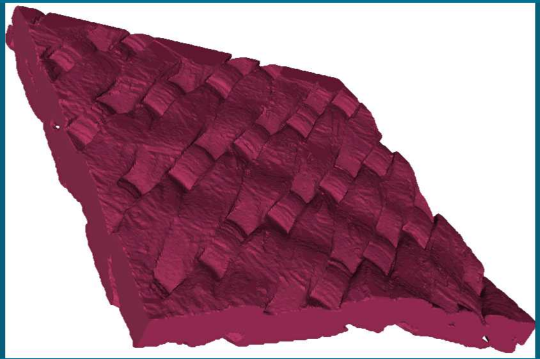
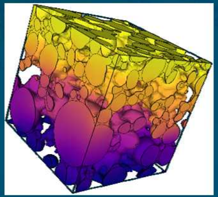
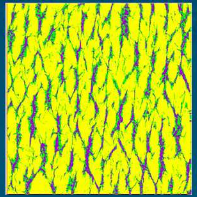
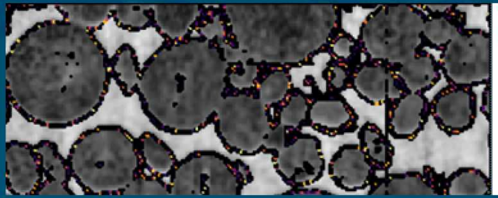
SAND2019-14183PE

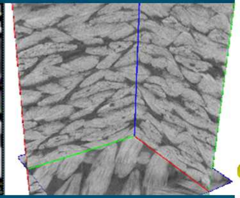
CAMI LDRD: Overview and Highlights

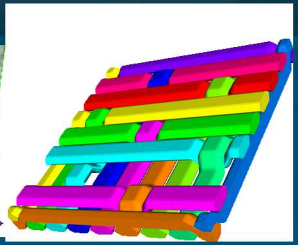










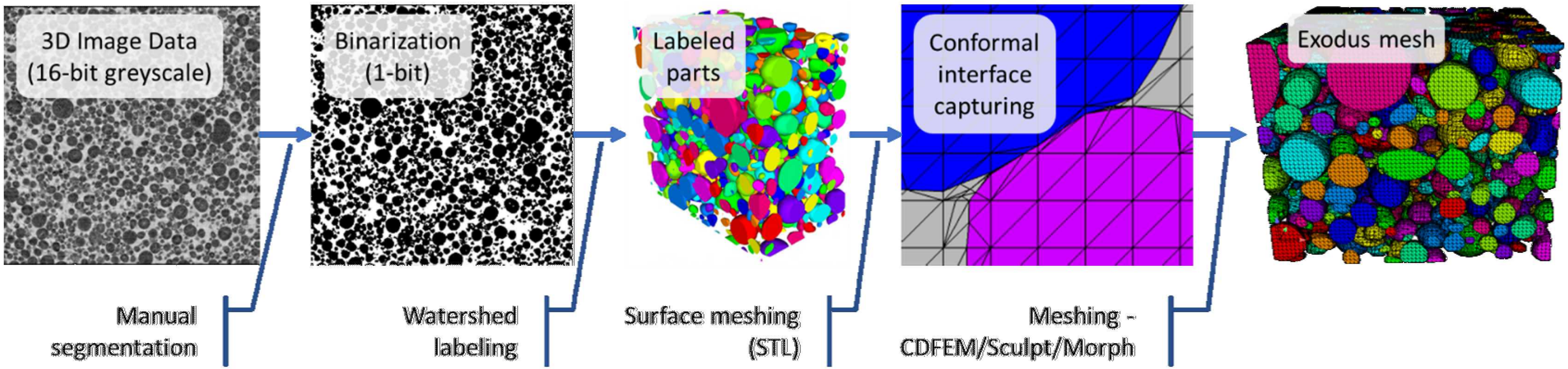


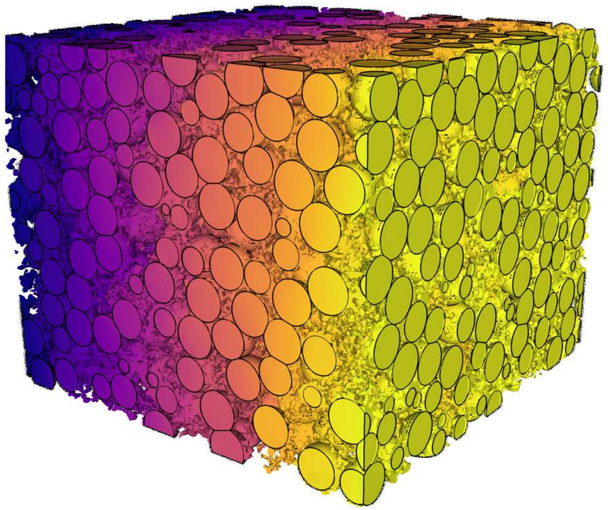
PRESENTED BY

Scott A. Roberts, Ph.D.

