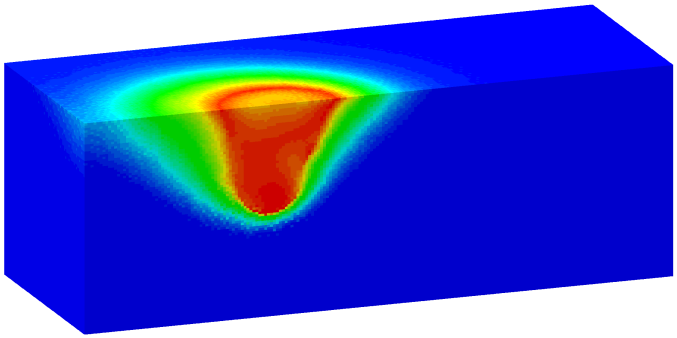
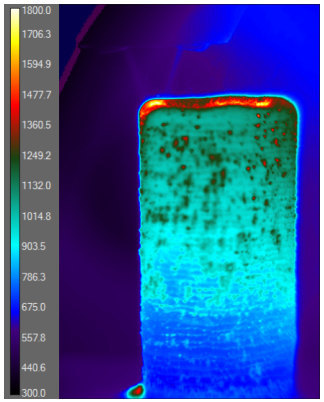
SAND2017-8925PE

Exceptional service in the national interest

Sandia National Laboratories





Grand Challenge LDRD "Born Qualified": Integrate Data, Modeling, Optimization, and UQ for Additive Manufacturing

Bart van Bloemen Waanders, Timothy Wildey, and Daniel T. Seidl.

(Optimization and Uncertainty Quantification1441)

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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-NA-0003525 SAND2017-6418 C

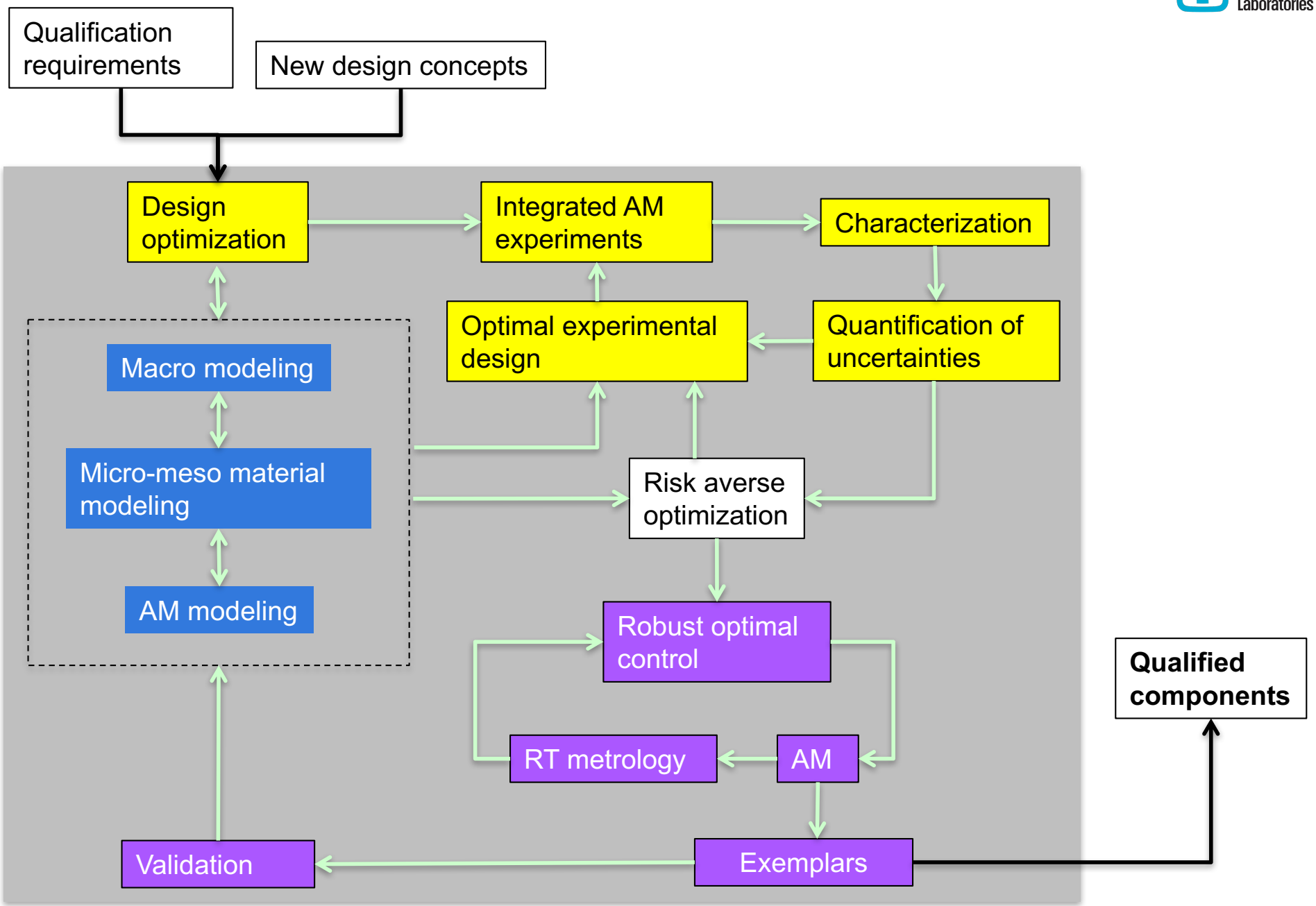
Sandia Commits Significant Resources to Transform the NW Enterprise

