SAND2018-8070C

Sandia National Laboratories

THE FUTURE OF ENGINEERING DESIGN AT SANDIA NATIONAL LABORATORIES

PRESENTED BY

Dr. Susan Seestrom

Associate Laboratories Director for Advanced Science and Technology and *Chief Research Officer*

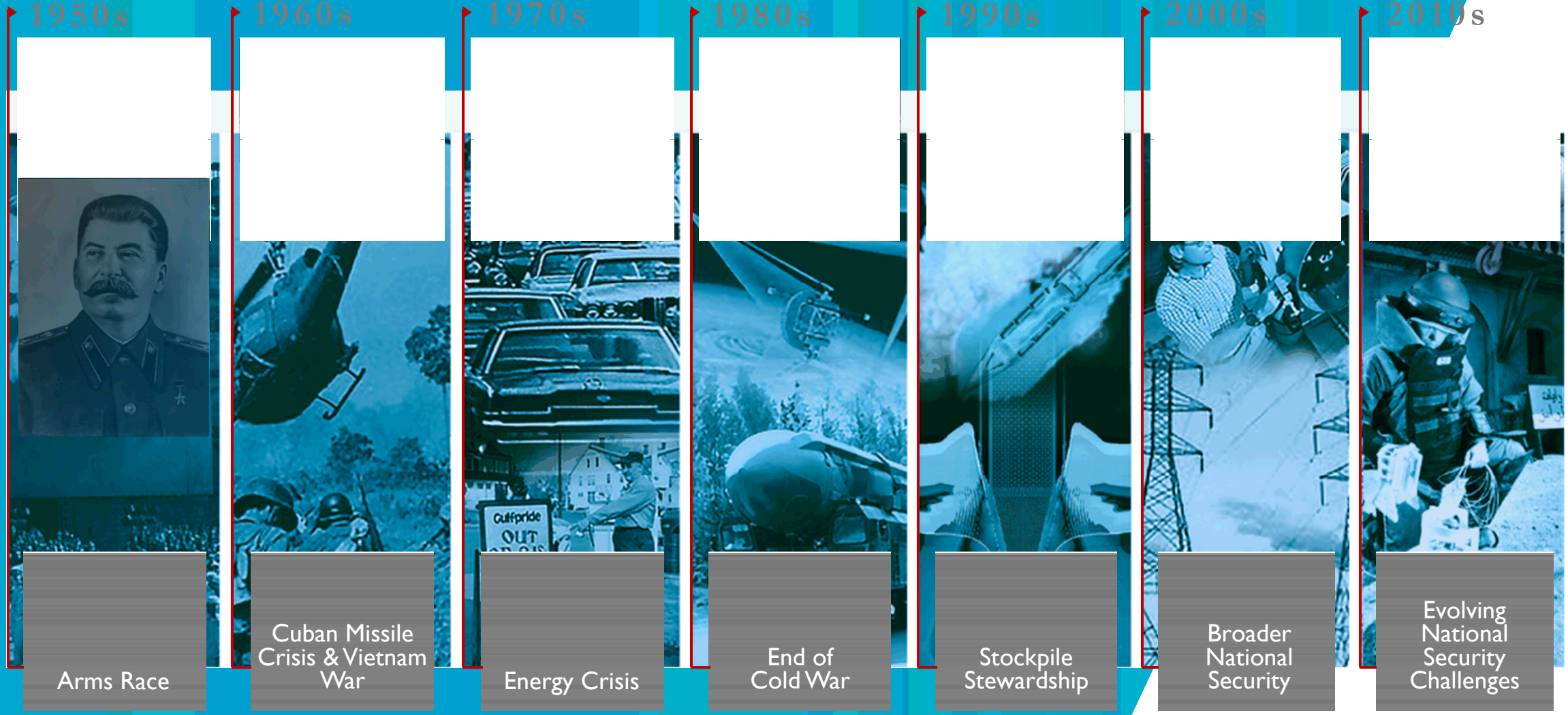
13th World Congress on Computational Mechanics

Jul 25, 2018

SAND REPORT NO.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

ADDRESSING NATIONAL SECURITY CHALLENGES SINCE 1949



SANDIA HAS FACILITIES ACROSS THE NATION

Main Sites

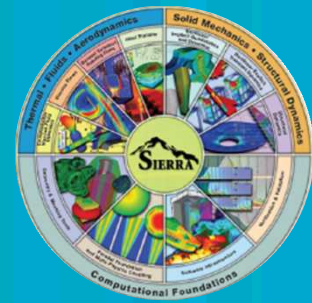
- Albuquerque, New Mexico
- Livermore, California

Activity Locations

- Tonopah, Nevada
- Waste Isolation Pilot Plant, Carlsbad, New Mexico
- Pantex Plant, Amarillo, Texas
- Kauai, Hawaii

SCIENCE-BASED ENGINEERING KEY TO MISSION SUCCESS

Integrating multidisciplinary efforts to advance the science of the possible for Sandia's missions

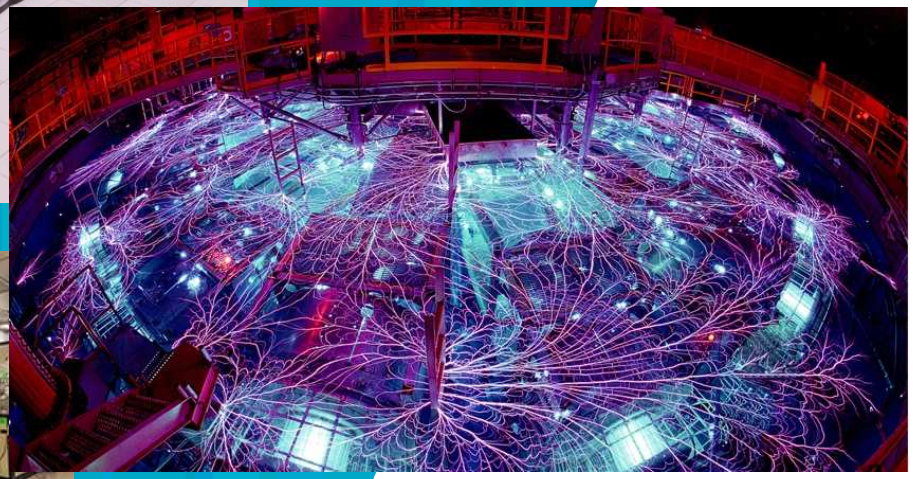


LAMMPS

DAKOTA
Explore and predict with confidence.

Modeling and Simulation

- High Performance Computing
- Software tools
- Uncertainty Quantification (UQ)

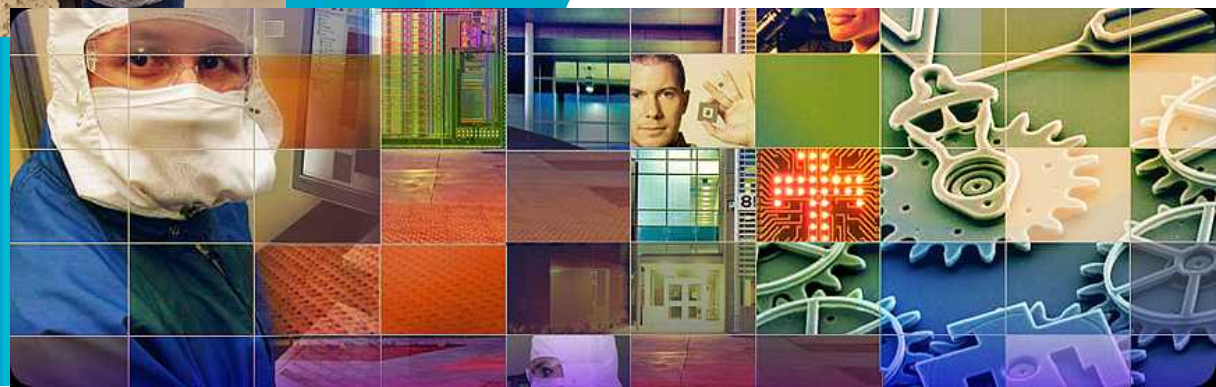


Advanced Experimental Capabilities

- Radiation effects
- Engineering environments
- Materials characterization and production

Microelectronics

- Microsystems & Engineering Sciences Applications (MESA) Fab
- Development of advanced semiconductor materials



SANDIA'S NUCLEAR WEAPONS MISSION

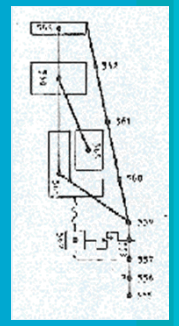
Sandia designs all non-nuclear components

- Warhead system integration
- Production
- Non-nuclear component design **and** qualification

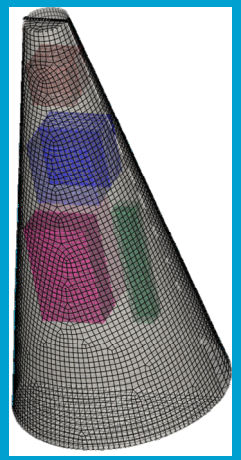
Fundamental science, computer models, and unique experimental facilities are used to understand, predict, and verify weapon systems performance.

WE HAVE DELIVERED INCREASING *MODEL* FIDELITY

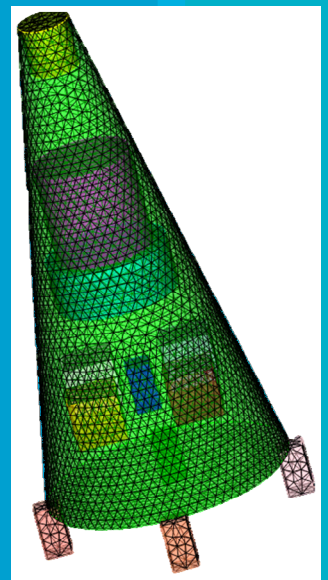
Enabled by platform and software advances