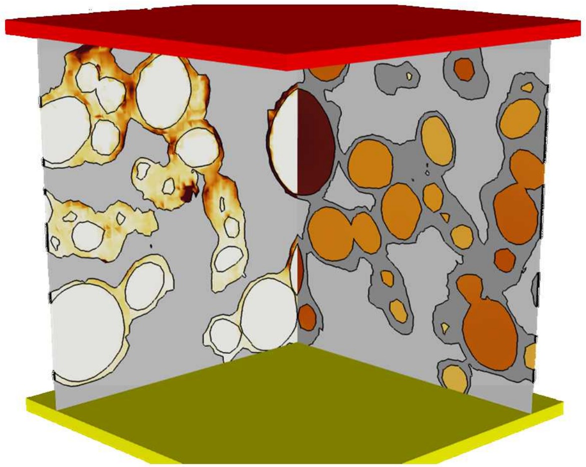
November 15, 2019

Prior art: Image-to-mesh for lithium-ion battery mesostructures

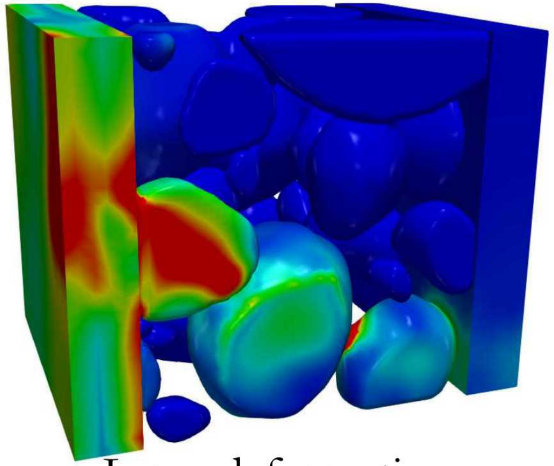




Effective electrode properties



Coupled electrochemical-mechanical performance

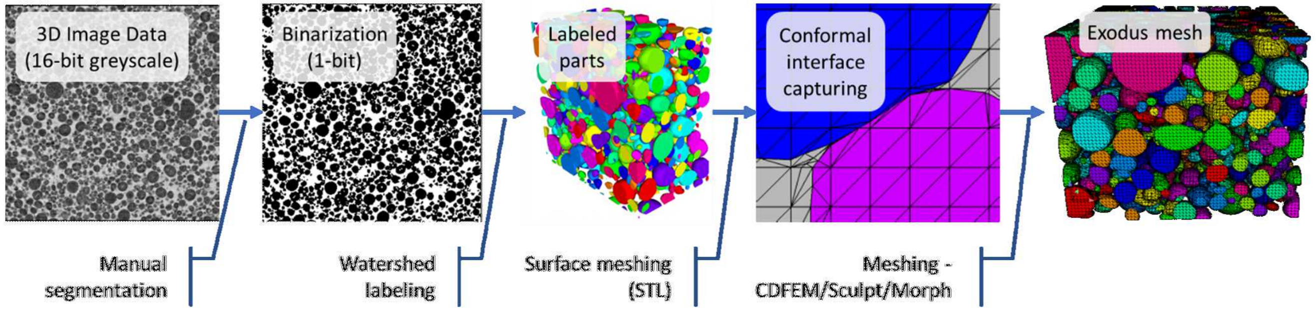


Large deformation mechanics

Pioneered large-scale image-to-mesh capabilities for lithium-ion battery mesostructures; 7 journal articles

Credible Automated Meshing of Images (CAMI) LDRD concept

Recent state-of-the-art processes are:
- Manual, SME-dependent
- Time-consuming
- Unknown credibility
- Don't capture all geometric features



Objective: We seek to develop a methodology for **automatically**, **efficiently**, and **reproducibly** creating **conformal** finite element meshes from **3D tomography** with **quantified uncertainty**.