- **Vision**: combines promise of additive manufacturing with deep materials & process understanding to revolutionize design, manufacturing, & qualification paradigms for the NW enterprise
- **Team**: 11 centers, 20 departments, 40 researchers, $4.5 M/year, 3 years
- **Challenges**: overcome uncertainties and variabilities, create large scale optimization for multi-scale/physics simulation, integrate with experiments
- **Why Sandia**: combination of unique qualification of NW components, computational science, experiments, and product targets
- **CIS contributions**: development of large scale multi scale/physics optimization under uncertainty, data science, and uncertainty quantification

References:

- T. Wildey, B. van Bloemen Waanders, and D. Seidl "Generalized Multiscale Mortar Methods for Multiphysics Applications", CMAME, 2017, (submitted).
- D. Seidl, B. van Bloemen Waanders, T. Wildey "Simultaneous Elastic Inversion of Shear Modulus and Traction Boundary Conditions", Inverse Problems in Science and Engineering, 2017, (submitted).

Research and Development Strategy Provides Roadmap with Optimization in a Central Role



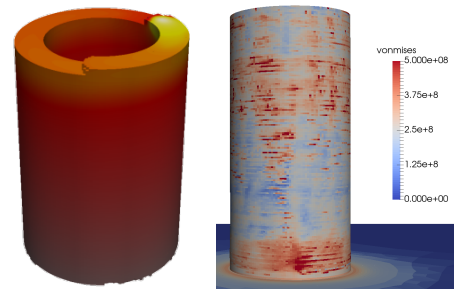
CIS Contributes Critical Computational Tools

- Mapping of multi scale/physics forward modeling from Sierra to Trilinos
- Leveraging Mortar methods achieves adaptivity, multiphysics, and multiscale
- Automation of adjoints and optimization interfaces provides large scale multi-scale/physics capabilities
- Demonstration of multiscale inversion and risk-averse control

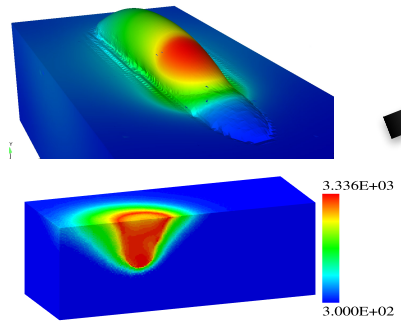
Large Spatial Resolution Motivates Multi-scale/physics Simulation with Optimization under Uncertainty Capabilities.

