Motivation, Development and Future Directions for Computational (Metallic) Materials at NASA

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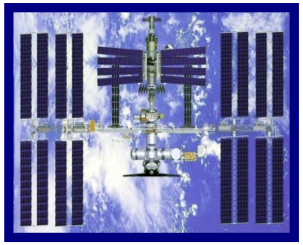
Outline

Background and Motivation
- Long Duration Spaceflight
- Some Problems of Interest

Computational Materials
- Material Performance
  - Next Generation D&DT
- Material Processing

Future Directions
- ARMD Vision 2040 Roadmap

A New Paradigm is Needed for Long Duration Missions



250 miles

International Space Station

Today's strategy for LEO does not work for tomorrow's deep space missions

Today, we rely on the 4 R's

Resupply

Repair by Replacement

Redundant Hardware

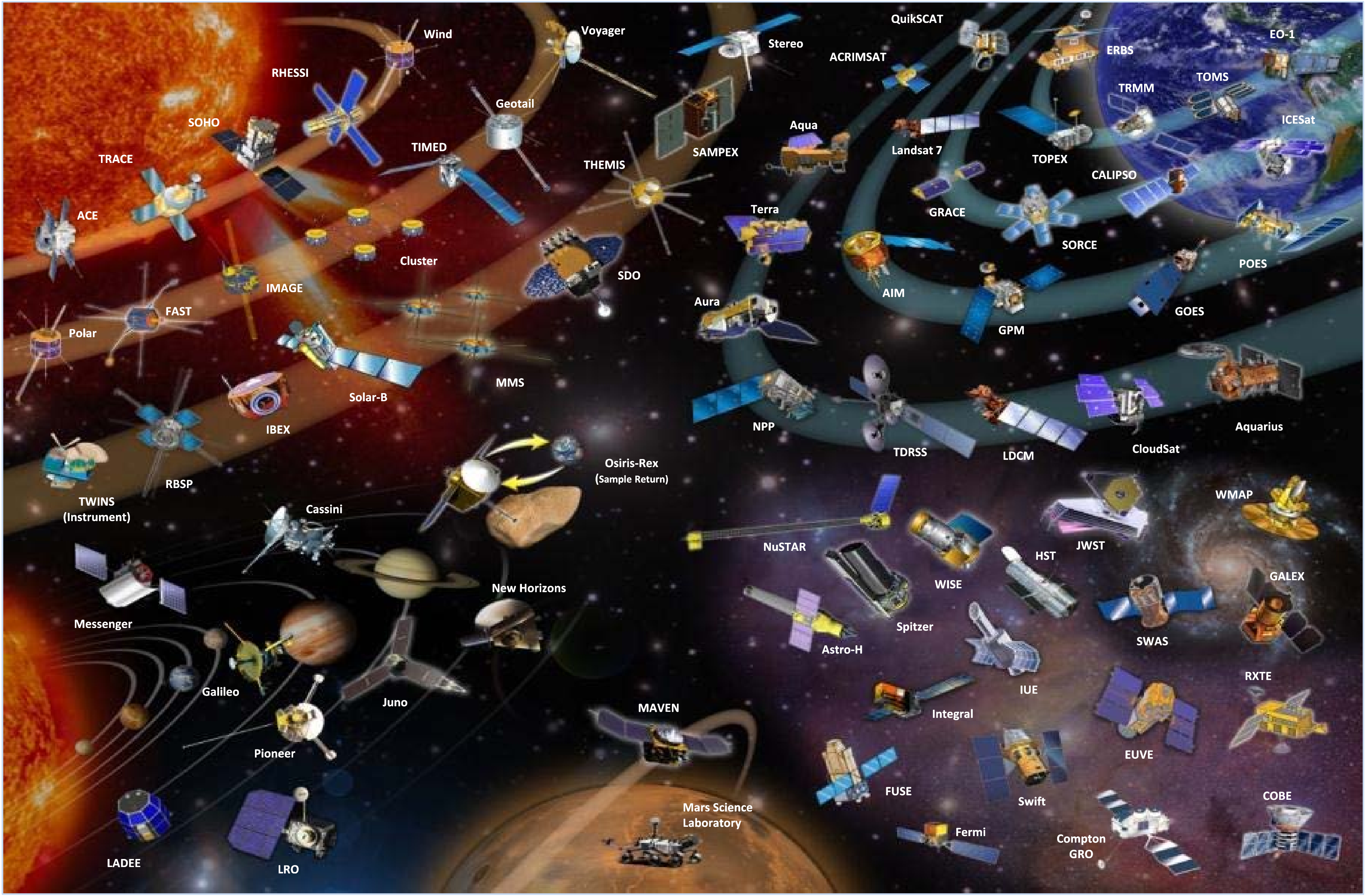
Retreat to Earth

For Mars and beyond: a new paradigm is needed – can basic research help?
History shows it has and will.

Martian Sunset

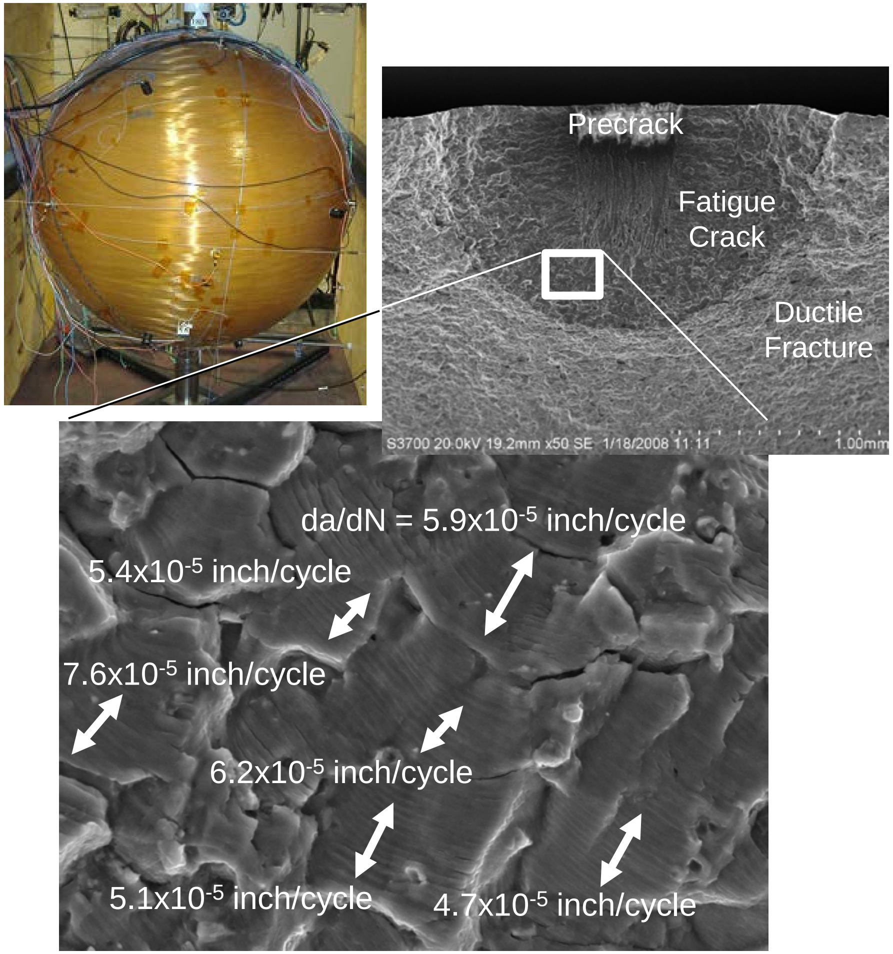
33,900,000 miles

The Diverse Mission Portfolio at GSFC*



* Mike Viens, GSFC

Ultra-Thin COPV Liners*



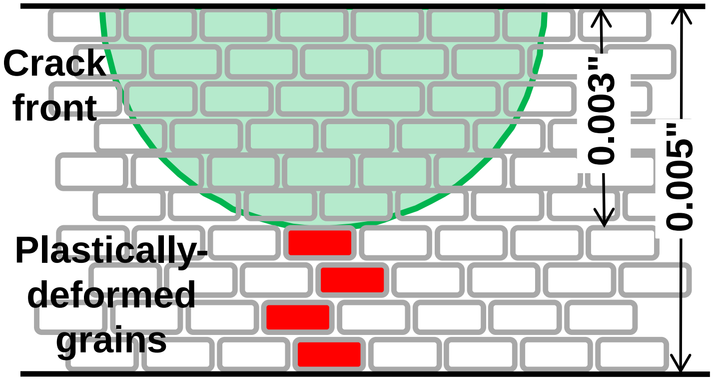
Loss of Similitude
Fatigue Striations (0.032” liner)*
Average: 5.8x10^{-5} inch/cycle Std. Dev.: 1.0x10^{-5}