Research thrusts – primary science questions:
- Deep machine learning algorithms (ML)
- Automatic conformal tetrahedral mesh creation (ATM)
- Uncertainty quantification and propagation (UQ)
- Application exemplar: Thermal protection system materials (TPS)
- Purdue AA: Battery mesostructures

Uncertainty quantification and propagation

Deep learning algorithms
- Image segmentation
- Part identification

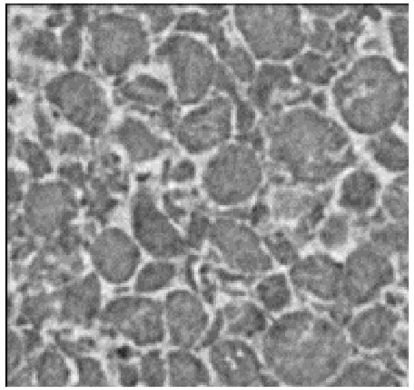
Automatic tetrahedral meshing
- Conformal interfaces
- Feature-governed mesh resolution

Physics solve
- Finite element method predictions
- Exemplar: TPS material mesostructures

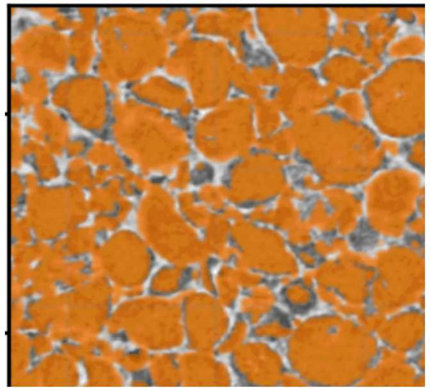
Automated, credible image-to-mesh capabilities would revolutionize engineering analysis workflows!

Deep learning produces accurate segmentations with per-voxel UQ

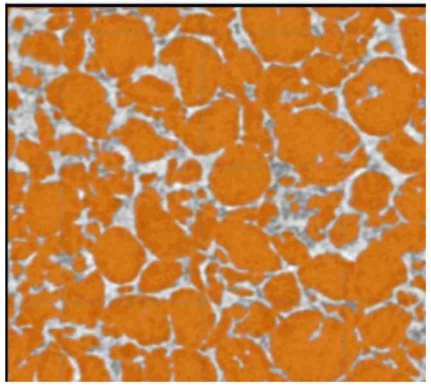
Slice from CT image of graphite electrode



Human label (orange) overlaid on CT scan of battery

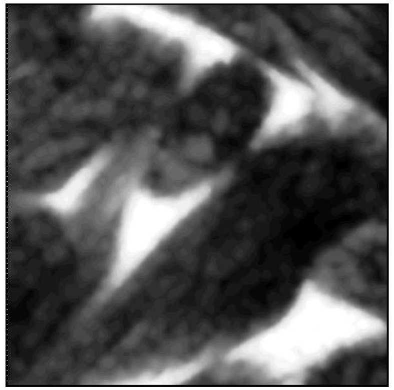


Deep learning label (orange) overlaid on CT scan of battery

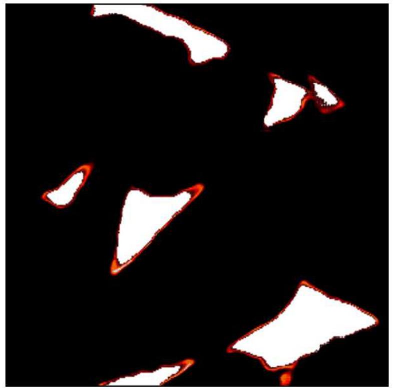


LIB: Incrementally trained DL model segments to high accuracy, higher than human labels in some cases

Slice from CT scan of TPS



Deep learning segmentation with uncertainty map

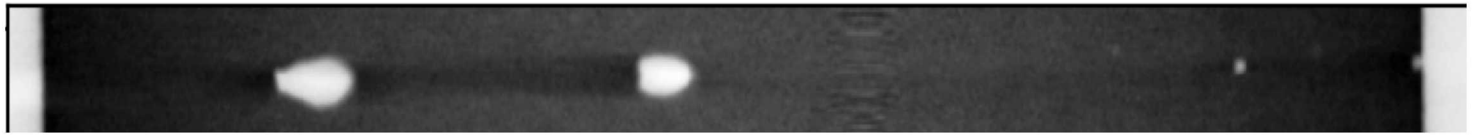


TPS: Accurate segmentations on held-out sub-volumes, with per-voxel UQ

Laser welds: 99.2% accuracy to manual labels with uncertainty maps on ambiguous features. Beginning to propagate into simulations using Sculpt

DL inferences takes minutes on GPU vs. hours to days manually!