Challenges:
multiscale
multiphysics
large optimization space
manage uncertainties

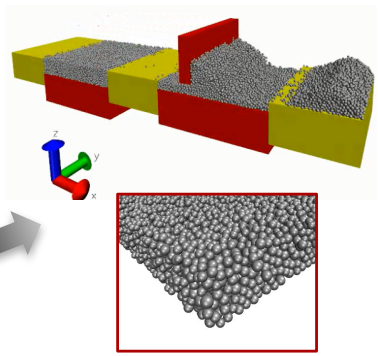
Part Scale Thermal & Solid Mechanics



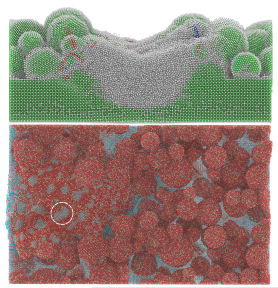
Mesoscale Thermal Behavior



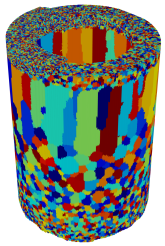
Powder Spreading



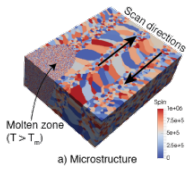
Powder Behavior



Part Scale Microstructure



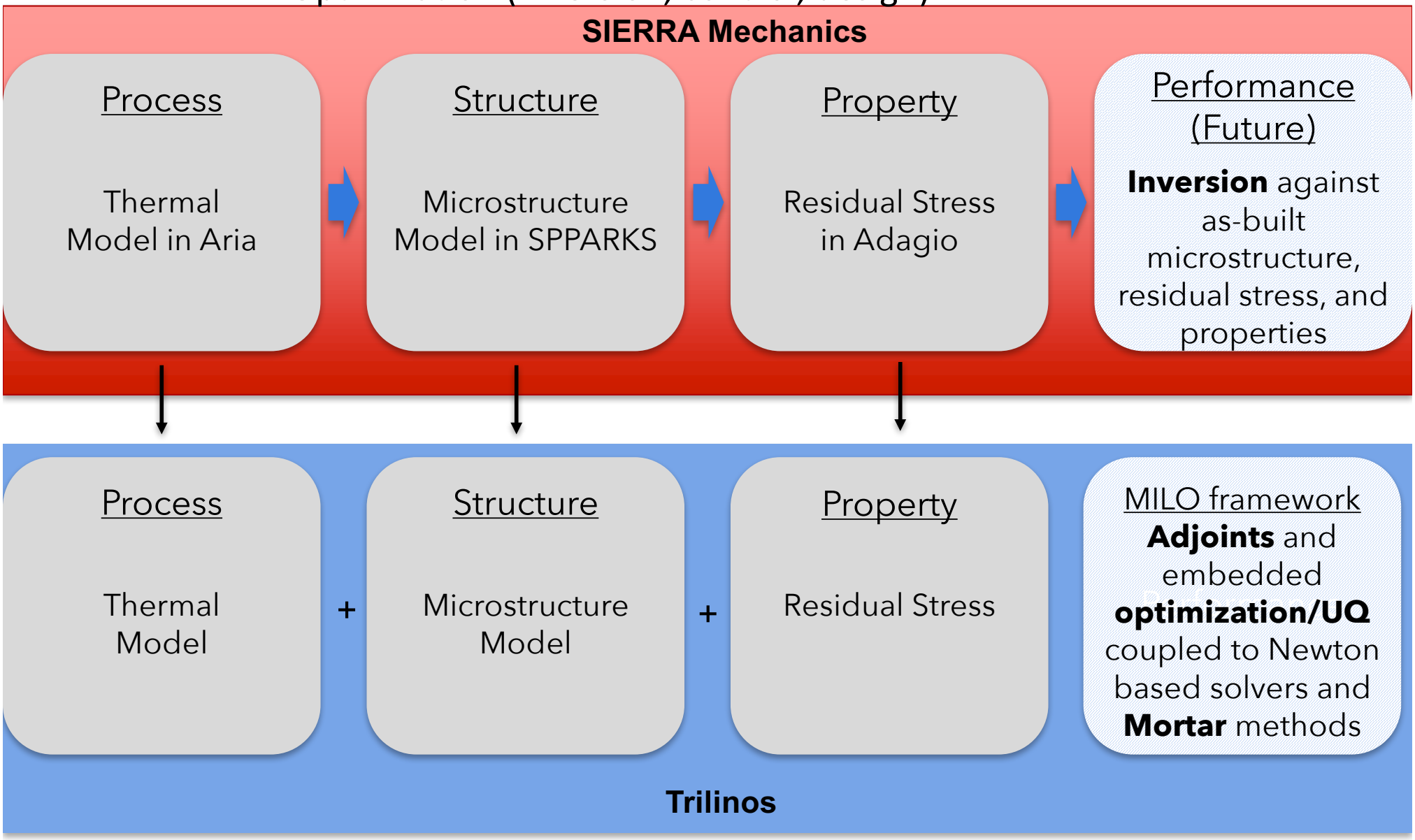
Mesoscale Texture/Solid Mechanics/CX



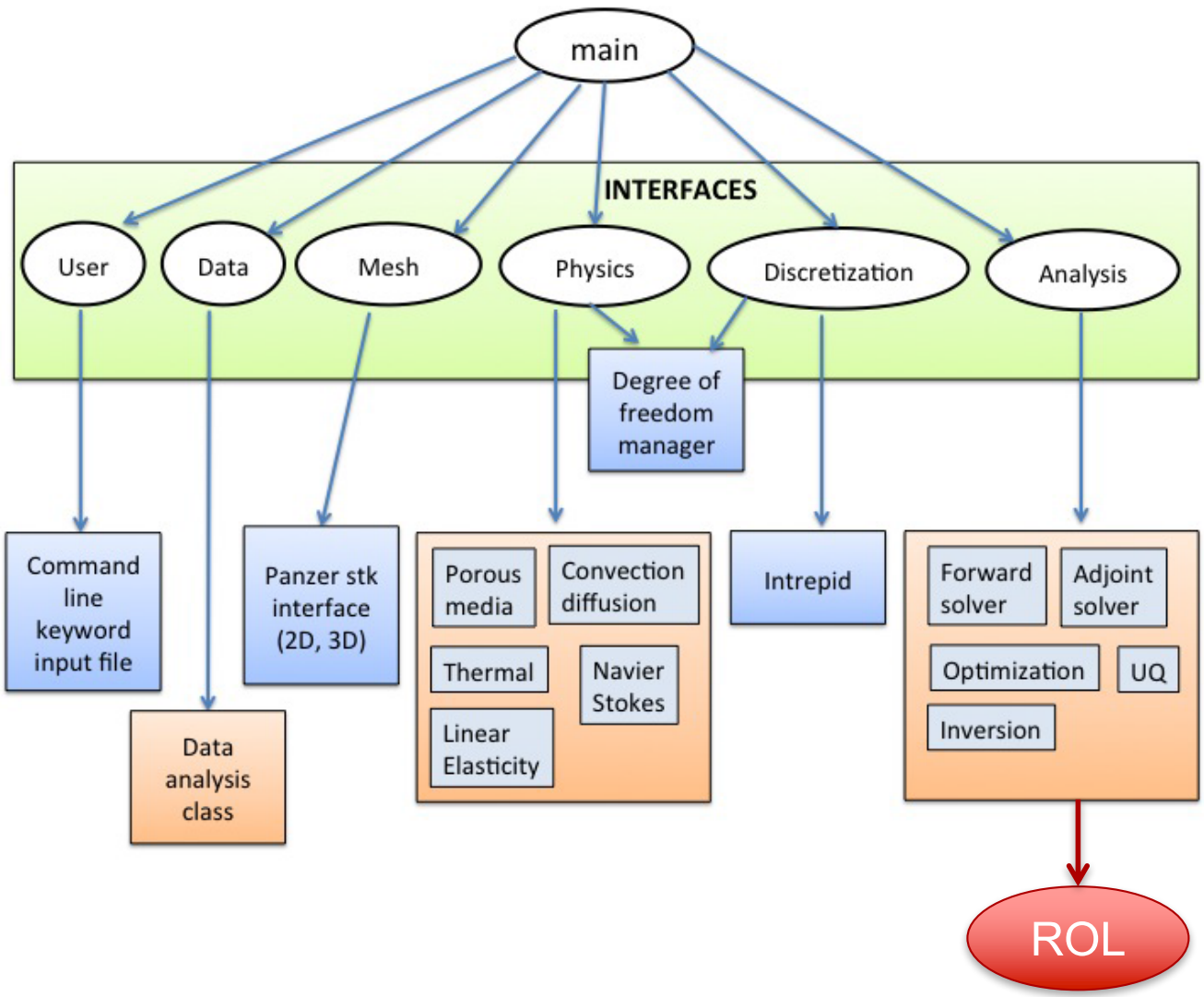
10^{-6} 10^{-3} 1

Length Scale (m)

Sierra Forward Modeling is Mapped to Trilinos Framework to Enable Optimization (inversion, control, design)



Multi scale/physics Interface for Large scale Optimization (MILO)



strong form:

$$\frac{\partial T}{\partial t} - D\frac{\partial T}{\partial dx} = f$$