Mass saving requirements are driving liner thicknesses to as low as 0.005”

- Engineering fracture mechanics & similitude assumptions break down as thickness and critical crack size decrease

Assuming an “ultra-thin” 0.005" liner

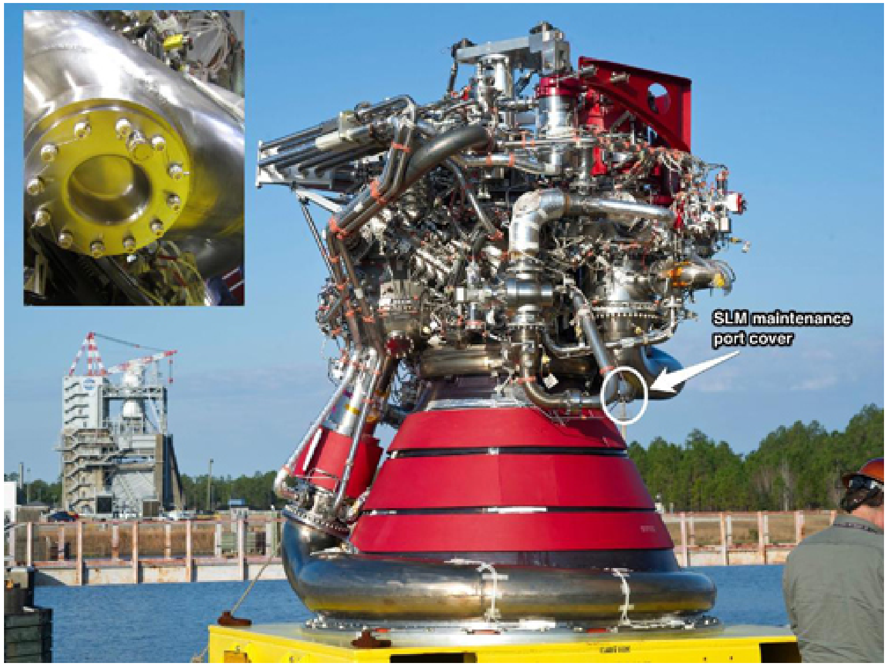
- Crack is large compared to liner thickness and material microstructure
- Microstructural variation is expected to be very large
- Plastic zone is also relatively large



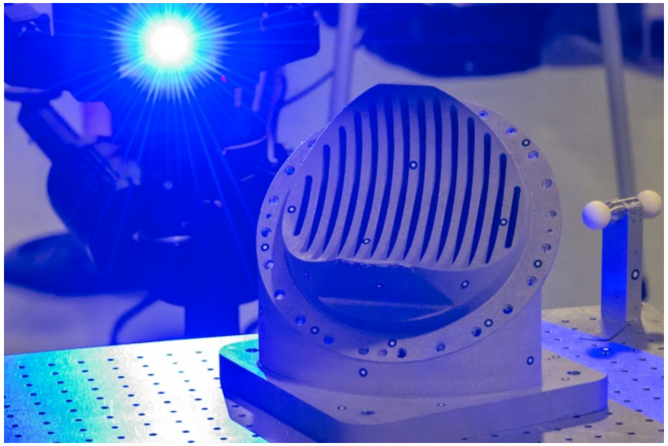
Surface Crack in 0.005” liner

* with Lorie Grimes-Ledesma, JPL

Additive Manufacturing in SLS (and numerous other spaceflight components)



RS-25 Engine prior to testing
at Stennis Space Center

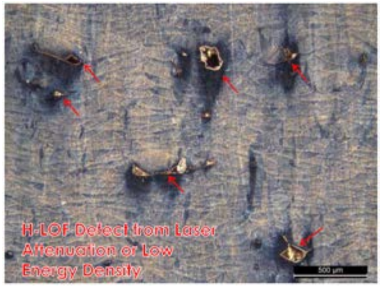


Pogo Z-Baffle made from
Selective Laser Melting (SLM)

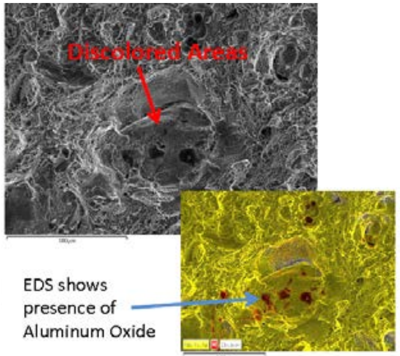
Computational Materials for SLS
- **Improve Process Certainty**
  - **Design / Tailor Process**
- **Improve Part Certainty**
  - **Meet material specifications**
  - **Certify components**

Issues Posed by Hot Isostatic Pressed (HIPped) AM Components*

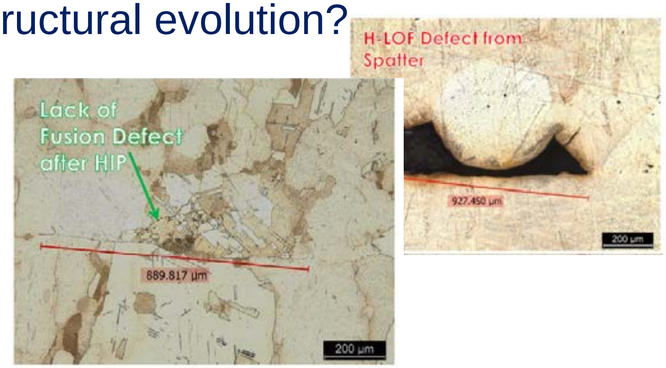
- Does the HIP process actually improve reliability? Under what service conditions?
- What types and sizes of AM induced defects cannot be removed through HIP
- How does the mechanism of defect creation affect the ability of HIP to remove defects? (e.g., can defects associated with oxidation be healed?)
- How does the atmosphere during AM play a role? Vacuum versus Argon?
- Are the defects that HIP can remove already below a size that is of consequence?
- Does HIP reduce volume of defects but not eliminate them. Does this make them harder to detect in NDE? Are all "healable" defects below NDE detection limits?
- Do unhealed defects of reduced volume actually create a more damaging flaw with higher stress concentration or crack-like tendencies?
- Does pressure (in addition to temperature) influence microstructural evolution?



Defects due to inadequate ventilation on the powder bed.



Defects unhealed in HIP with apparent oxidation related cause.



Large lack-of-fusion defect **post-HIP** with near zero volume. Do not know strength (if any) of the interface.