CT scan of laser welded material



Accurate deep learning segmentation

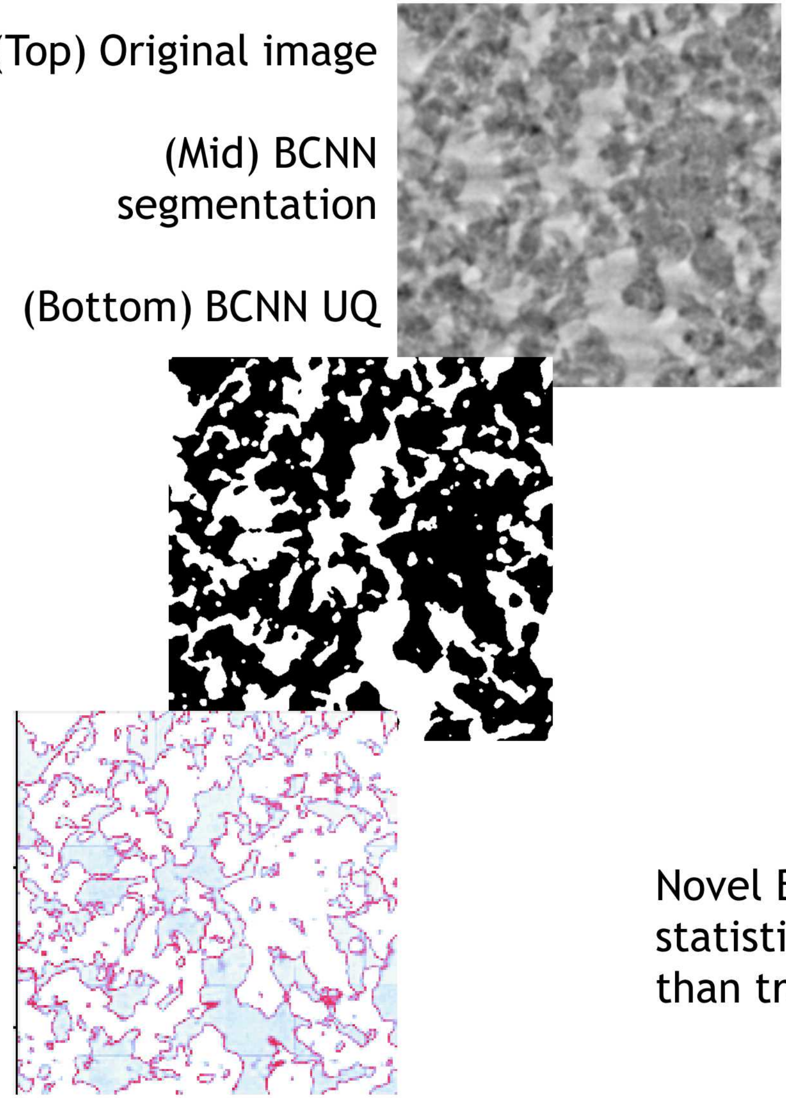
We have proven DL models capable of flexible and accurate image segmentation with rigorous per-voxel UQ estimates