weak form:

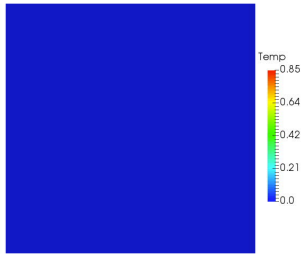
$$\int_\Omega \rho c_p \frac{\partial T}{\partial t} v + D\frac{\partial T}{\partial x}\frac{\partial v}{\partial x} - f \cdot v d\Omega = 0$$

code:

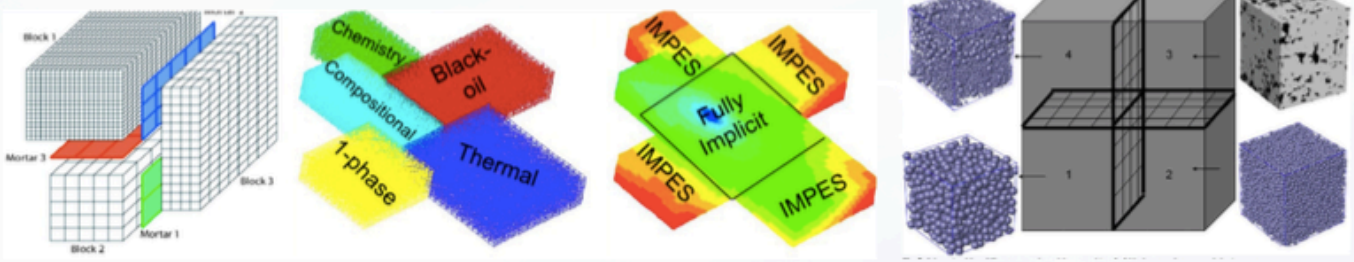
```
Res=rho(k)*cp(k)*udot*v+diff(k)*dTdx*dvdx –f*v
```

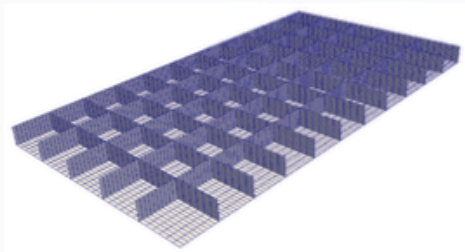
Automates:

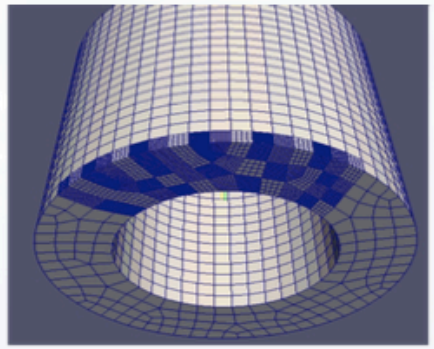
- 3D Parallel
- Adjoints
- Opt under uncertainty
- Unstructured
- Multiscale
- Multiphysics



Novel Development of Multiscale Capability using Mortar Methods at Element Level







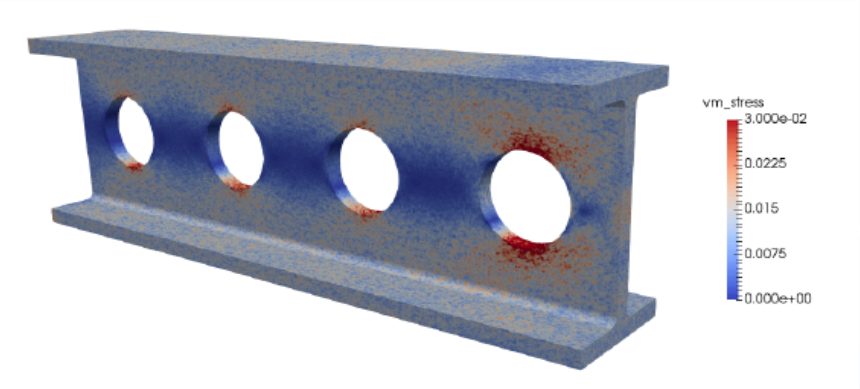
$\mathcal{O}(1)$ $\mathcal{O}(10)$ $\mathcal{O}(100)$ $\cdots$ $\mathcal{O}(10^7)$ $\mathcal{O}(10^8)$ $\mathcal{O}(10^9)$

Number of Subdomains

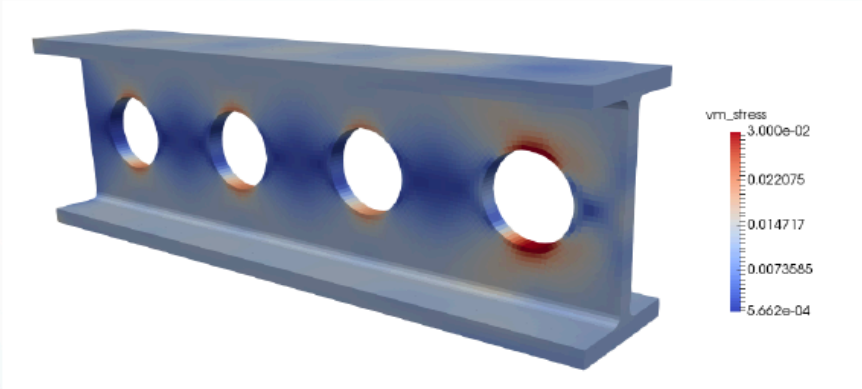
Domain Decomposition

Current Work

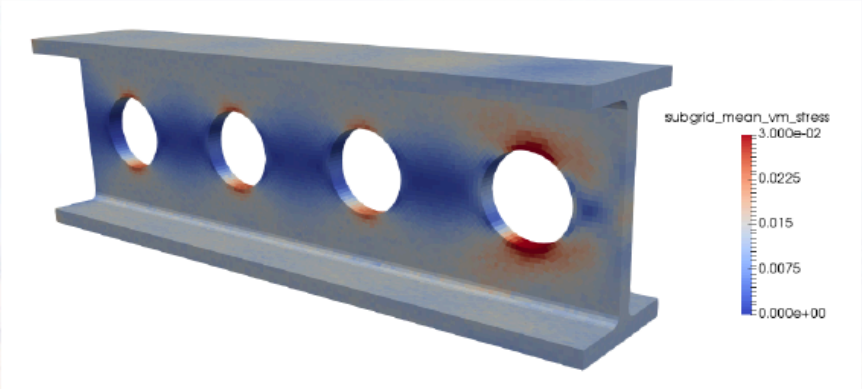
Mortar Approach Achieves Fine-scale Crystal Elasticity at Reduced Computational Cost (and produces an adjoint) for Large Scale Optimization