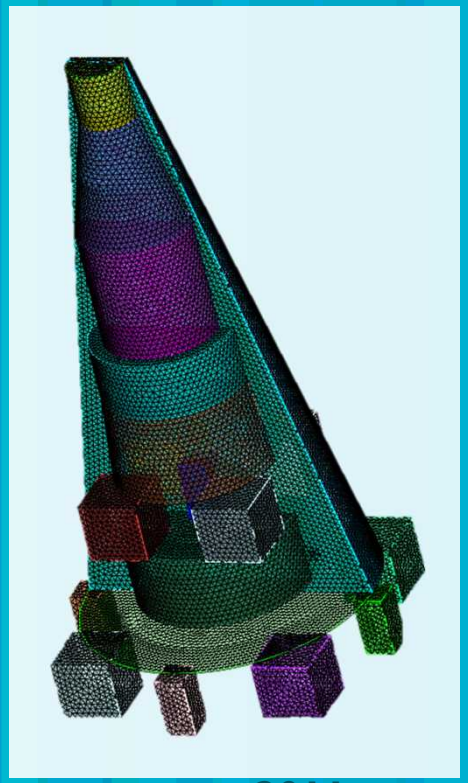
ca. 1988
200 DOF
Shellshock 2D



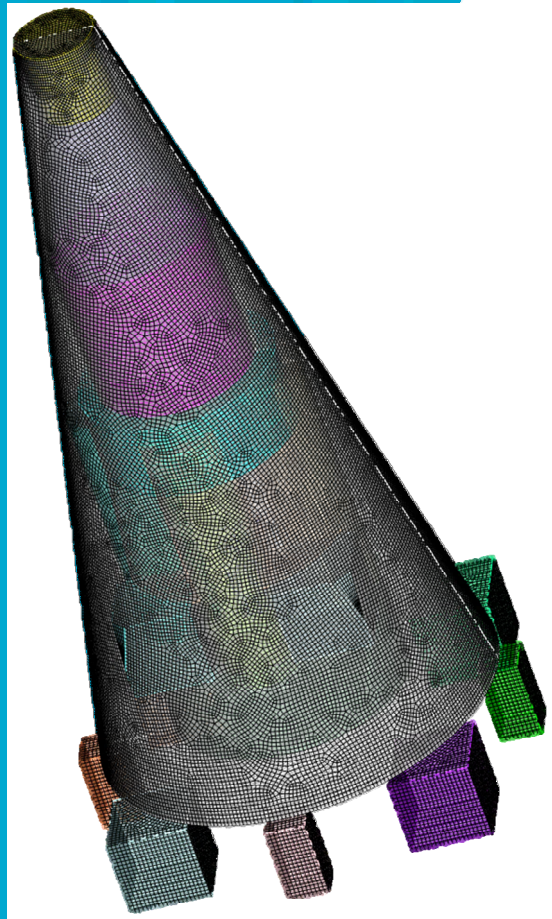
ca. 1995
40,000 DOF
NASTRAN



ca. 1998
400,000 DOF
SIERRA
Structural
Dynamics



ca. 2011
1.1M DOF
SIERRA
Structural
Dynamics

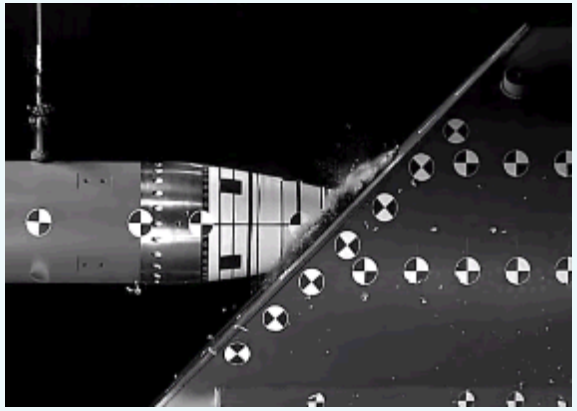


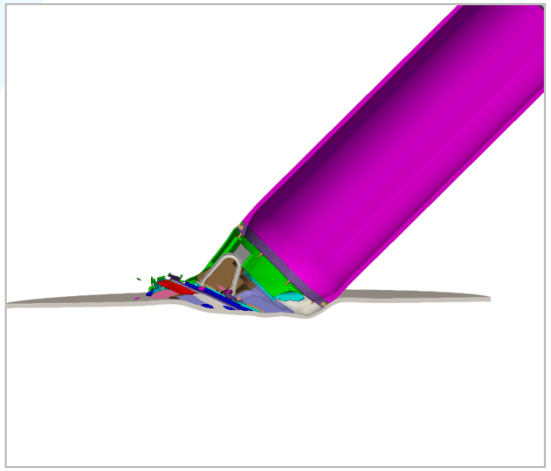
ca. 2018
10.6M DOF
SIERRA
Structural
Dynamics

MISSION REQUIRES INCREASING SYSTEM FIDELITY

Experiments and simulation work together

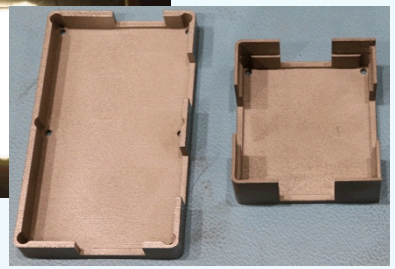
- Optimize performance of impact fuze in various environments
- Use of ‘virtual builds‘ to explore design trade space
- Simulations used to optimize tests
- Simulations provide insight into damage that is not experimentally accessible

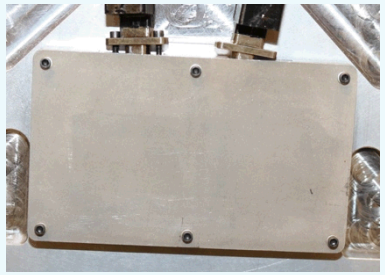




100s of virtual builds
1000s of virtual tests
Millions of CPU hours

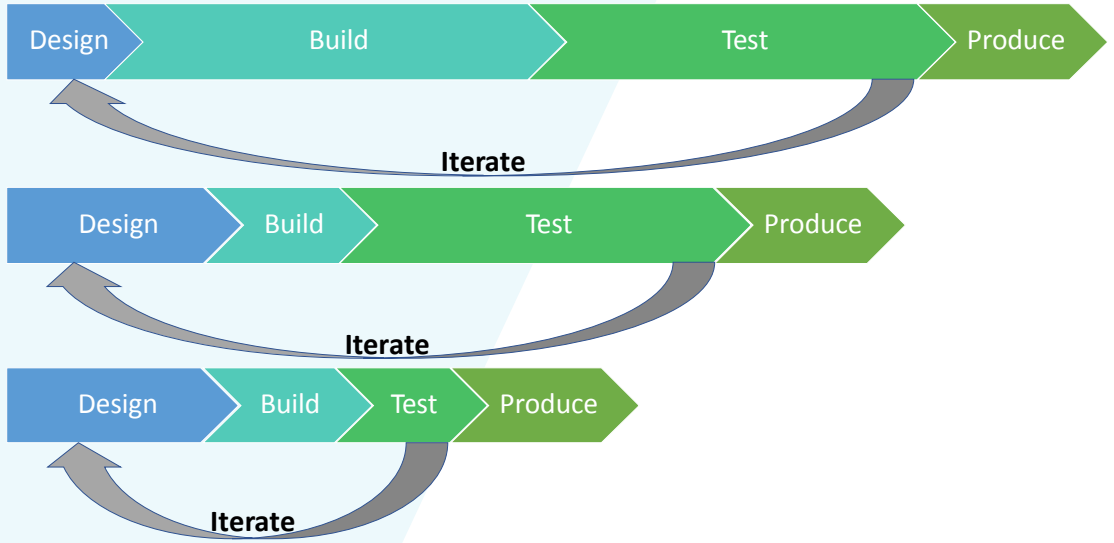
Modeling/simulation and additive manufacturing can reduce the number and speed of design-build-test iterations





316L SS ESD faraday cage covers for sounding rocket telemetry circuit boards. Printed parts (above, right); assembled (bottom right).

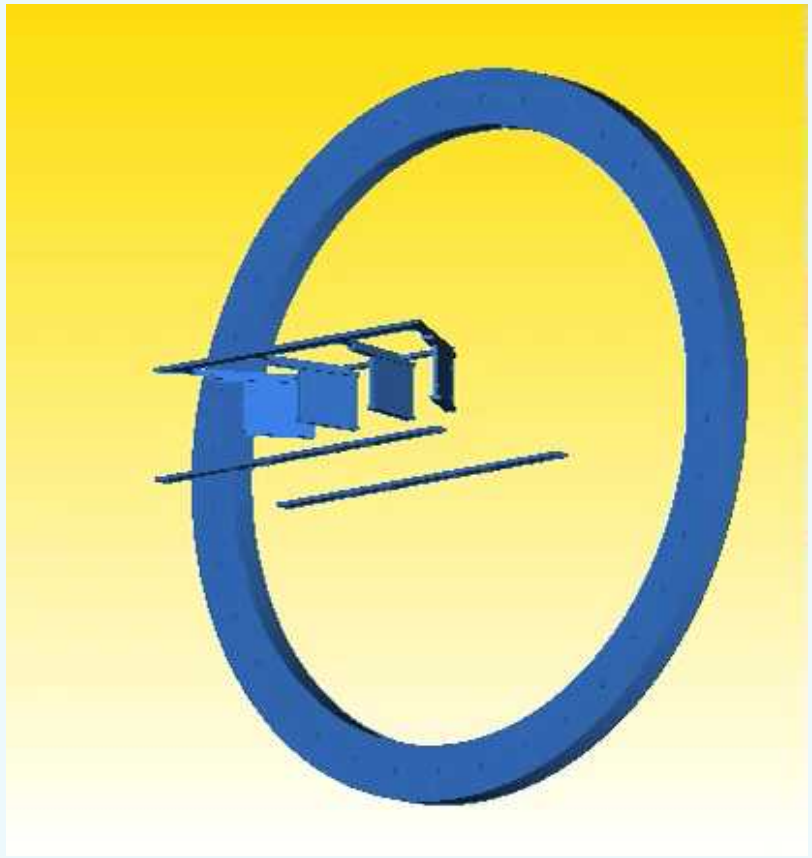
- Short turn-around production of metal parts needed
- Metal laser powder bed fusion was used
- Additional material test coupons were printed
- Estimated time and cost savings of roughly 60%



Topology optimization using PLATO

Impact on Design:

- Topology optimization explodes design space
- Take advantage of new materials with unique properties
- Enabled by HPC & high fidelity mod/sim
- Use additive manufacturing to realize organic designs



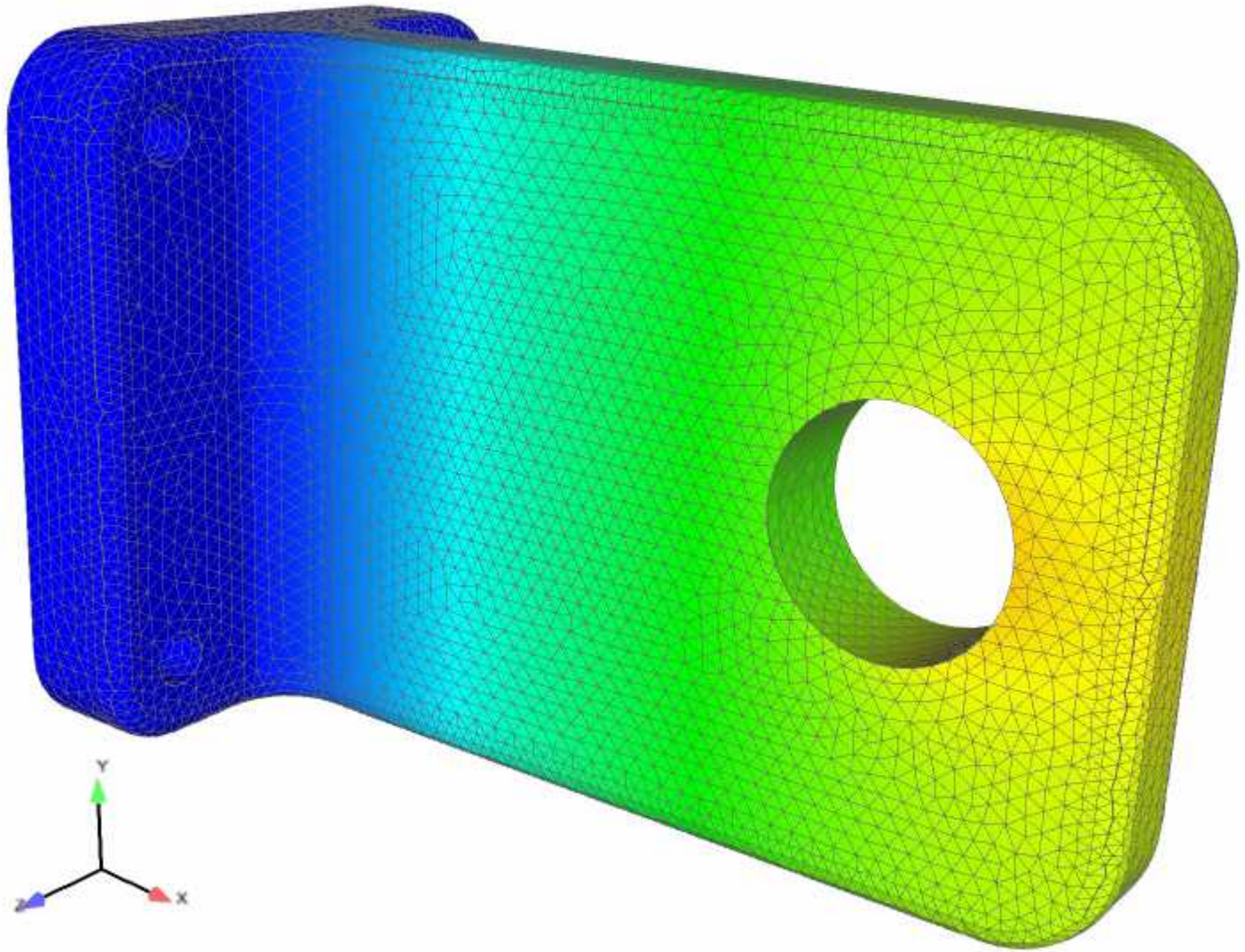
Example: satellite bracket design with increased stiffness, 40% weight reduction