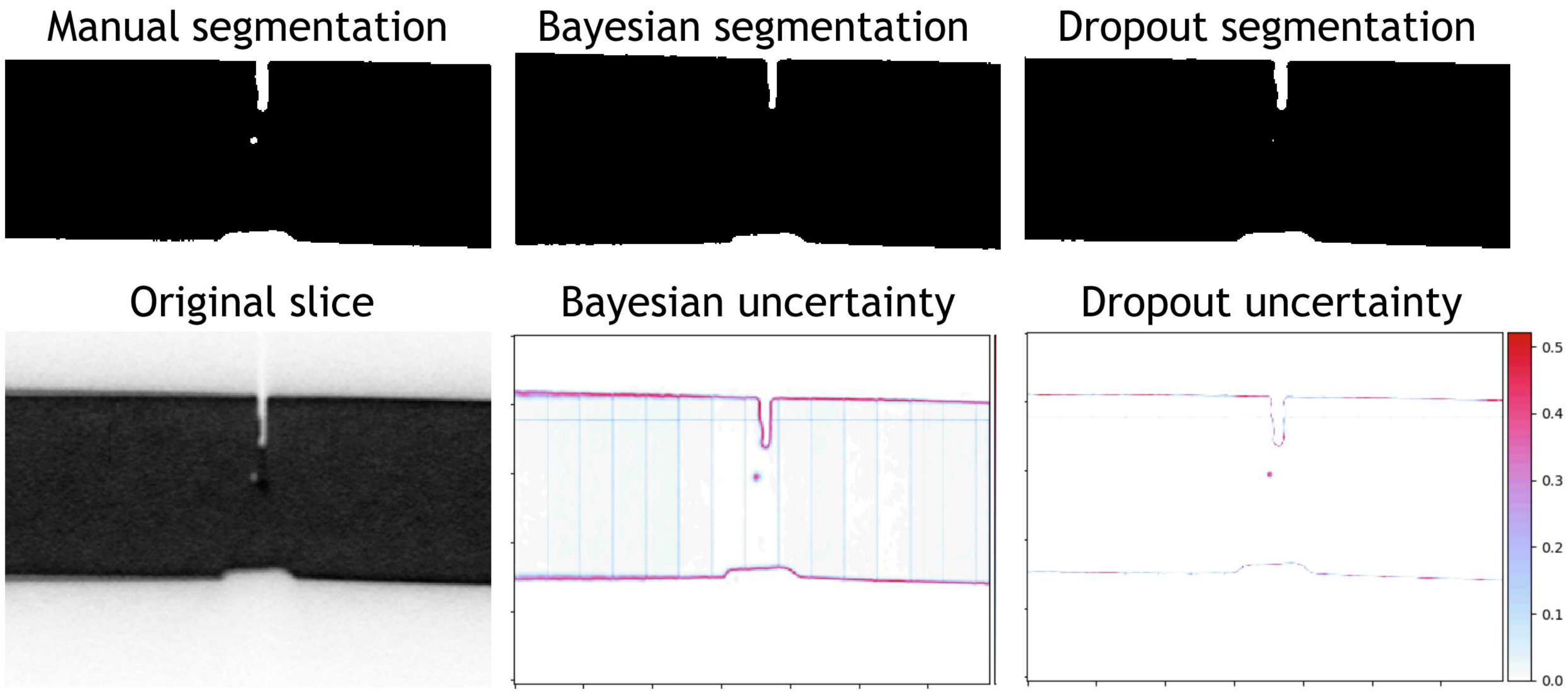
Interpretable uncertainty using Bayesian CNNs

(Top) Original image

(Mid) BCNN segmentation

(Bottom) BCNN UQ





Novel Bayesian Convolutional Neural Network (BCNN) framework provides more statistically grounded, interpretable, and smoother uncertainty quantification (UQ) than traditional Monte Carlo dropout approach. Preparing paper for CVPR.

Bayesian CNNs show promise for interpretable and usable per-voxel uncertainty estimates

Improving segmentation through uncertainty refinement

CNNs trained to segment images

If human labels are poor, trained CNN will be poor

Uncertainty quantification on poorly trained CNN used to refine binary predictions

Improved model used through domain shift to segment images of different contrast and resolutions

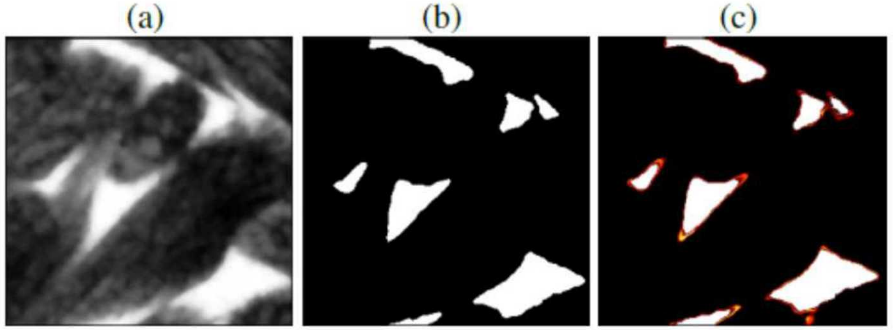


Figure 1. Binary segmentation results on held-out test examples from training domain. (a) Slice of CT scan of woven composite material. (b) Human binary labels for slice. (c) 3D CNN predicted binary labels for slice with uncertainty overlaid.