**Wells, West, MSFC*

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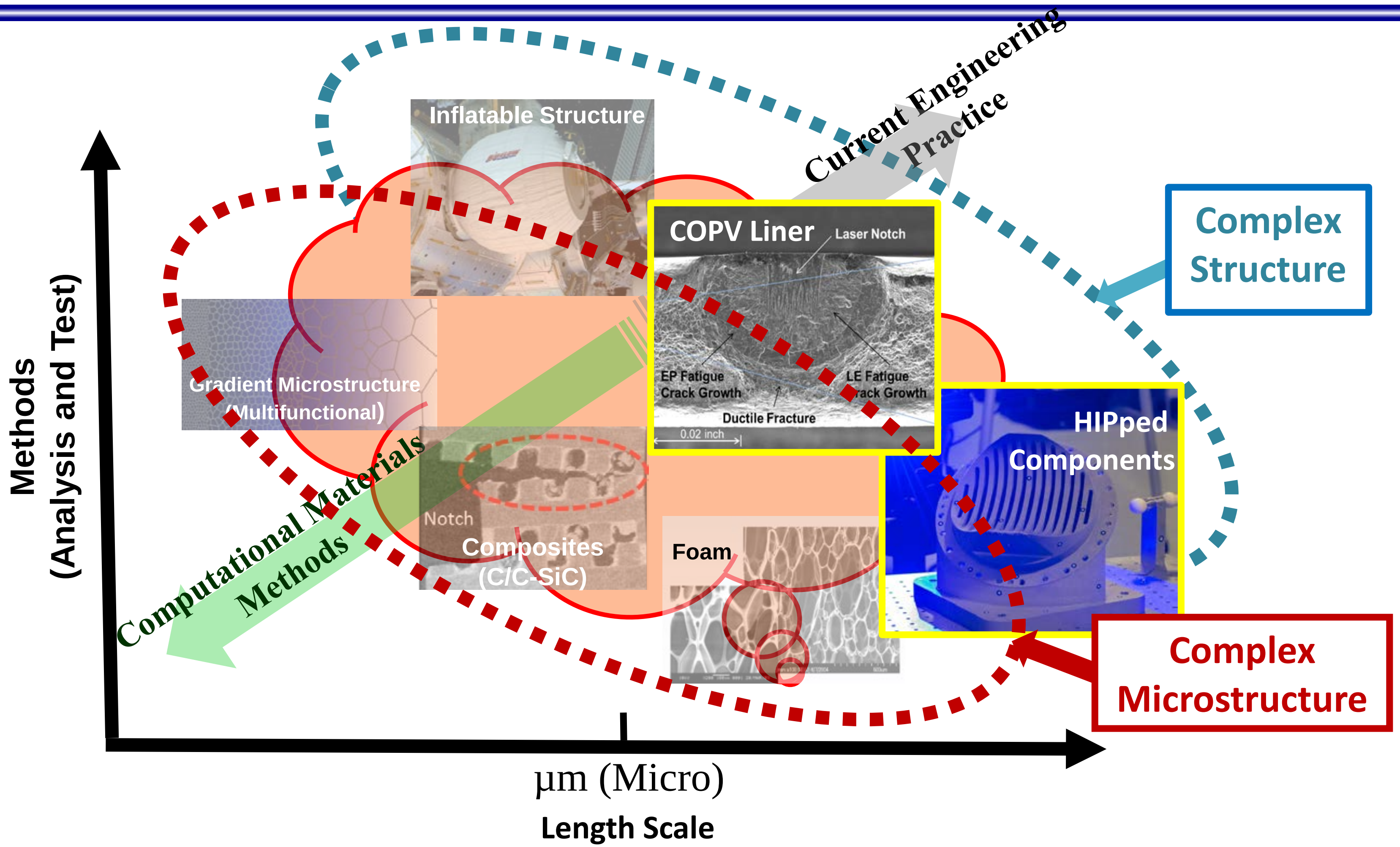
D&DT Analysis and Test Shortfall

(Micromechanics Regime)*

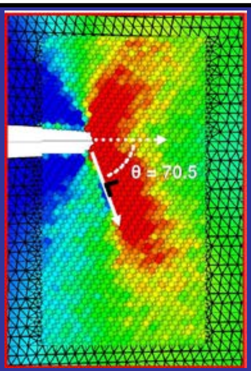


Future designs include microstructure-dependent D&DT influences:

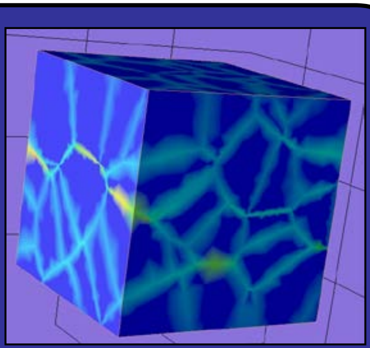
- Very thin or functionally-graded structural components (where traditional methods are suspect)
- Advanced materials and manufacturing, which preclude brute-force testing programs

**NASA/TM-2017-2017-219621; NESC-NPP-17-01, R. Piascik & N. Knight, Re-Tooling the Agency's Engineering Predictive Practices for D&DT*

Computational Materials for Material Performance



Modeling Plasticity at a Crack Tip



Simulation of Crack Growth in a Material Microstructure

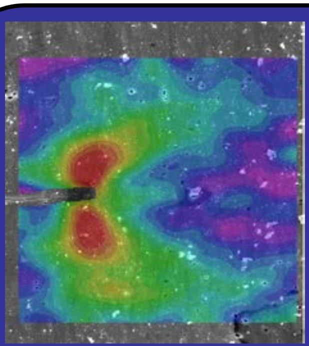
Simulate Operative Physical Processes at Relevant Length Scales

- Simulate critical damage processes
- Develop micro-/nano-structure-based simulations that interrogate damage processes at local length scales and local environments
- Propagate uncertainties across length scale to predict component reliability
- Design materials to extend structural life

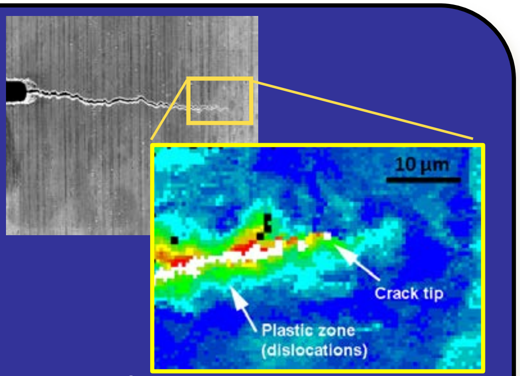
Physics-Based Material Design & Certification Requires Close Integration of Analysis and Experimentation

Characterize the Physics of Damage via Experimental Evaluation

- Develop micro-/nano-structure-based testing & characterization that interrogates damage processes at local length scales and local environments
- Validate damage models and understand operative processes
- Fabricate and evaluate model materials

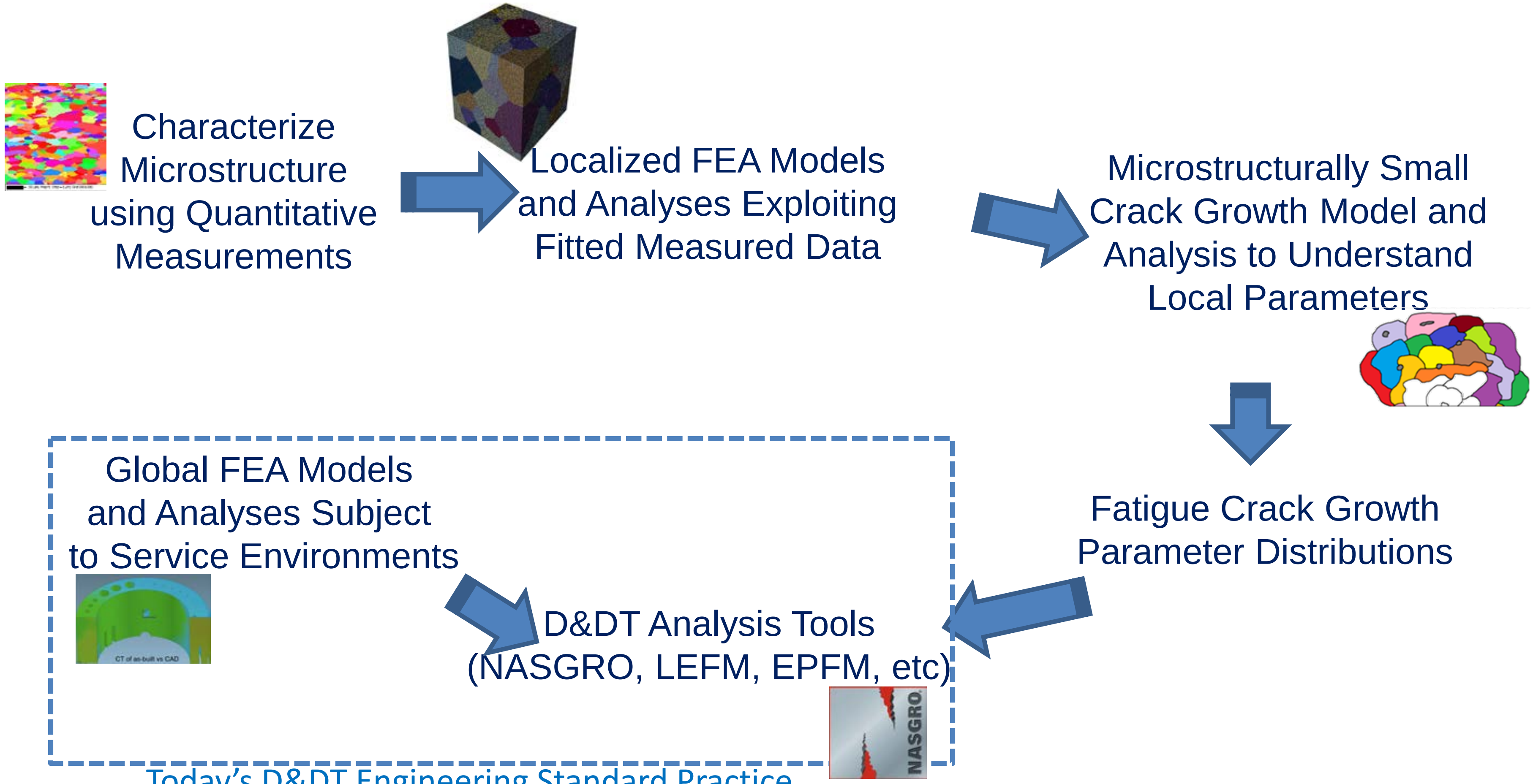


Measure Deformation at Crack Tip



Characterize Damage Evolution

Development of Microstructurally-Informed D&DT -Work Flow



Characterize Microstructure using Quantitative Measurements

Localized FEA Models and Analyses Exploiting Fitted Measured Data

Microstructurally Small Crack Growth Model and Analysis to Understand Local Parameters

