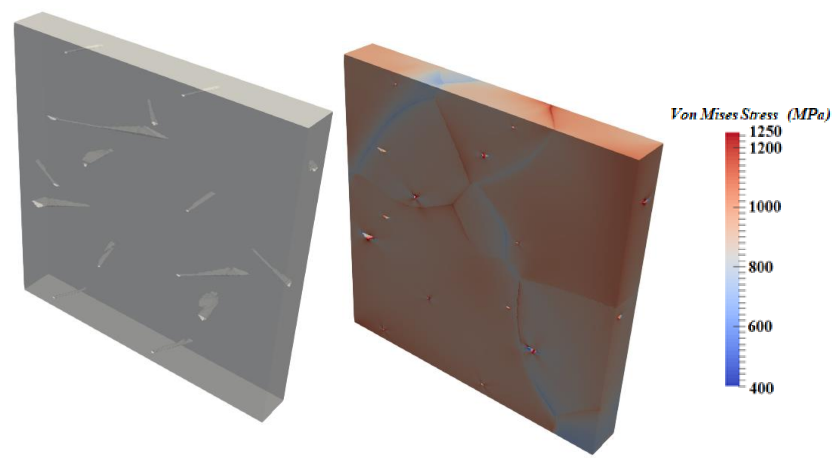



Cut section views of 3D microstructure

[1] spparks.sandia.gov
[2] dream3d.bluequartz.net
[3] http://gmsh.info/
[4] https://software.nasa.gov/software/LAR-18720-1



# For more detailed discussion

**Saikumar R. Yeratapally,** Christapher G. Lang, Edward H. Glaessgen, *"A Computational Study to Investigate the Effect of Defect Geometries on the Fatigue Crack Driving Forces in Powder-Bed AM Materials"* AIAA SciTech 2020 forum. DOI:10.2514/6.2020-1386

# 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

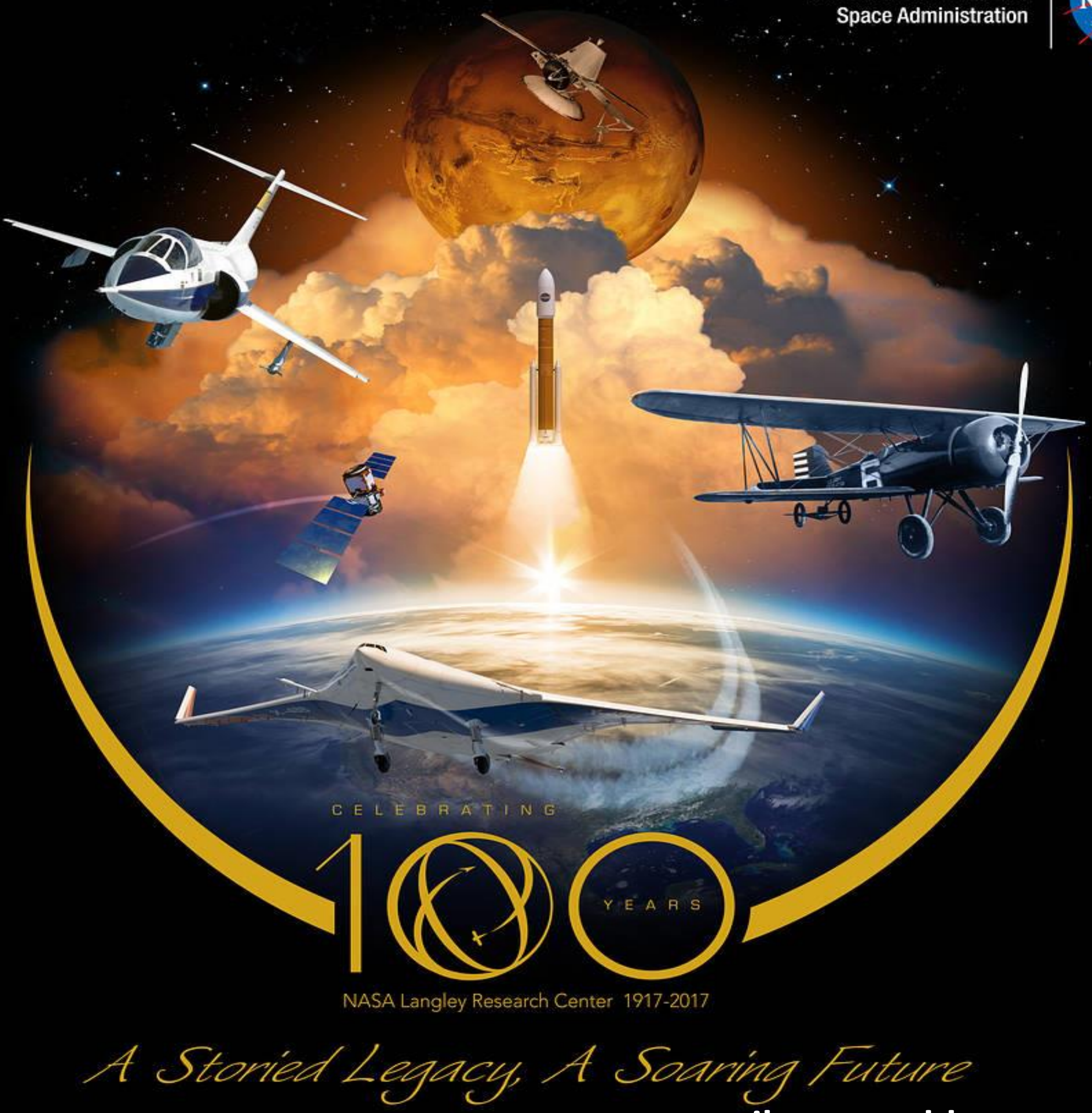
# Acknowledgements


- The work discussed in the presentation has been supported by:
  - 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!

National Aeronautics and
Space Administration

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