PLATO Features:

- Print ready design
- UQ-enabled designs
- Multi-material designs
- Designs with lattice metamaterials
- Automated conversion back to CAD surfaces

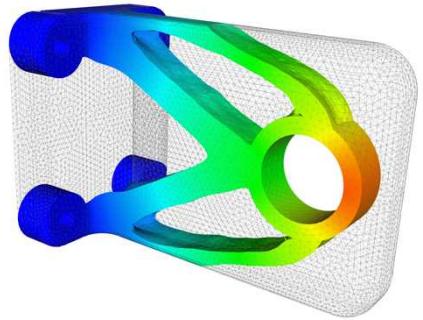
REAL TIME MULTI-PHYSICS DESIGNS ARE POSSIBLE

Incorporating the right physics is essential

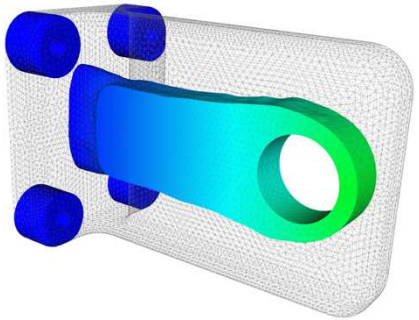


- GPU enabled solver package
- Optimized for stiffness and thermal conductivity

Mechanical Optimization Only



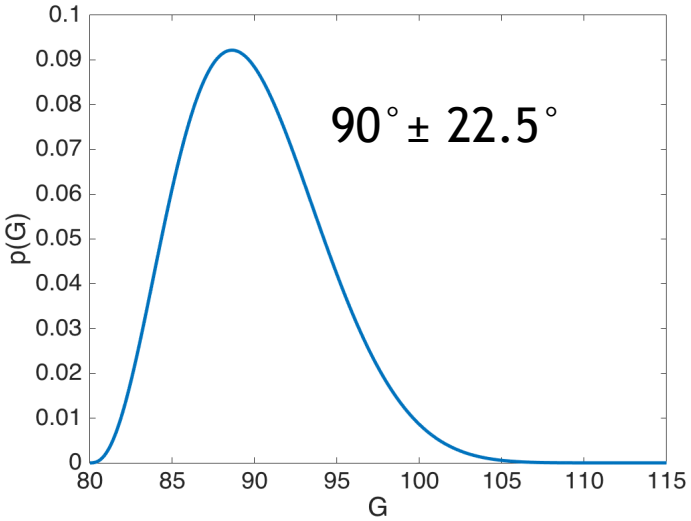
Thermal Optimization Only

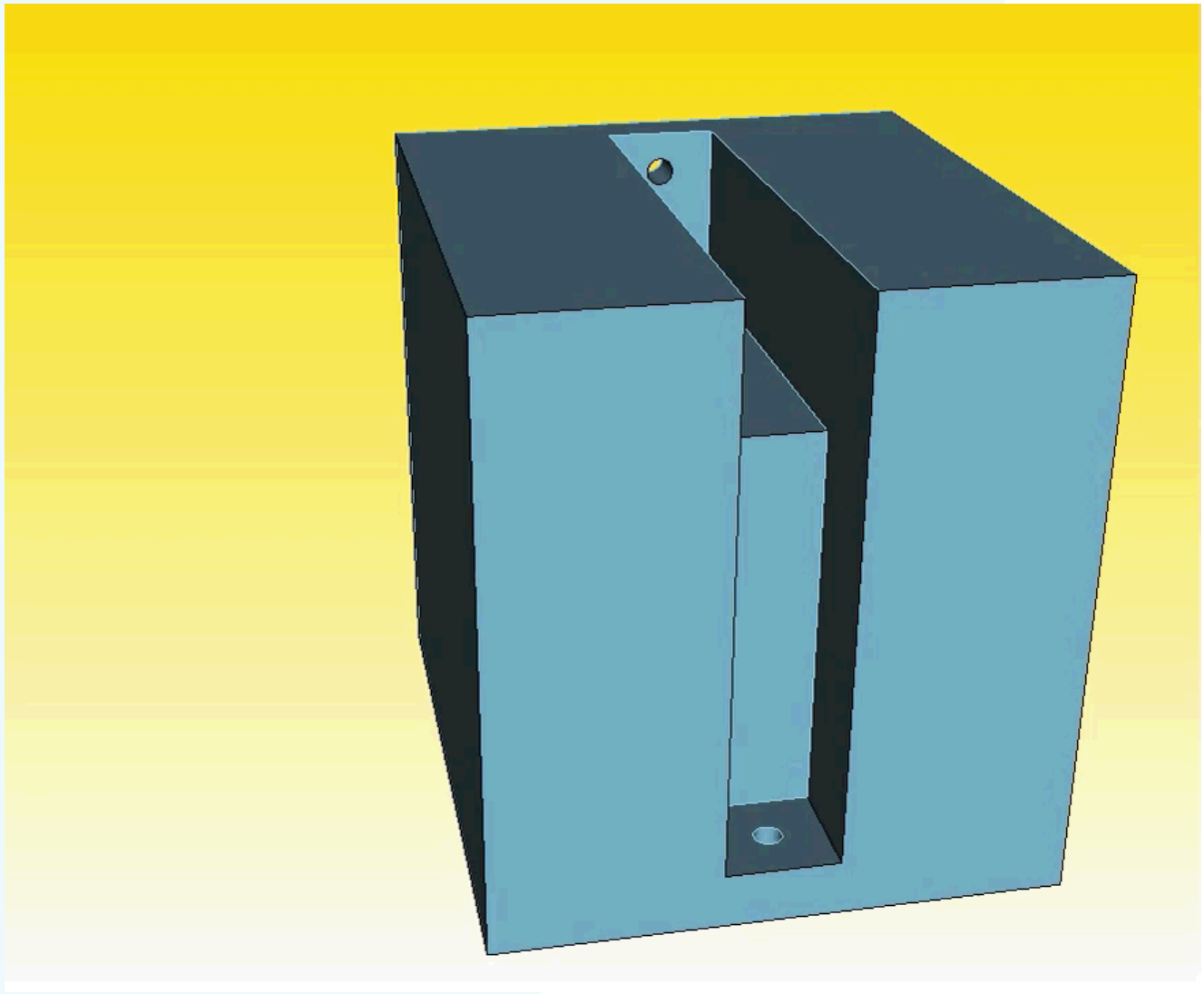


UQ ENABLES ROBUST DESIGNS

Insensitive to naturally occurring load variations

- Uncertainties in load angle included
- Optimized sampling (only 5-15 samples)
- User specified probability density function (here for load direction)

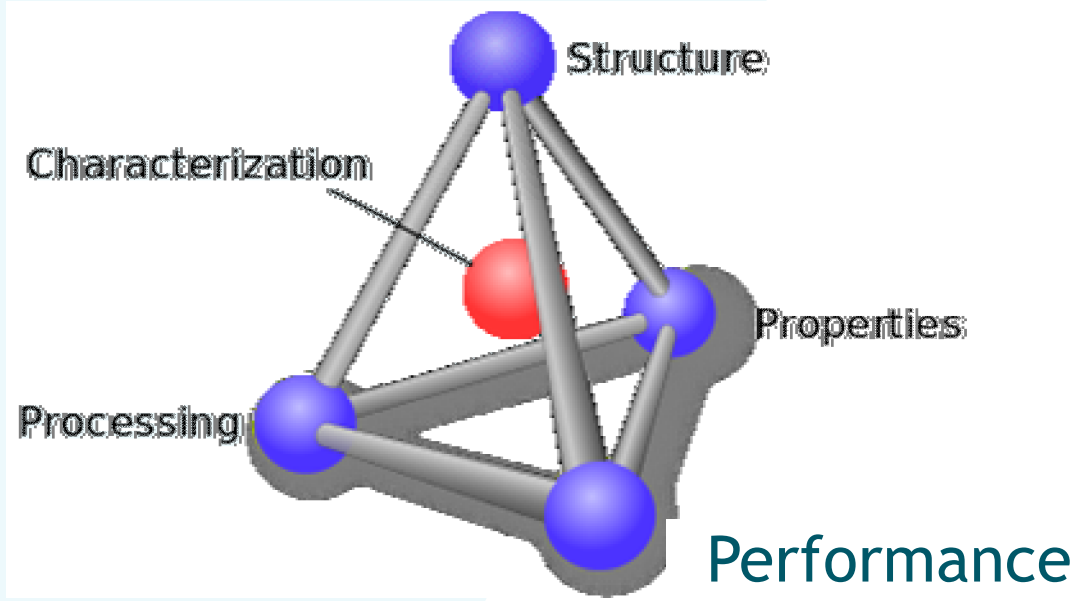




ADVANCED MATERIAL MODELING NEEDED

Our vision: born qualified

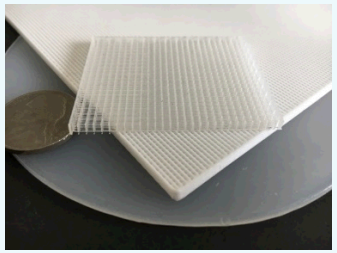
- In AM, metals experience extreme melting/solidification environments not present in traditional manufacturing.
- Understanding and predicting detailed thermal/fluid phenomena will lead to improved part quality and ultimately **prediction of performance**.
- Computation is driving process development.