Fatigue Crack Growth Parameter Distributions

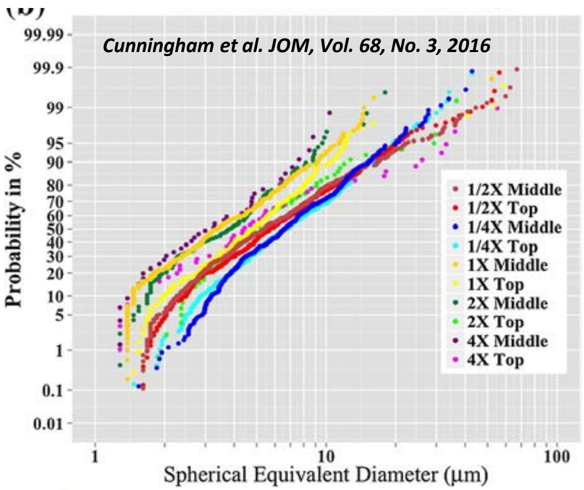
D&DT Analysis Tools (NASGRO, LEFM, EPFM, etc)

Global FEA Models and Analyses Subject to Service Environments

Today's D&DT Engineering Standard Practice

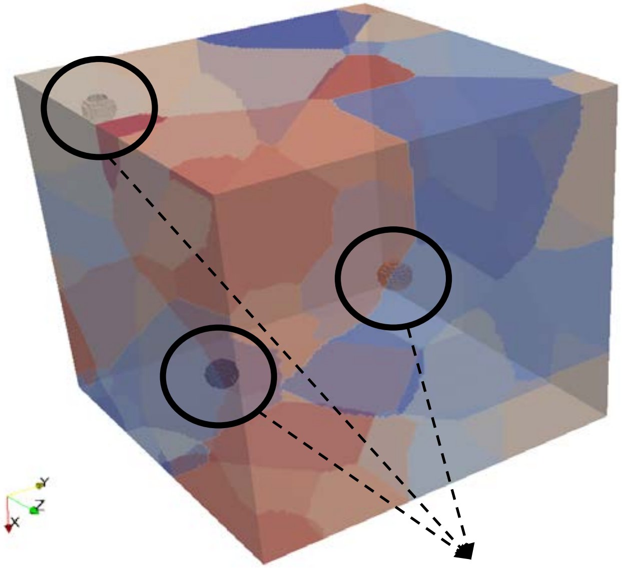
- Today's standard D&DT engineering practice relies on continuum assumptions
- Microstructurally-informed D&DT will consider local length scales, environments and material properties
  - Expanded effort on small-scale testing and physics-based material model calibration
  - Produce distributions of behavior by relying more heavily on modeling and simulation

Assessing Hot Isostatic Pressing (HIP) Treatment for Additively Manufactured Hardware

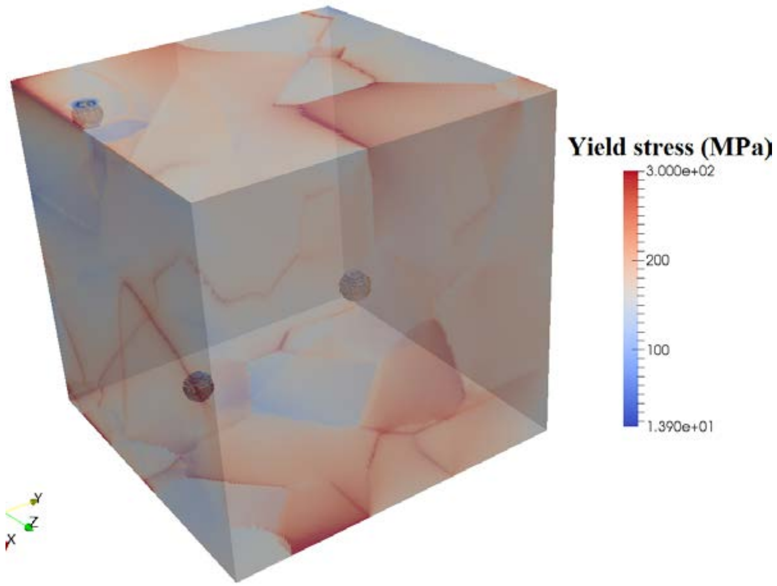

Cunningham et al. JOM, Vol. 68, No. 3, 2016

*Incorporation of Process-Specific Defects in 3D Simulations**

Example case: *Entrapped gas porosity / Key-Hole porosity (SPHERICAL IN NATURE)*



Pores



* Sai Yeratapally, LaRC

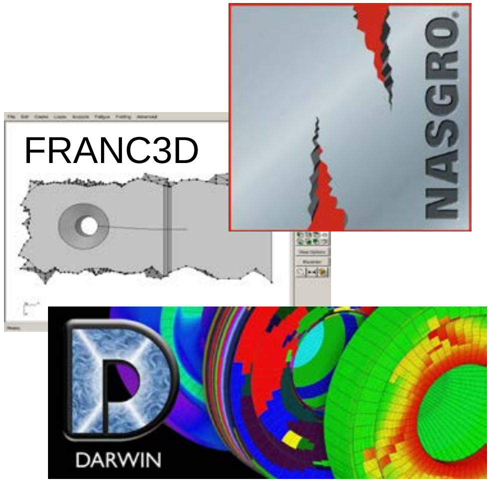
Development of Microstructurally-Informed D&DT - Research Solutions for Engineering Problems

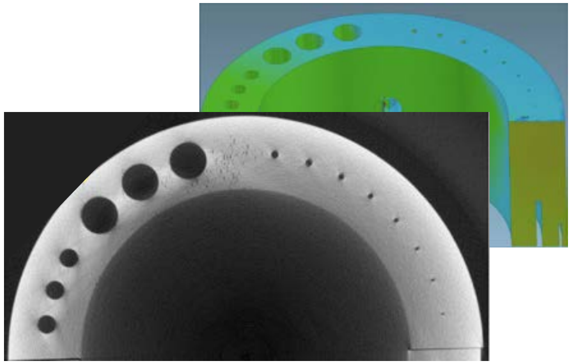
Microstructurally-Informed D&DT of Fracture-Critical Components

Fatigue Crack Growth Material Parameter Distributions

Embed these Relationships within Engineering Codes

Component Level Inputs





*

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

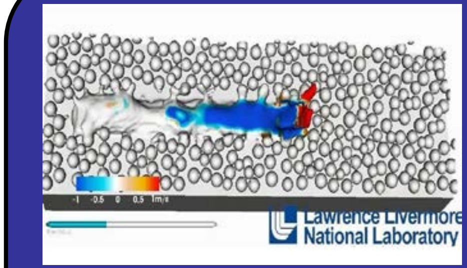
Apply microstructurally-informed D&DT simulation to determine fatigue life of fracture-critical components having small length scale features

- Important because of new processing methodologies, desire to save weight leading to thin structures, etc
- Produce materials whereby small length scale features will increasingly become root cause for failure

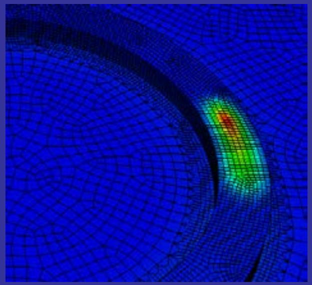
→ New approaches are required to understand and work at these length scales