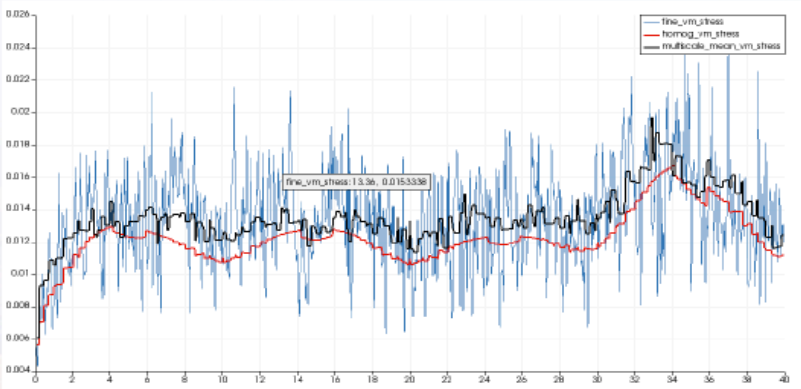
Fine scale



Homogenization

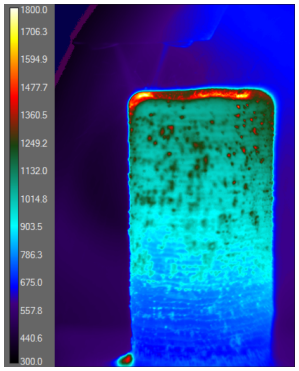


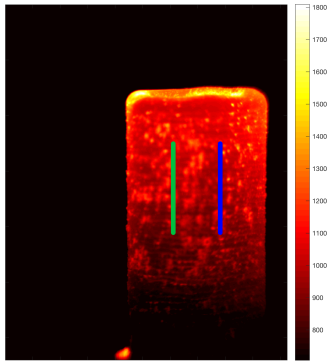
Multiscale

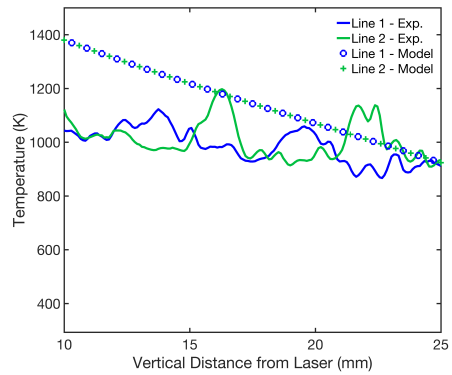


Comparison along line through middle below holes.

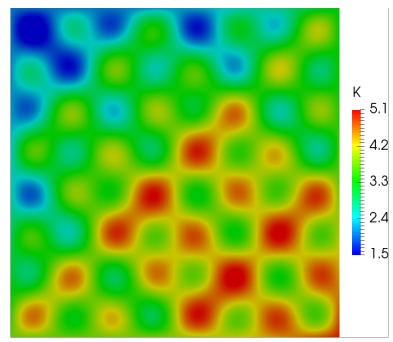
Spatial Variation of IR Thermal Measurements Motivate Multiscale Inversion