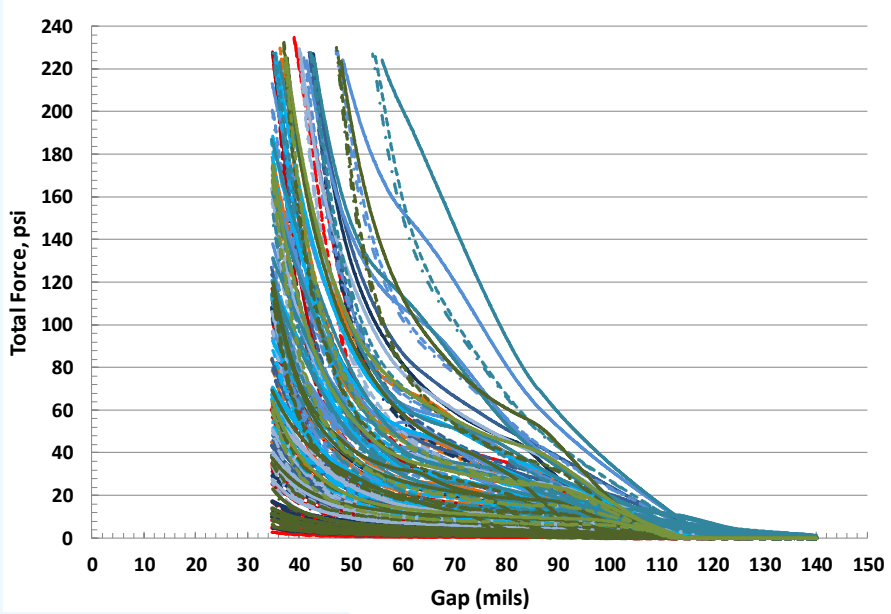
TRANSITIONING DESIGNS INTO MISSION SOLUTIONS

Ensuring repeatability and reliability

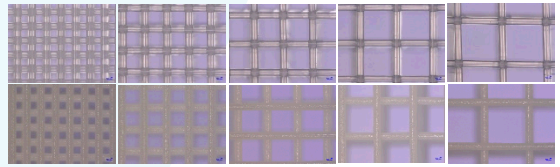
- Design parts for extreme mechanical conditions
- Make parts for high-consequence applications
- Validate part performance
- Perform R&D to improve understanding

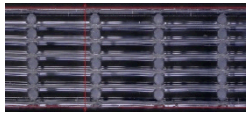


Mechanically tunable compression pads



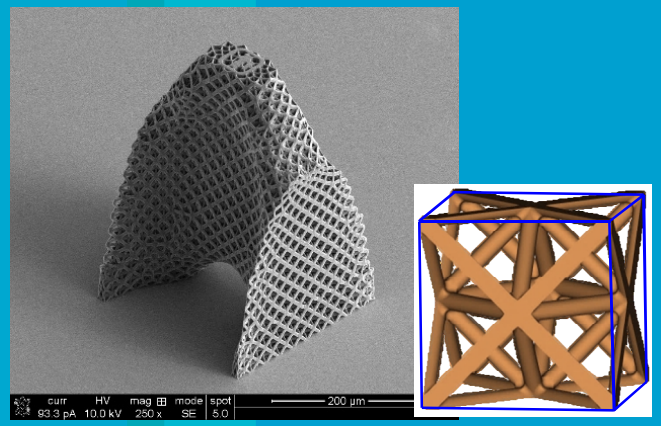
Process tunable to specific performance

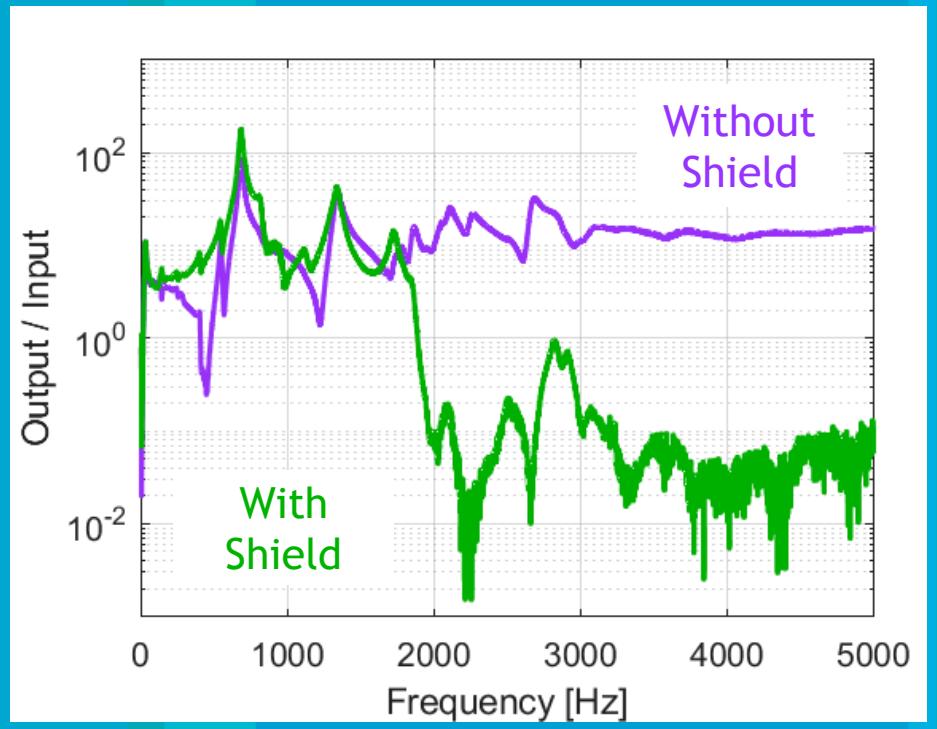




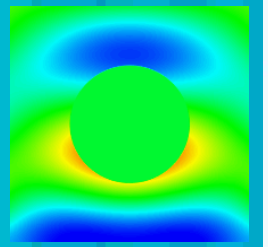
Printed compression pad cross section

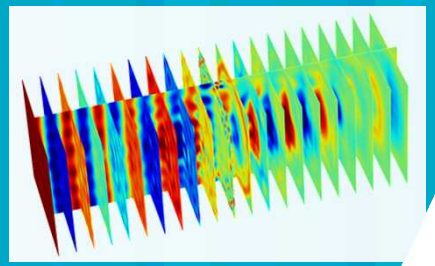
Example: acoustic metamaterials



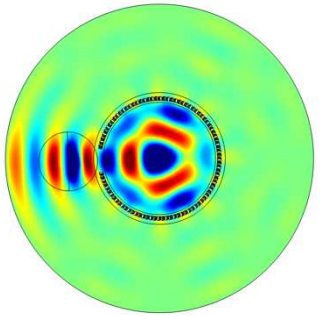


Multiphase composite materials designed to produce dynamic material properties not found in nature

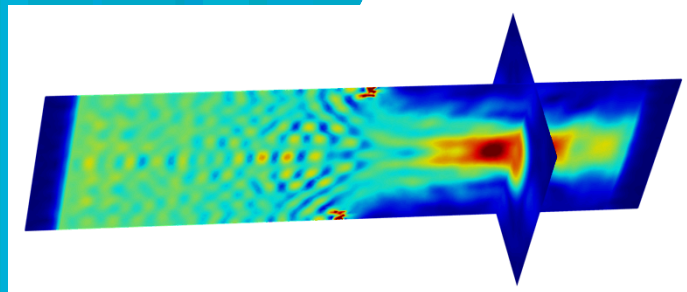




Wave Bending



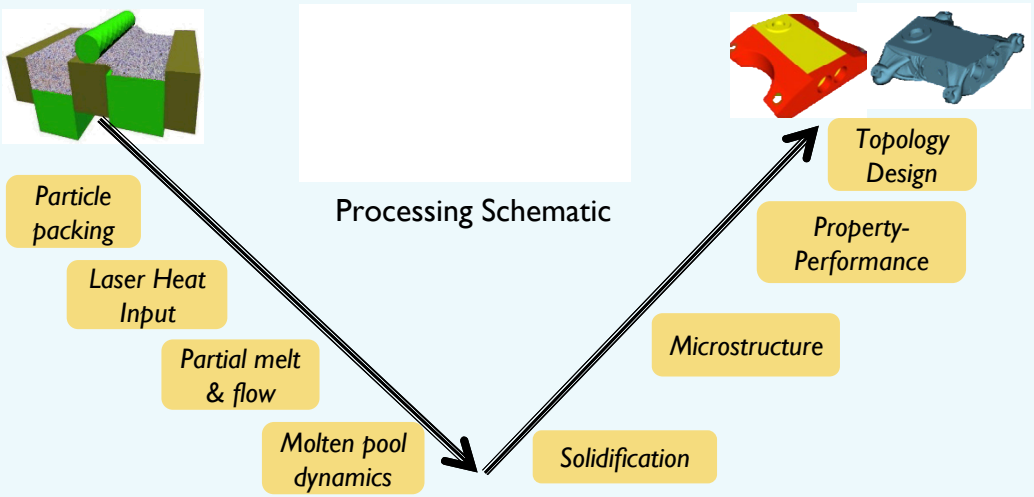
Wave Steering



Wave Focusing

VALIDATED MULTISCALE MULTIPHYSICS MODELING

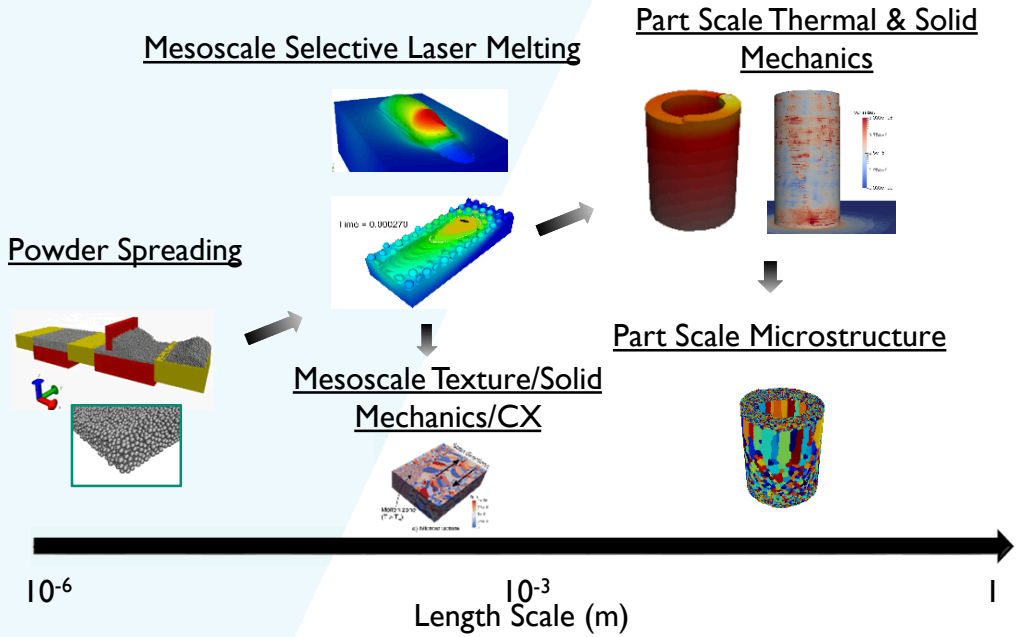
Required to take full advantage of AM capabilities



Critical modeling issues:

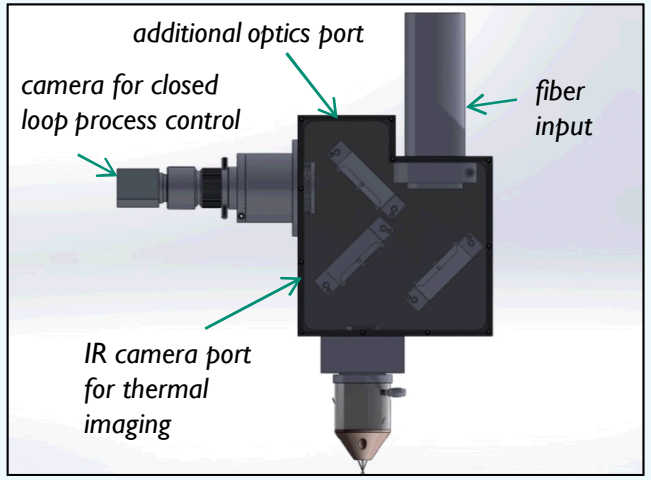
- Wide range of length scales
- Variability of raw materials
- Physics models are young
- Need new numeric techniques