**Beshears, R., "Computed Tomography Inspection and Analysis for Additive Manufacturing Components," ASNT Annual Conference, November 2, 2017.*

Computational Materials for Material Processing



Simulation of Laser-Powder Bed Interactions



Prediction of Local Heat Distribution

Simulate Fundamental Physics Governing Processing

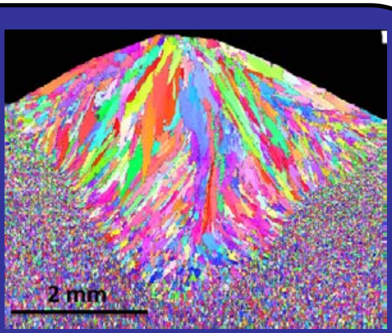
- Determine role of processing parameters on location-specific properties
- Simulate physical processes including laser beam absorption in powder bed, heat transfer via conduction and radiation, and fluid flow at the melt pool, particle flow
- Simulate residual stress, distortion, microstructural evolution and precipitate growth

Develop Physically Correct Models Needed to Support Certification of AM Feed Stock and Manufacturing Process

Characterize Material Evolution using Experimental Methods

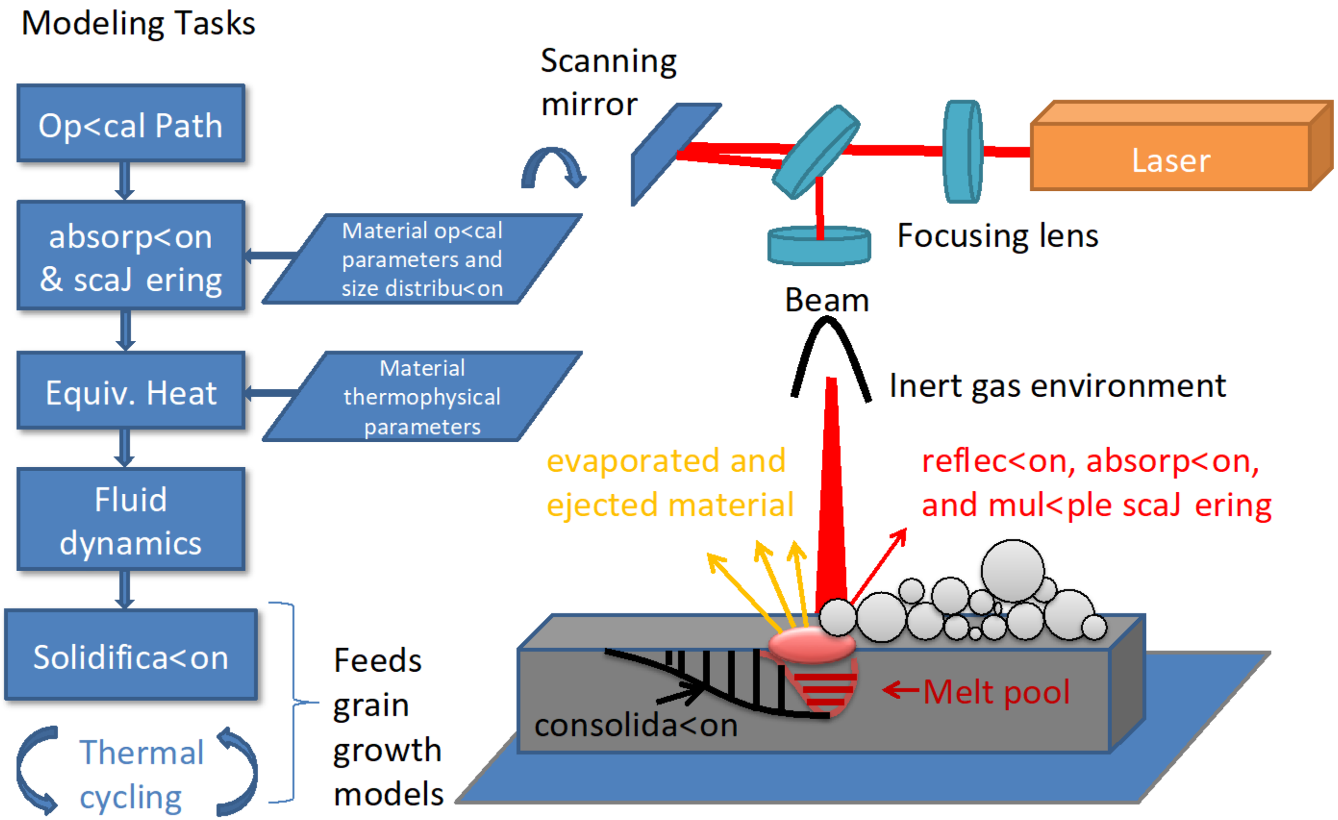
- Employ heavily-instrumented SLM machine and synchrotron beam lines (APS, CHESS)
- Produce coupon-size specimens using well-controlled parameters
- Understand details of the relationship between processing parameters and resulting microstructure

Selective Laser Melting



Grain Structure from Additive Process

Powder Scale to Solidification*



Laser – Laser electromagnetic scattering on spheres is translated into equivalent computationally efficient heat source

Heating – Laser energy is translated into heat on spheres and subsequent conduction

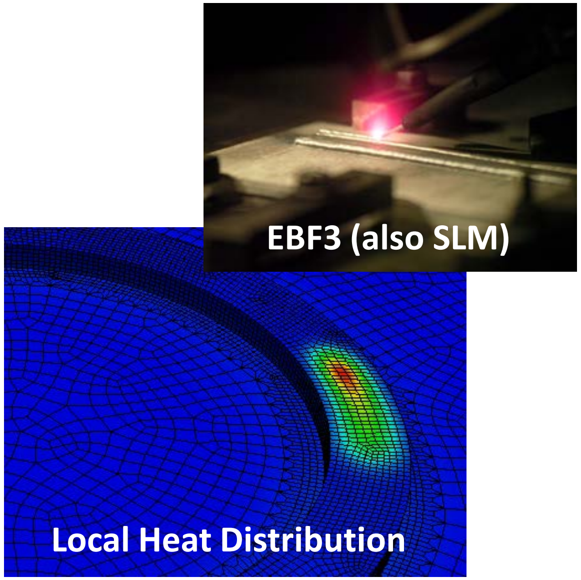
Melt pool

- **Fluid flow –** Metal changes phase from solid to liquid and subsequently flows
- **Evaporation/Recoil pressure –** Significant sparking and metal evaporation occurs which impacts depth of weld penetration and subsequent grain growth structure
- **Grain growth –** Models such as CALPHAD can be coupled with thermal cycling history simulated here

* K. Wheeler, D. Timucin, ARC

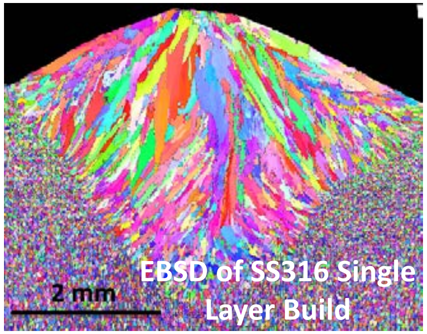
Thermal Modeling*

- Description of the FE Model
  - Transient heat diffusion with phase change
  - Set up model using final part geometry
  - Activate elements for the added powder per layer
  - Heat input model defines the distribution of volumetric heat source (units are J/m^3-sec)
- Details
  - Currently only heat diffusion is modeled in order to predict the thermal history for the entire part (thermal cycling will occur in the layers)
  - Convection and radiation boundary conditions included
  - All of the “action” takes place in the melt pool, requiring a very fine mesh to capture the steep gradients. This leads to high computational costs when modeling numerous layers.
  - Convection within the melt pool is captured by artificially increasing the conductivity of the melted material (factor of 2 [Yaghi 2012])
  - The effect of different heat input models is insignificant away from the melt pool zone



EBF3 (also SLM)