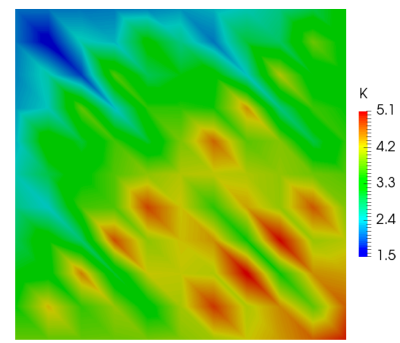


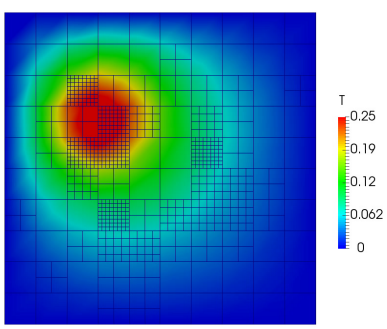


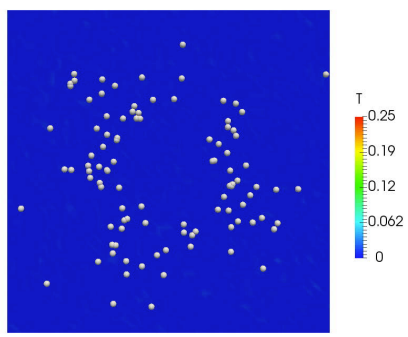


$$K(x,y) = 2 + z_1 \sin(\pi x)\sin(\pi y) + z_2 x^3 + z_3(1-y)^2 + z_4 \sin(5\pi x)\sin(5\pi y) + z_5 \sin(10\pi x)\sin(10\pi y)$$









Parameter	Exact	Single-scale	Multiscale
z_1	1.5	0.91	1.36
z_2	1.25	1.11	1.25
z_3	1.75	1.19	1.73
z_4	0.5	0.58	0.55
z_5	0.75	2.53	0.69

Risk-averse Prototype Demonstrates Complicated Algorithms and Software Capabilities

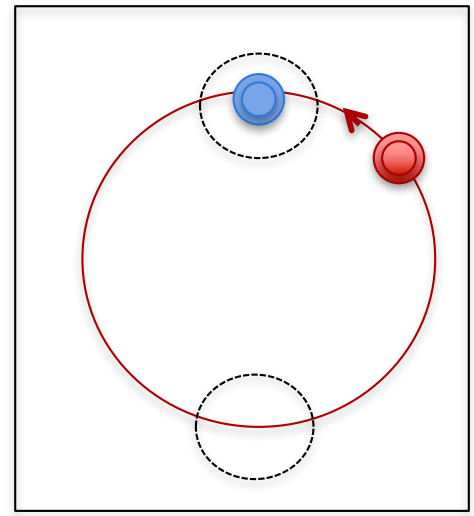
$$\min_{z} \quad \mathcal{J} = \sigma\left[\frac{1}{2}\int_0^T \int_\Omega (u(\xi)-\bar{u})^2 \, dx \, dt\right] + \frac{\beta}{2}\int_0^T \int_\Omega z^2 dx \, dt$$

where u solves:

$$\frac{\partial u}{\partial t} - D\Delta u + = \bar{f}(z,\xi)^* \quad \in \Omega \times (0,T)$$

$$u = \tilde{u} \quad \text{on} \quad \Gamma \times (0,T)$$

$$u = u_0 \quad \in \Omega, \; T = 0$$



CVaR	Obj fcn	control	VAR	time	iter
0.5	1.093E-1	47.23	0.10593	1241	73
0.7	1.108E-1	47.798	0.1079	1278	73
0.9	1.136E-1	48.738	0.1116	1820	105
0.95	1.155E-1	49.333	0.113	4531	133

At the Two Year Mark, BQ Has Developed Foundational Tools and is Set to Deliver Qualified Exemplars in the Third and Final Year

- **BQ** combines promise of additive manufacturing with deep materials & process understanding to revolutionize design, manufacturing, & qualification paradigms for the NW enterprise BQ LDRD research and development to support the transformation of NW program.
- **CIS contributions** consists of development of large scale multi scale/physics optimization under uncertainty, data science, and uncertainty quantification.

Future work - third year goals:

***Integration** of computational sciences and experimentation to achieve qualified exemplars.*

Thank you!