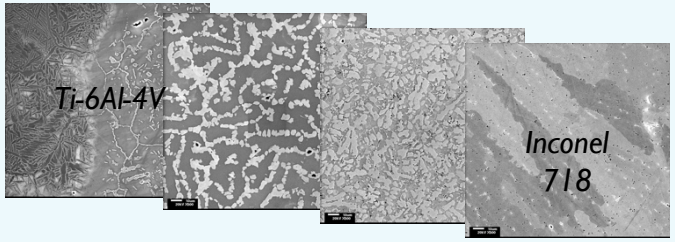
- Parallel attack on interdependent modeling areas
- Powder spreading and flowability
- Melt pool dynamics modeling
  - Robust solvers
- Grain morphology estimation based on actual build processes



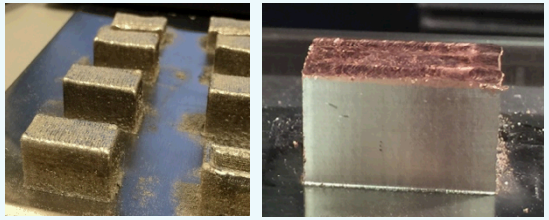
Tuning AM process requires sophisticated diagnostics

- Physics of melt pool is key
- Understanding process parameters is critical
- Multiple material constructs are possible

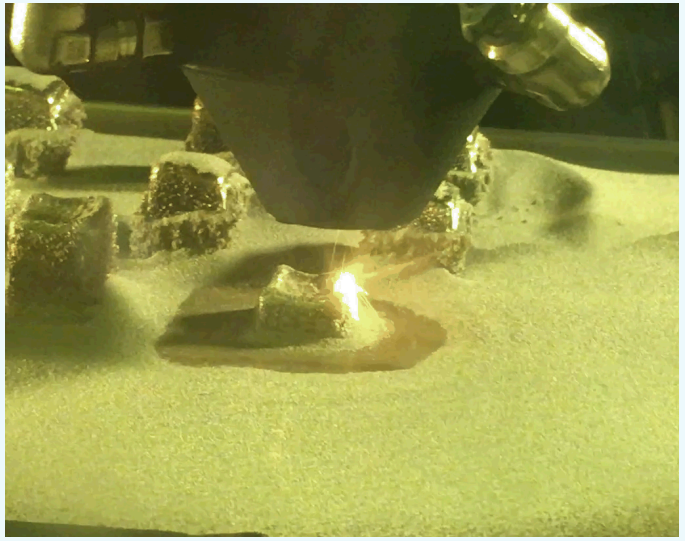




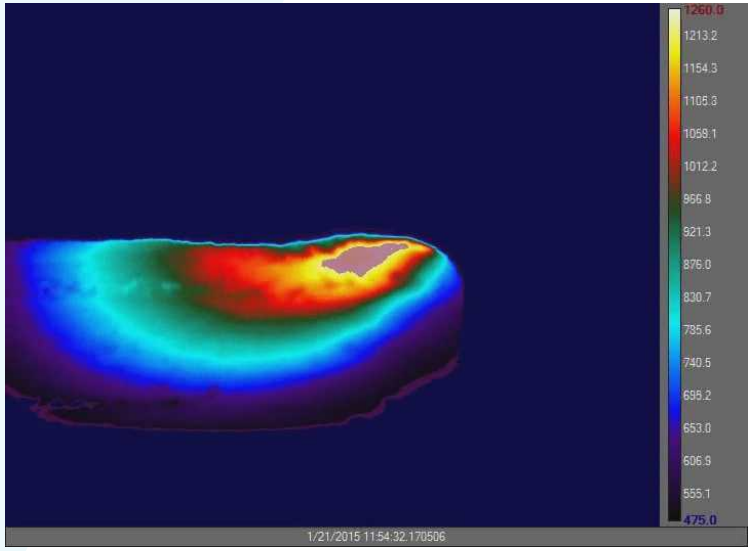
LENS functionally graded materials



304L SS / Cu multi-material thermal concentrator



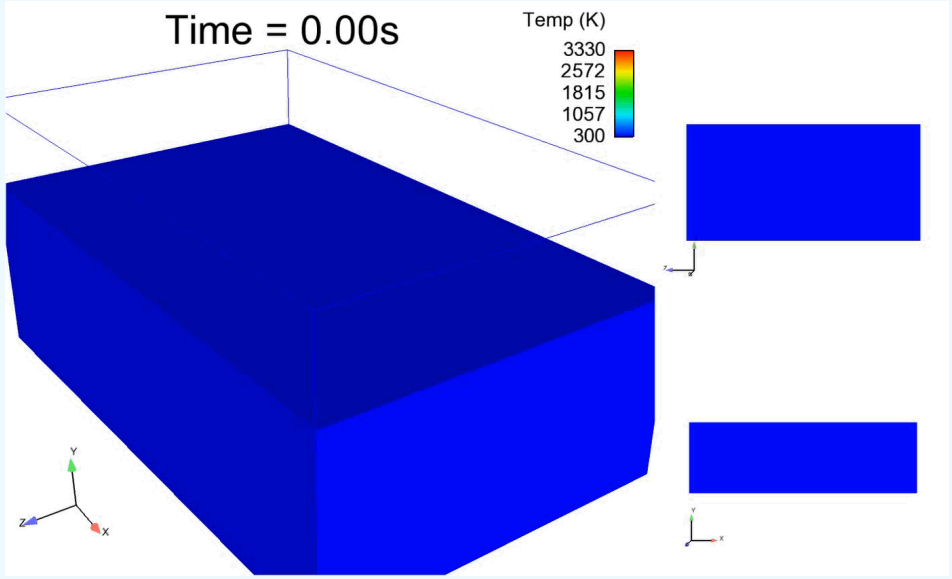
Laser engineered net shaping (LENS®)



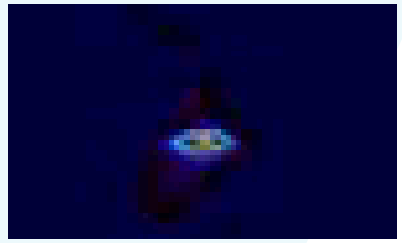
Thermal history during bi-directional metal deposition

Melt pool controls process results

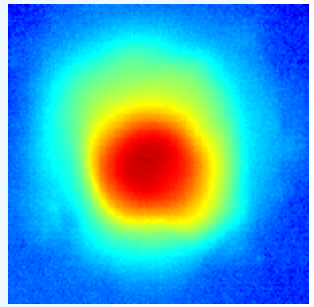
- Complex phenomena must be modeled
  - energy and mass deposition, heat transfer, melt propagation
- 3D model physics required
- Model validation experiments needed



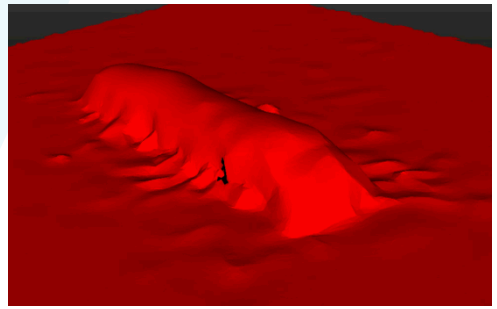
Sandia's Sierra/Aria FEM code Conformal Decomposition FEM (CDFEM) allows for evolving mesh



IR Camera



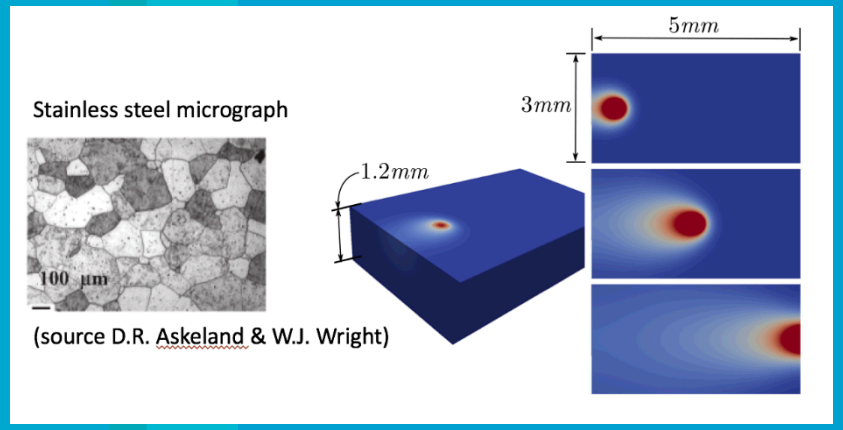
2-color pyrometer

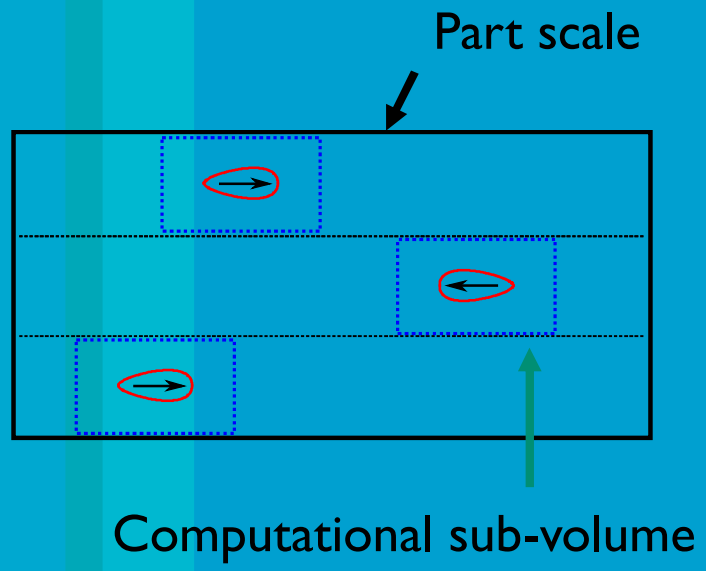


Surface Topology Scan

NEW COMPUTATIONAL CAPABILITY REQUIRED

Focus calculation on regions where grain structure is created





It is prohibitively expensive to perform simulations across an entire final part geometry at its native scale due to length scale disparities

- Part: centimeter and larger
- Molten Zone: millimeters
- Grains: hundreds of microns and smaller

Proposed solution

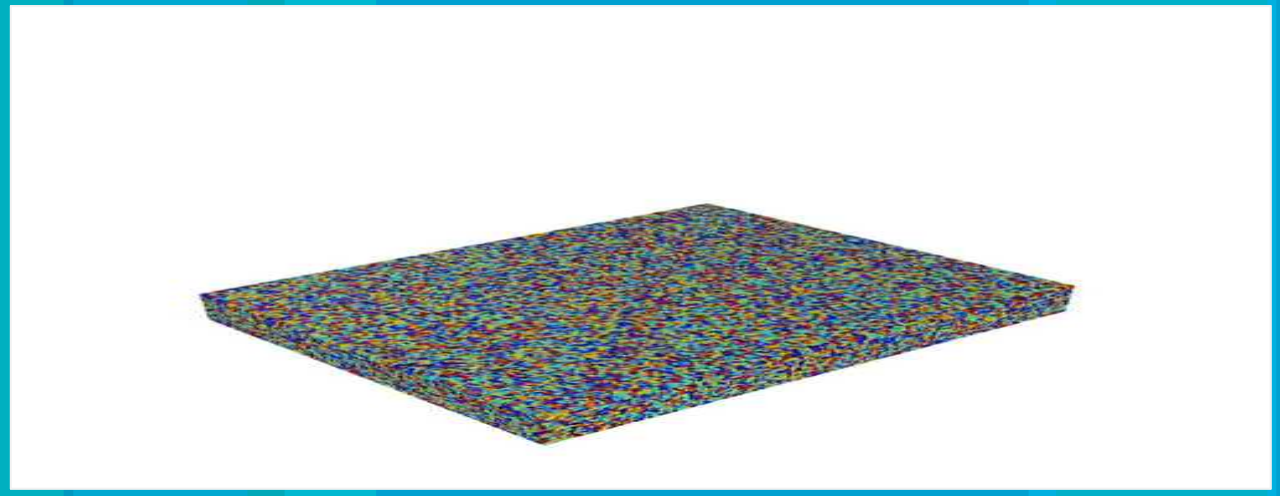
- Material deposition and heat source interaction are localized
- Model material deposition, grain growth, and evolution on moving computational sub-volumes
- Capability will scale down memory requirements for simulation exponentially to enable true build-scale simulation on a desktop