Local Heat Distribution



EBSD of SS316 Single Layer Build

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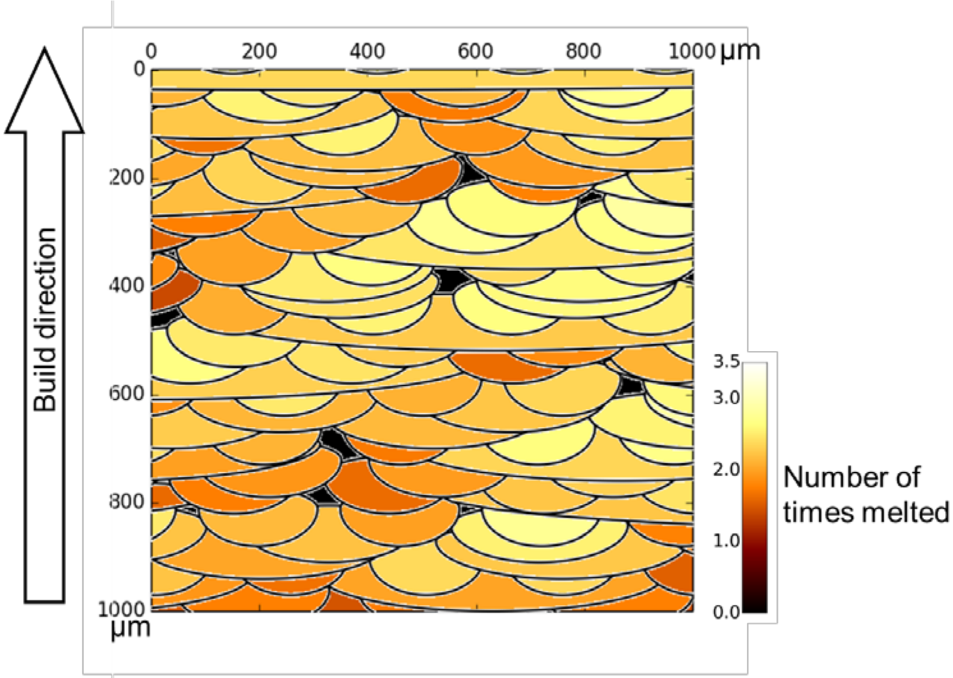
* Chris Lang, LaRC

Modeling of Microstructure Formation in AM IN718 with Emphasis on Porosity Prediction*



Research Objectives and Impact

- Development of a validated model for 3D printing of In 718 parts
    - Incomplete melting
    - Porosity
    - Microstructure
- Increase confidence in manufacturability via powder bed AM
- Enabling for production of specialized, low production volume parts

Three major components to the approach

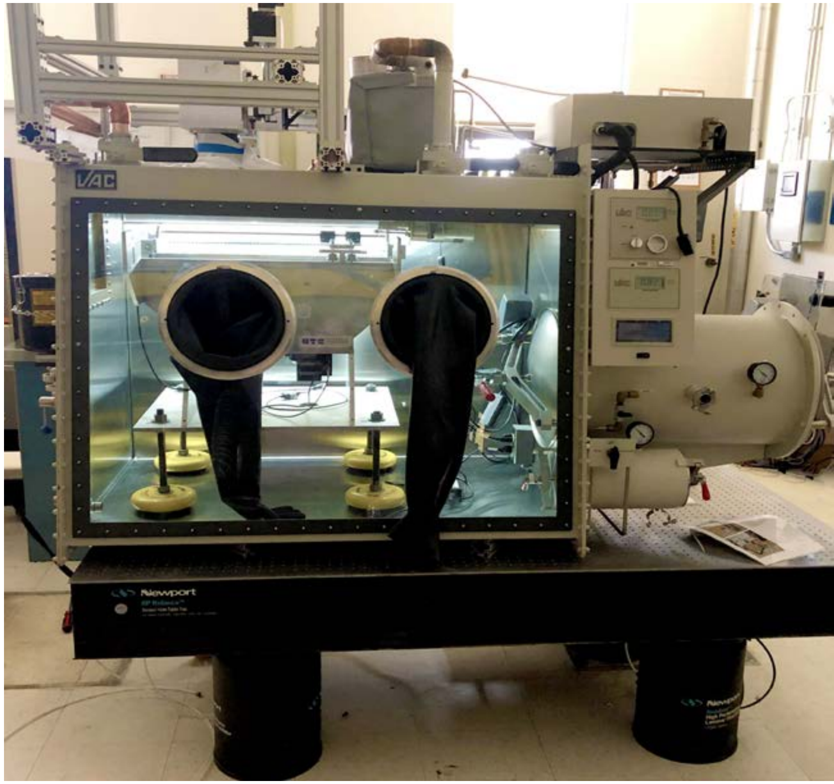
- An incomplete melting model based on scan geometry, deposited layer thickness and melt pool dimensions
- A gas bubble in melts model that is based on a hybrid of the Potts model with the cellular automaton method
- A model for hardness that is based on combining a computational thermodynamics package, such as Thermo-Calc, with kinetics, e.g., from available TTT, with thermal histories, measured or computed

*with A. Rollett and C. Pistorius, CMU (1 of 6 ESI on simulation of AM processing)

Configurable Architecture Additive Testbed*

Description

Support development of *validated* capabilities for optimization, certification and sustainment of new designs that are enabled by laser-powderbed AM.



Approach

- Use CAAT as a development platform:
  - Experiments to calibrate, validate and increase confidence in models
  - In-situ data: Video and Thermal cameras (include laser inline), plume emissivity, in-situ accelerometers, in-situ thermocouples, ppm humidity, ppm O_2 monitoring
  - Post-build: material & defect characterization
  - Pursue statistically significant relationships between in-situ monitoring and defects
  - "Tune / Calibrate" the instrument hardware for precise experimentation

*Samuel Hocker, LaRC

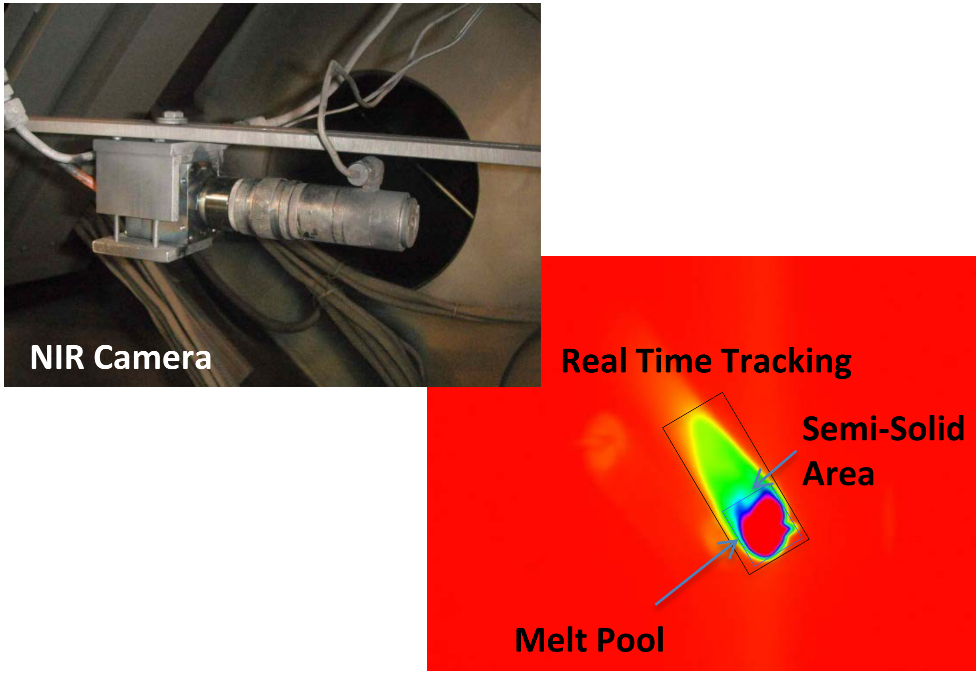
In-Situ Monitoring of Additive Manufacturing*

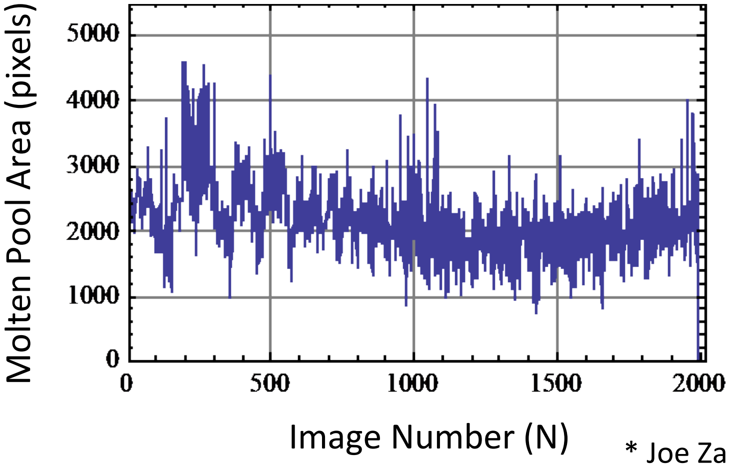
Approach

- Employ heavily-instrumented AM machine
- Spatial and radiometric calibrated infrared thermography
- Remotely acquire temperature images and apply advanced image processing techniques to determine deposition parameters such as molten pool size and semi-solid area in real time using tracking algorithm.

Results

- Imaged and measured deposition parameters such as melt pool area and semi-solid regions.
- Tracked melt pool and semi-solid area independent of orientation.
- Provided much greater resolution than previous measurements of melt pool system (1,000’s pixels vs. 9 pixels).





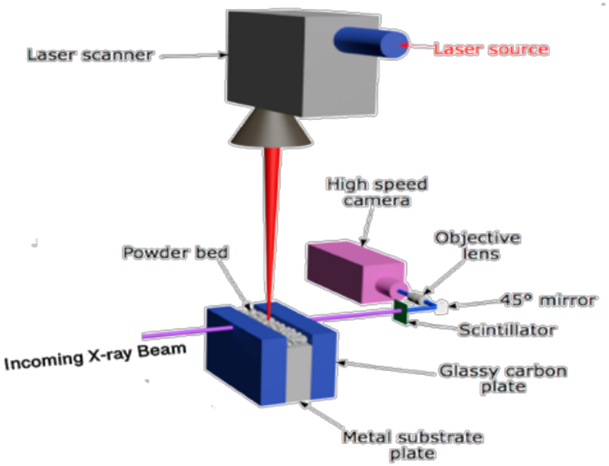
* Joe Zalameda, LaRC

In-Situ SLM Process Characterization

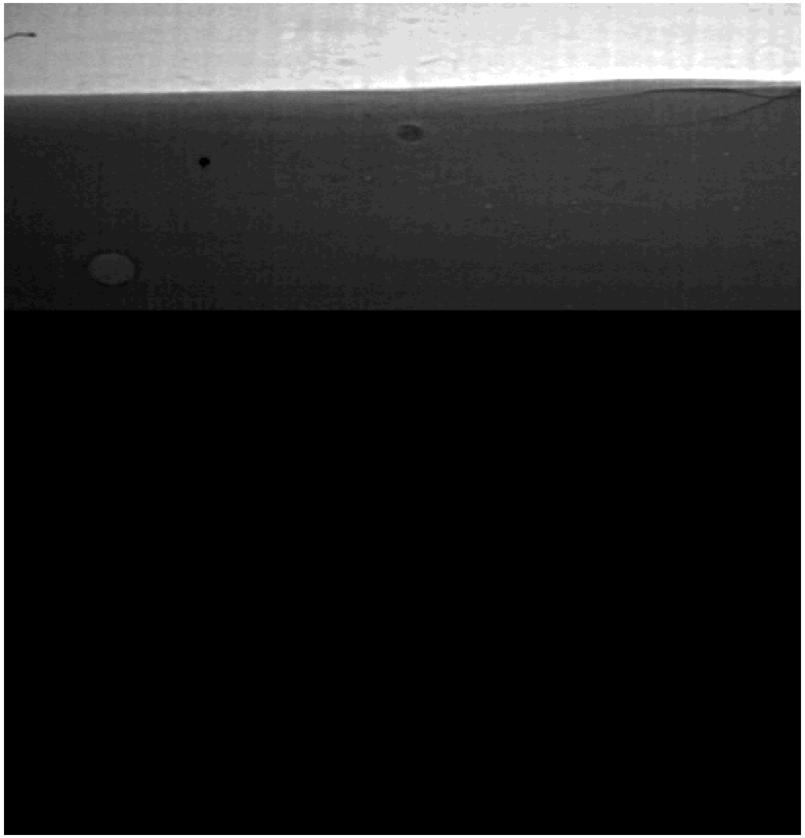
Advanced Photon Source (APS) at Argonne National Laboratory

Image credit: Argonne National Lab

Collaboration with APS and Carnegie Mellon University



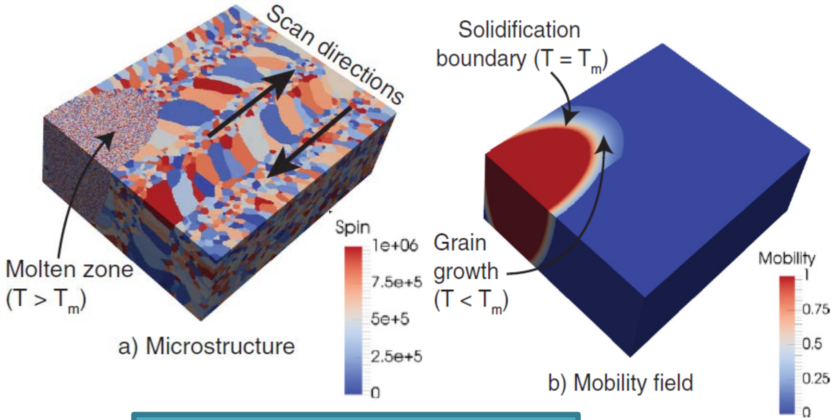
Parab, et al. J Synchrotron Radiation, 2018.

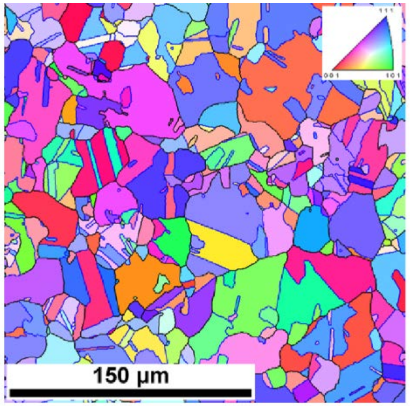


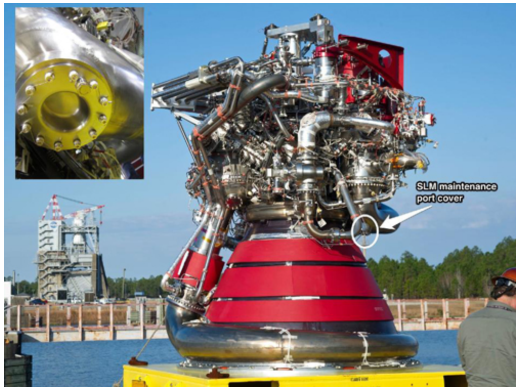
Combined DXR and Near-IR Movie

Image credit: Tao Sun (APS)

Process-Structure-Property Linkage







Process Simulation*

Microstructure

Property/Performance

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*T.M. Rodgers et al. / Computational Materials Science 135 (2017) 78–89