PREDICTING DESIGN AT THE MICROSCALE

SPPARKS: Stochastic Parallel PARticle Kinetic Simulator

SPPARKS

- A tool for designing AM fabrication processes
- Simulates microstructural evolution

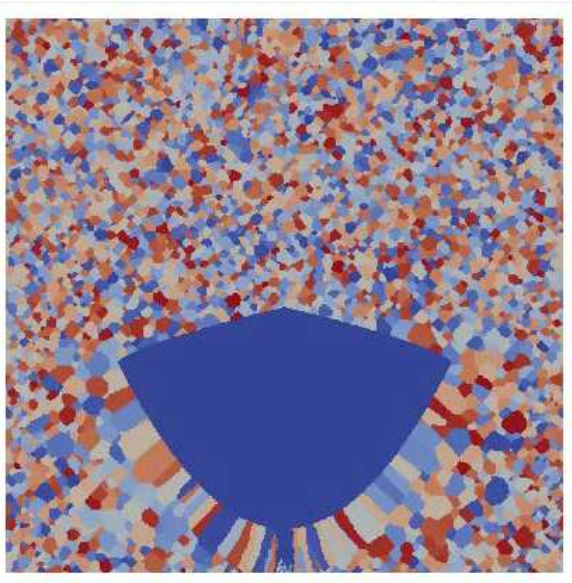


AM processes (melting, solidification, grain growth)

T. M. Rodgers, J. D. Madison, V. Tikare,
Computational Materials Science 135 (2017) 78-89

Grain Growth

Welding

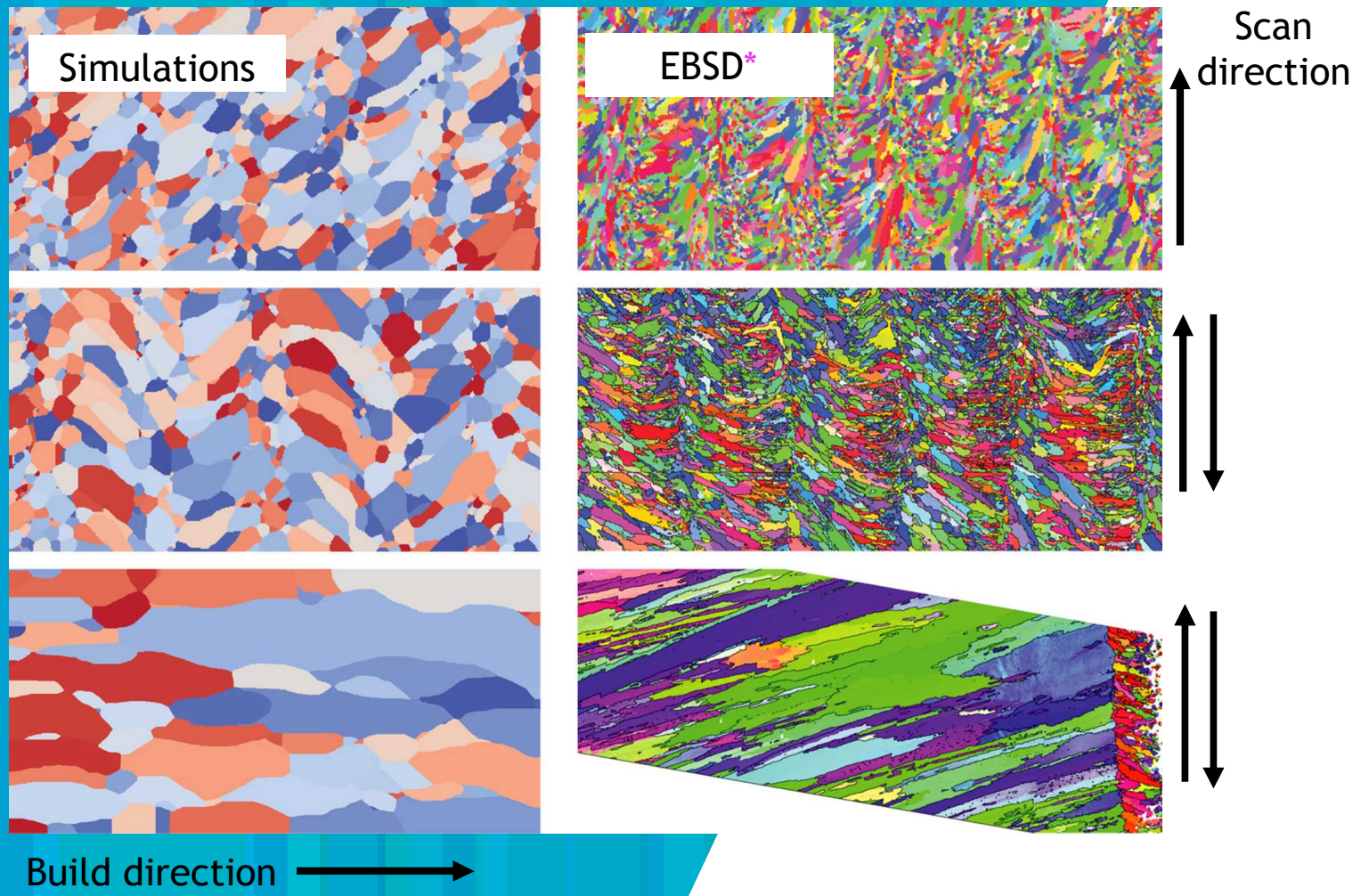


WHY IS A MICROSTRUCTURE SIMULATOR IMPORTANT?

Microstructural variations within and between different components control variation in engineering properties

Simulation of microstructural evolution during fabrication will inform:

- Design of process variables
- Uncertainty quantification in final components produced

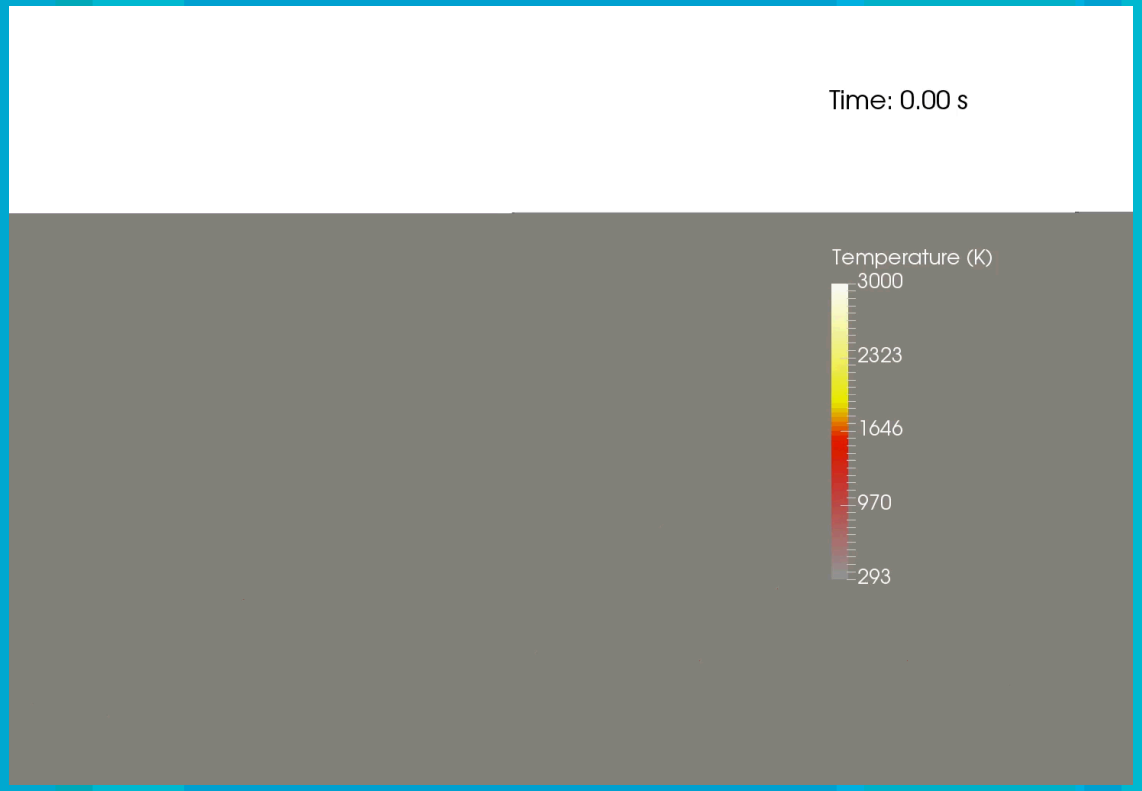


T. M. Rodgers, J. D. Madison, V. Tikare, Computational Materials Science 135 (2017) 78-89

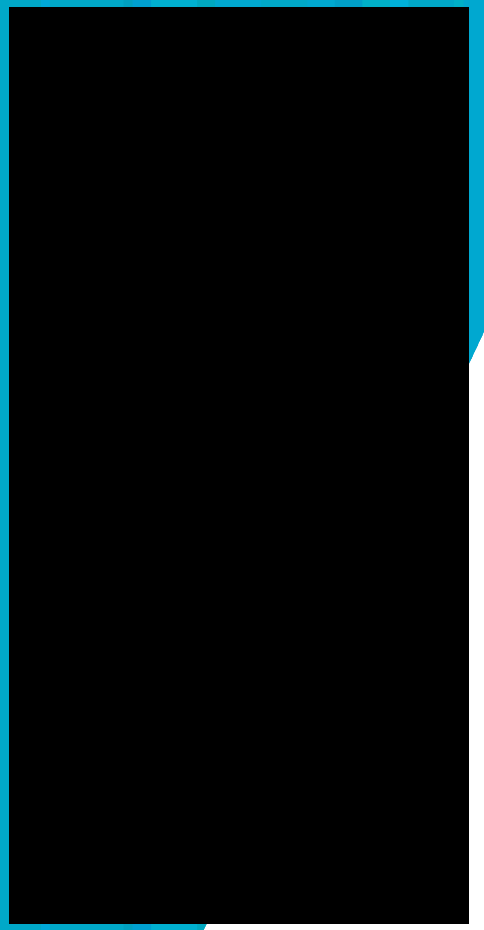
*L.L. Parimi, G. A. Ravi, D. Clark, M. M. Attallah, MATERIALS CHARACTERIZATION 89 (2014) 102-111

PROCESS PARAMETERS – MICROSTRUCTURE – PERFORMANCE

Process determines structure



Sierra FEA Thermal Model



SPPARKS kMC Model

Coupling with SIERRA thermal models

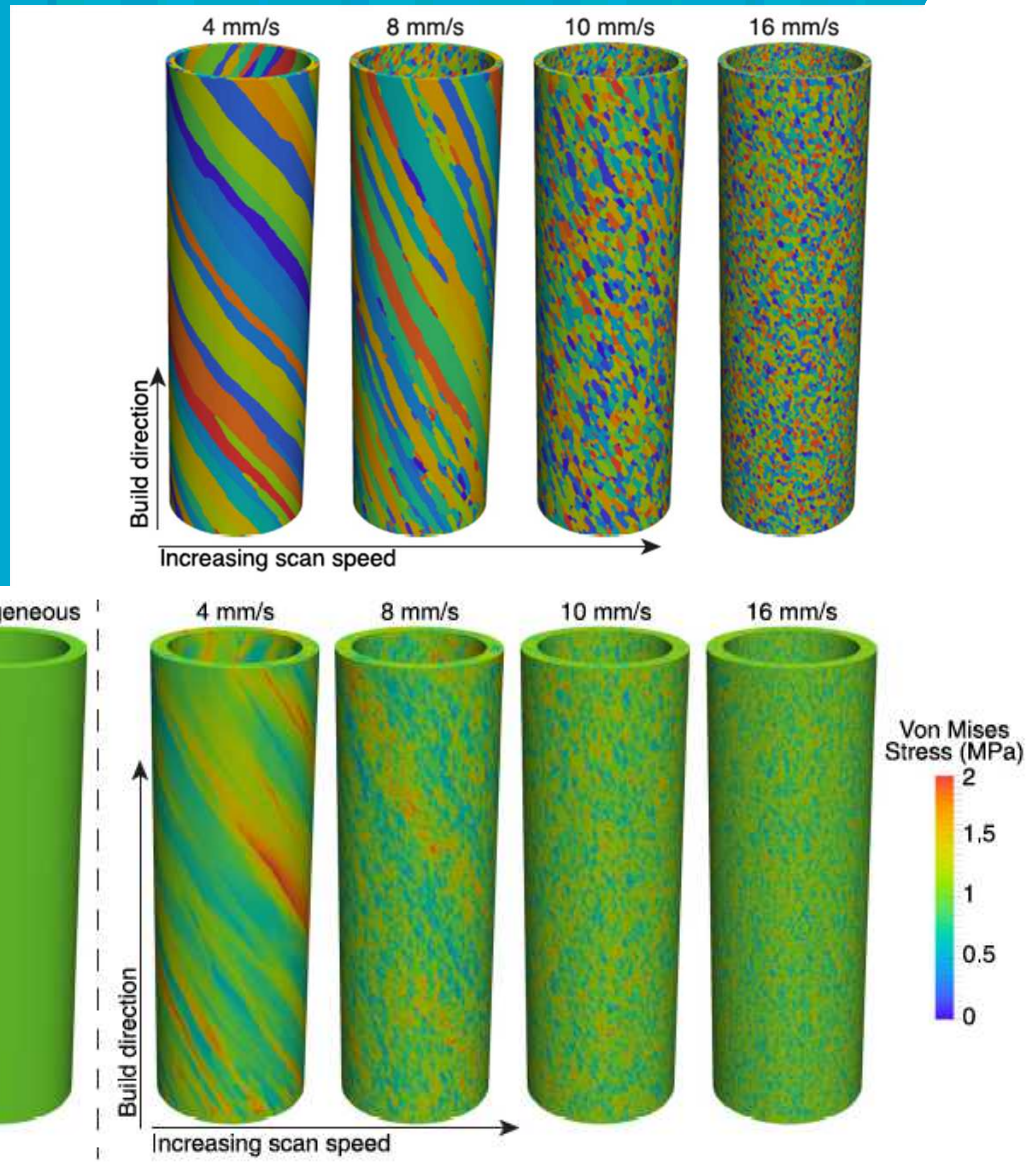
K.L. Johnson, T.M. Rodgers, O.D. Underwood, J.D. Madison, K.R. Ford, S.R. Whetten, D.J. Dagel, J.E. Bishop, Comp. Mech., vol. 61, no. 5, (2018) pp. 559-574

MICROSTRUCTURE PREDICTS PERFORMANCE

SPPARKS & SIERRA

- Processing creates microstructure
- Microstructure controls performance
- Coupling kinetic Monte Carlo (SPPARKS) with direct numerical simulation of mechanical behavior (SIERRA)

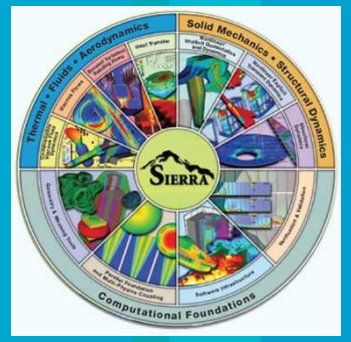
T. M. Rodgers, J. E. Bishop and J. D. Madison
Modelling Simul. Mater. Sci. Eng. 26 (2018) 055010



QUALIFIED BY DESIGN

The future vision for UQ

Integrated Materials Models: Evolving with Quantified Uncertainty



PRIME

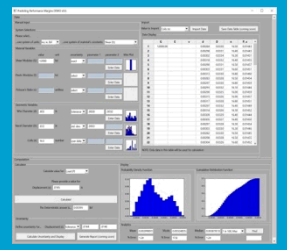
DAKOTA

GRANTA
MATERIAL INTELLIGENCE

LAMMPS

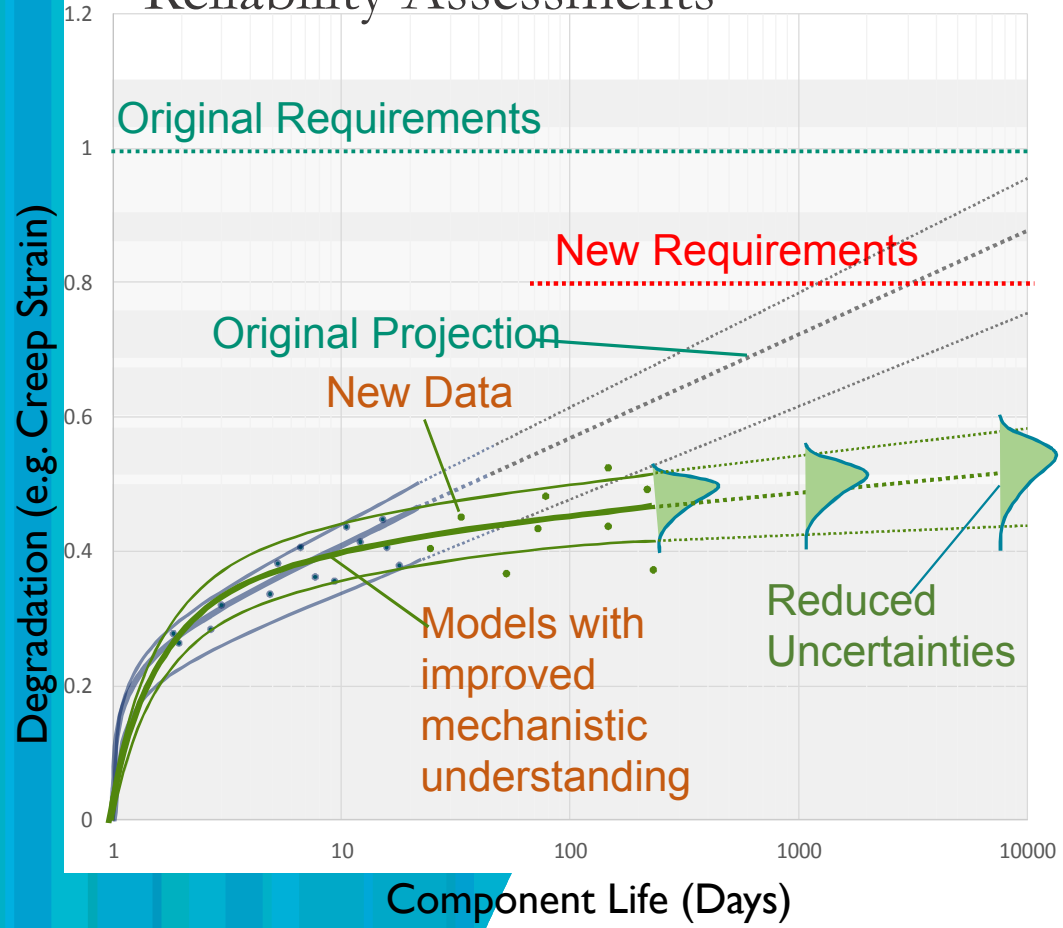
CUBIT

github repo



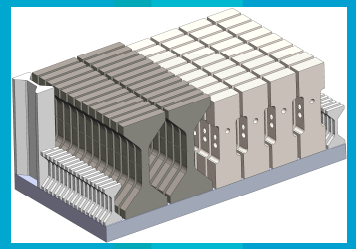
SPPARKS kMC Model

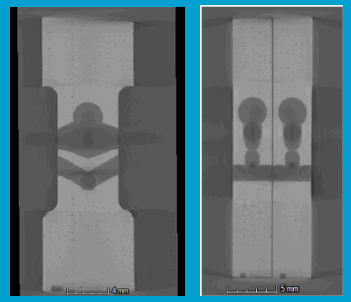
Evolving, Serial-Number Specific Reliability Assessments



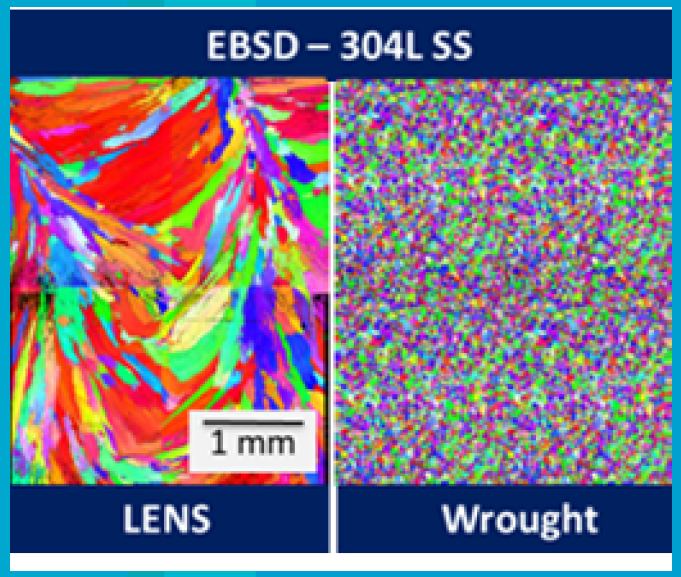
THE FUTURE – UNCERTAINTY QUANTIFICATION

2017 Sandia Fracture Challenge

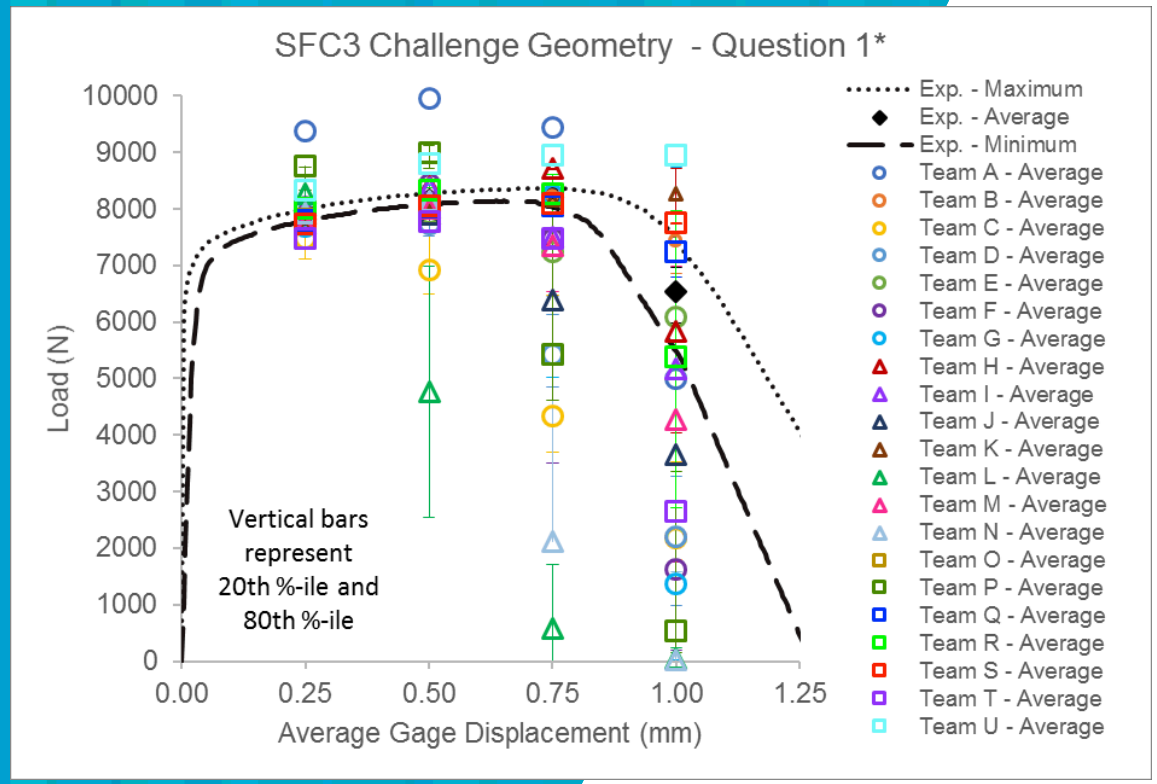




Complex sample geometry



Structure varies with process



Computational predictions still highly variable

Models that used microstructure information performed best!