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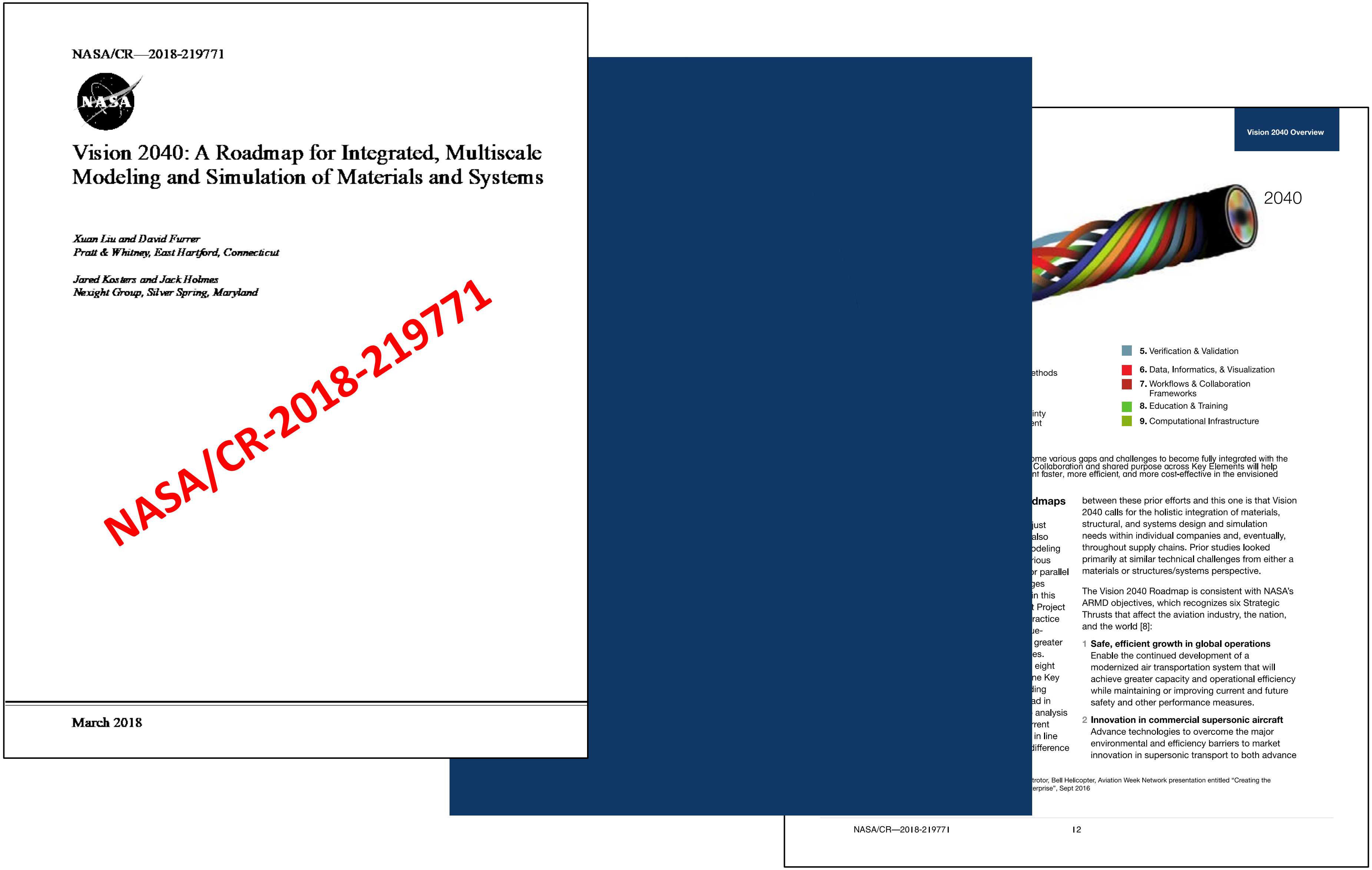
Vision 2040 for Integrated, Multiscale Materials and Structures Modeling / Simulation



NASA/CR—2018-219771

Vision 2040: A Roadmap for Integrated, Multiscale Modeling and Simulation of Materials and Systems

Xuan Liu and David Furrer
Pratt & Whitney, East Hartford, Connecticut

Jared Kosters and Jack Holmes
Nexight Group, Silver Spring, Maryland

NASA/CR-2018-219771

March 2018

Vision 2040 Overview

ethods

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ent

- 🟦 **5.** Verification & Validation
- 🟥 **6.** Data, Informatics, & Visualization
- 🟥 **7.** Workflows & Collaboration Frameworks
- 🟩 **8.** Education & Training
- 🟩 **9.** Computational Infrastructure

ome various gaps and challenges to become fully integrated with the Collaboration and shared purpose across Key Elements will help nt faster, more efficient, and more cost-effective in the envisioned

dmaps

just also odeling rious or parallel ges in this t Project ractice ue- greater es. eight ne Key ding ad in analysis rrent in line difference

between these prior efforts and this one is that Vision 2040 calls for the holistic integration of materials, structural, and systems design and simulation needs within individual companies and, eventually, throughout supply chains. Prior studies looked primarily at similar technical challenges from either a materials or structures/systems perspective.

The Vision 2040 Roadmap is consistent with NASA's ARMD objectives, which recognizes six Strategic Thrusts that affect the aviation industry, the nation, and the world [8]:

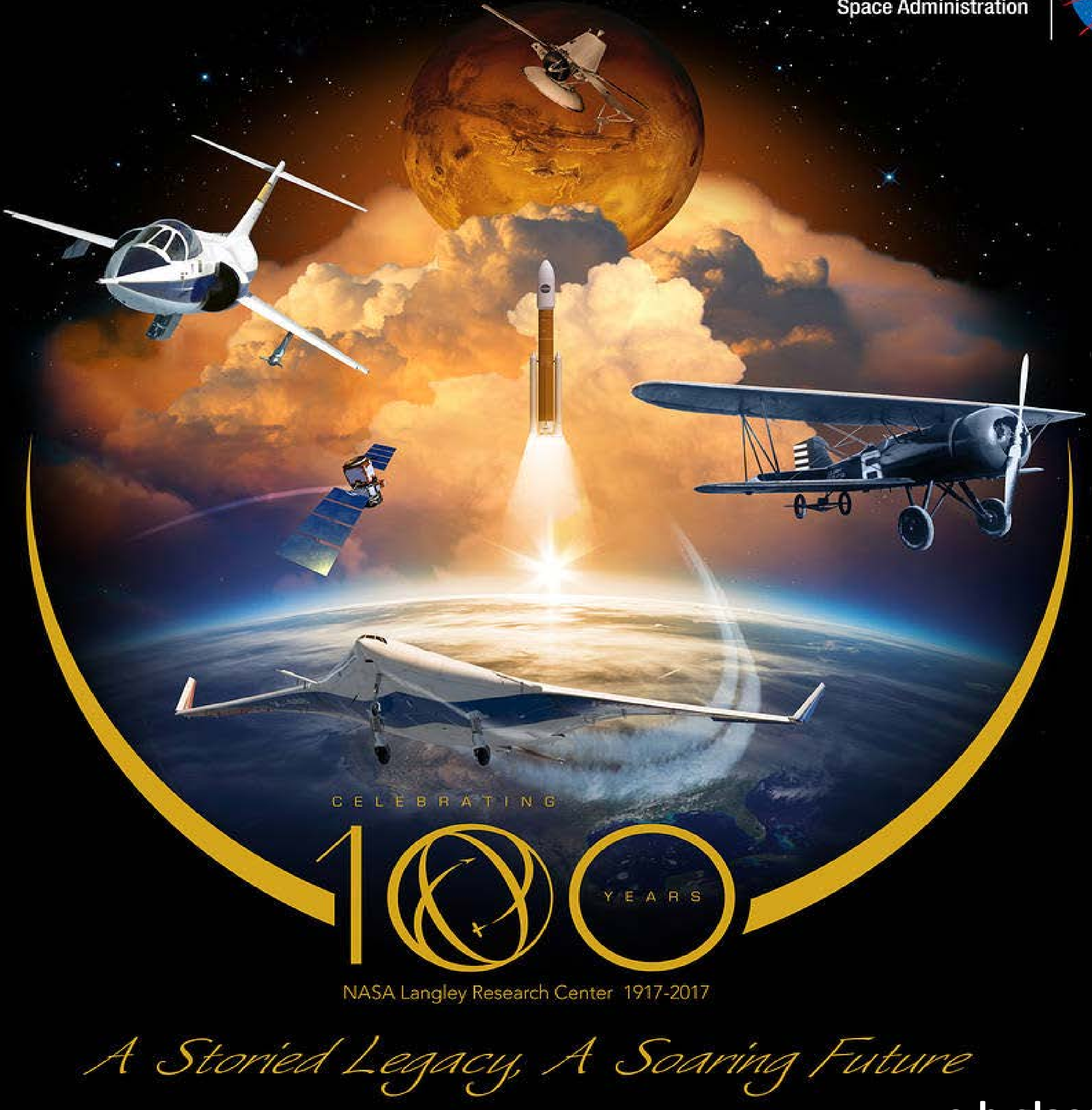
1 **Safe, efficient growth in global operations**
Enable the continued development of a modernized air transportation system that will achieve greater capacity and operational efficiency while maintaining or improving current and future safety and other performance measures.

2 **Innovation in commercial supersonic aircraft**
Advance technologies to overcome the major environmental and efficiency barriers to market innovation in supersonic transport to both advance

trotor, Bell Helicopter, Aviation Week Network presentation entitled "Creating the erprise", Sept 2016

NASA/CR—2018-219771 12

National Aeronautics and
Space Administration



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