FRACTURE CHALLENGE PARTICIPANTS

Multidisciplinary perspectives

Sandia National Laboratories

ONERA
THE FRENCH AEROSPACE LAB

GE

The American University in Cairo

Univerza v Mariboru

RWTH AACHEN UNIVERSITY

UT DALLAS

UIC
UNIVERSITY OF ILLINOIS AT CHICAGO

UCLA BRUINS

GLOBAL ENGINEERING & MATERIALS, INC.
Engineering and Innovative Solutions

UNIVERSITY OF MIAMI

RUHR UNIVERSITÄT BOCHUM
RUB

MINES ParisTech

MISSOURI

Natural Resources Canada / Ressources naturelles Canada
CanmetÉNERGIE
Leadership en écoInnovation

THE UNIVERSITY OF ARIZONA.

Massachusetts Institute of Technology

UNIVERSITY OF Cincinnati

Cornell University — Founded A.D. 1865

Northwestern University — Quaecumque Sunt Vera — 1851

Tsinghua University — 1911

Zhejiang University — 1897

Chongqing University — 1929

Dalian University of Technology — 1949

Naval Surface Warfare Center NSWC — A Tradition of Excellence

NASA

The University of Texas at Austin

WHAT WE NEED FOR FUTURE ADVANCES

New tools to make this work possible now and in the future

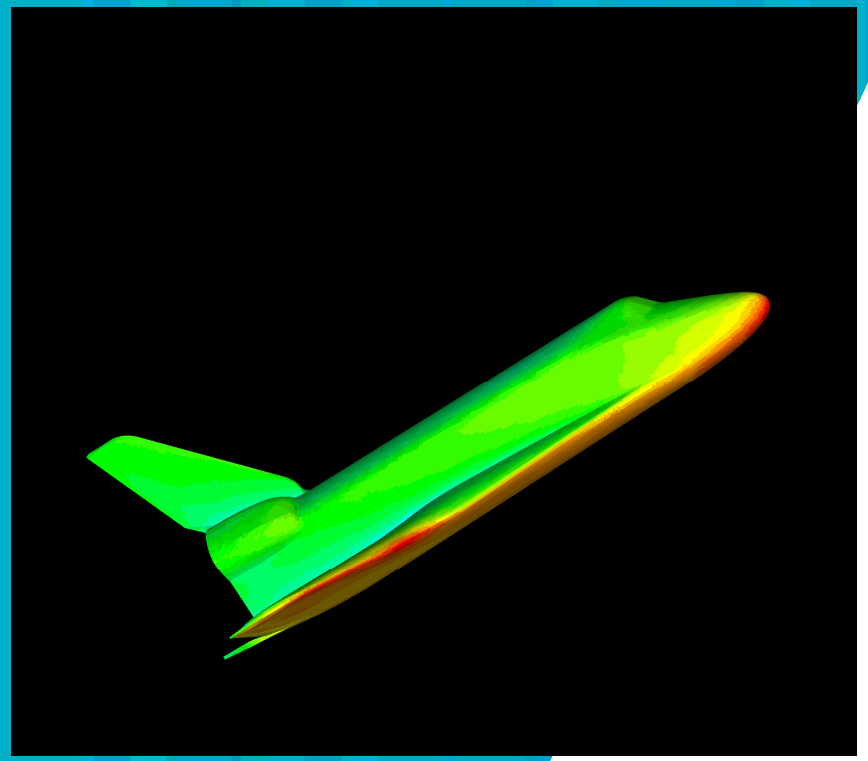
- Sandia's engineering missions are pushing us in new directions
  - Complex full-system engineering models that span a system's lifecycle
  - Explicit focus on how humans and computers interact to enable critical decisions
  - Adding automation, data-analytics, and intelligence throughout computational simulation
    - See WCCM mini symposia on data science
- But advances in computing overall are also important:
  - Exascale Computing Project—enabling 50x improvement in capability by 2021-23
  - Sandia's new ARM-based supercomputer prototype (Astra) helps open the door for future custom hardware options
  - Neuromorphic and quantum efforts also moving forward
- Diverse partnerships and diverse staff will help achieve both

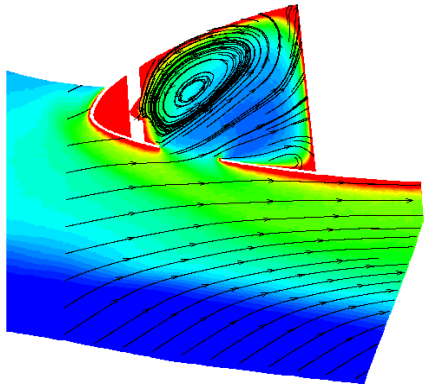
HIGH IMPACT DECISIONS REQUIRE HIGH-FIDELITY ANALYSIS

The Space Shuttle Columbia accident

- Accident attributed to insulating foam impact on the wing leading edge during launch
- Sandia provided NASA with aerodynamic, aerothermal, fluid dynamic and foam impact analysis
- Numerical simulations of fluid flow suggested a shock-shock interaction increased heating rates in the area of the impact
- Flow inside the wing accentuated the problem

The right physics and right model, at the right scale, might have identified a real-time solution to avoid the accident





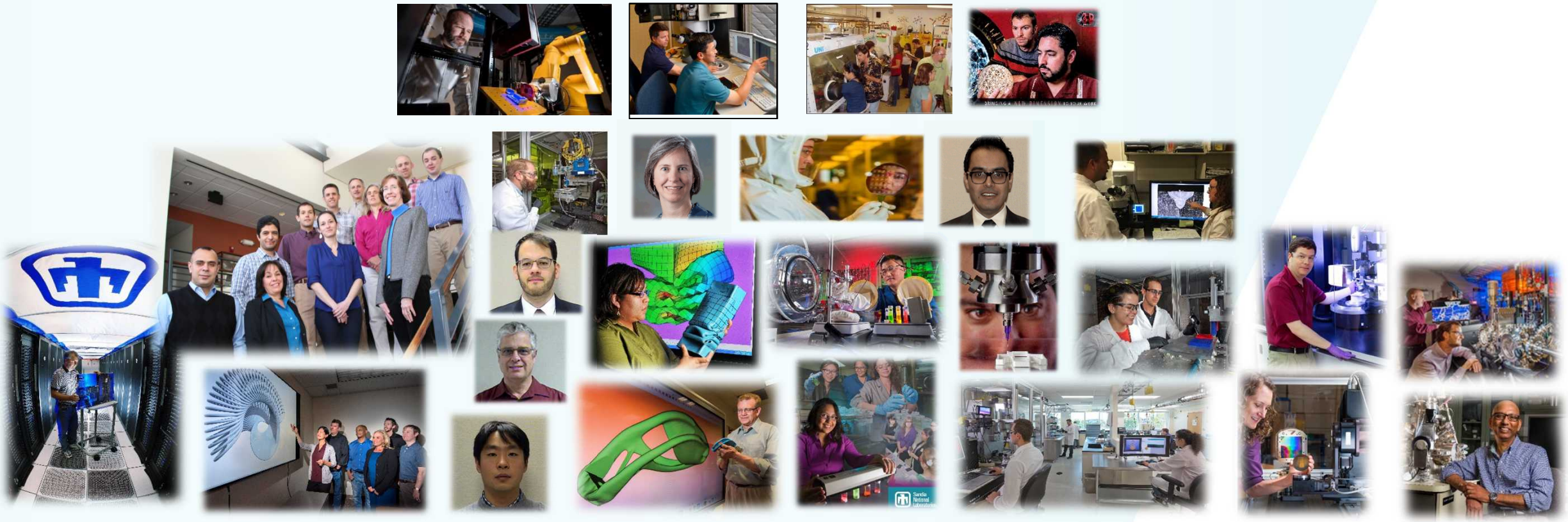
ACKNOWLEDGEMENTS

Fadi Dressler Abdeljawad
Miguel Aquilo
Nicolas Argibay
David Adams
Dorian K. Balch
Lauren L. Beghini
Joseph E. Bishop
Timothy Blada
Ted Blacker
Dan Stefan Bolintineanu
Brad Boyce
Judith Alice Brown
Harlan James Brown-Shaklee
Michael T. Brumbach
Dorean Chaleunphonh
Michael Evan Chandross
Blythe Clark
Brett Andrew Clark
Scott Collis
Adam Wade Cook
Bret Michael Curtis
Amber Dawn
Christopher B. Diantonio
Shawn Dirk
Kurtis Ross Ford
Eric Christopher Forrest
Michael Allan Guthrie
Lili Heitman
Bradley Howell Jared
Kyle Johnson
Daniel R. Kammler
David M. Keicher
Kristopher R. Klingler
Joshua Koepke
Andrew Kustas
Judith Lavin
Nicholas Leathe
Jeremy B. Lechman
Brian T. Lester
Gerald Fredrick Lofstead
Jonathan D. Madison,
Sethambal S. Mani
Mario J. Martinez
Joseph R. Michael
John A. Mitchell
Daniel Moser
David R. Noble
Steven J. Plimpton
Jim Redmond
Amy Riker
Allen Roach
Joshua Robins
Theron Rodgers
Randy Schunk
Daniel Thomas Seidl
Mark Smith
Paul Robert Stallings
Michael Stender
Jim Stewart
Samuel Subia
Joshua Daniel Sugar
Laura Painton Swiler
Samantha Taylor
Veena Tikare
Bradley Trembacki
Dede Valerio
Mike Valley
Mikhail Vorontsov
Bart G Van Bloemen Waanders,
Timothy Walsh
Jason W. Wheeler
Shaun R. Whetten
Timothy Michael Wildey
Mark Wilson
Michael K. Wong

… And Many More

DEFINED BY OUR OUTSTANDING PEOPLE!

SANDIA



High Performance Computing | Computational Modeling & Simulation | Microstructure Modeling | Design & Topological Optimization | Material Synthesis | Advanced Manufacturing | Material Characterization | Performance Qualification

Exceptional service in the national interest