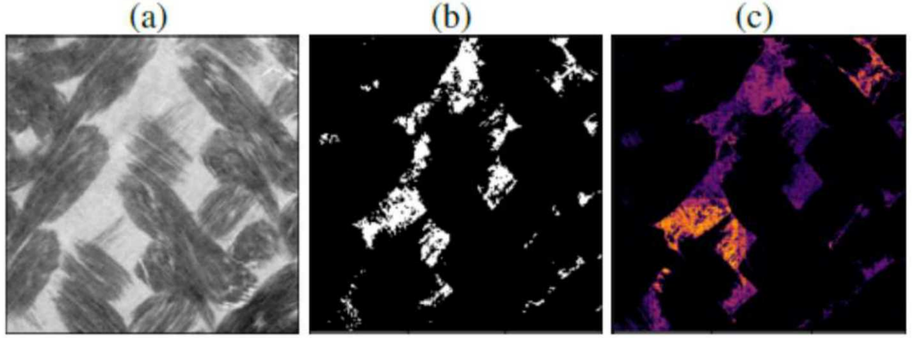
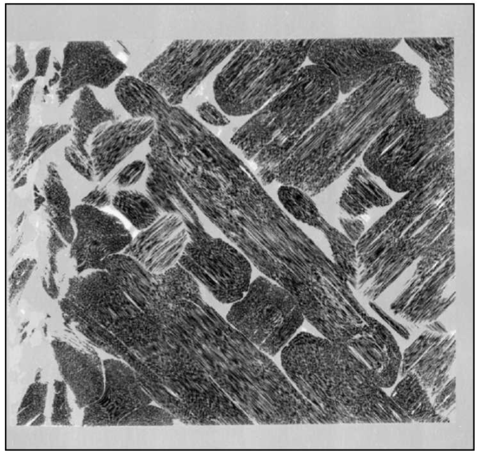


Figure 3. Binary segmentation results on domain-shifted CT scan from CNN without refinement. (a) Slice of CT scan from shifted domain. (b) 3D CNN predicted binary labels for slice. (c) Uncertainty maps for each voxel with brighter pixels representing more uncertainty.

Computer science advances impactful in computer vision field

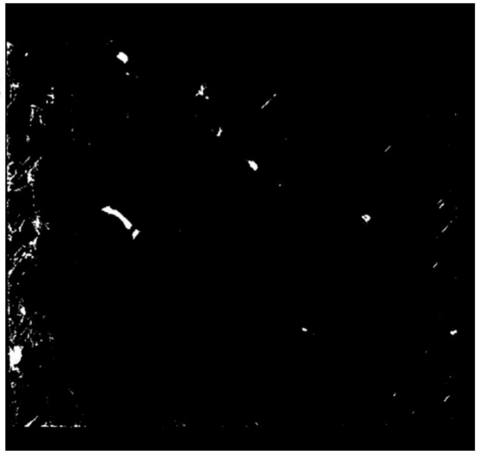
Novel applications of uncertainty maps drive new research directions

CT slice from shifted domain



Predict segmentation using model trained on original domain

Unusable segmentation



Apply advanced uncertainty based refinement method

Refined segmentation

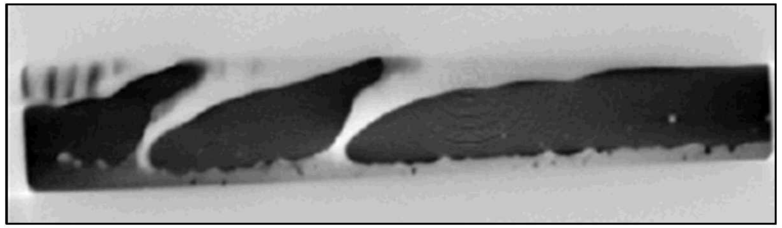
Uncertainty enables DL to overcome domain shift, improve segmentation quality

- Technical Advance SD15006: Segmentation Certainty Through Uncertainty
- Top computer vision conference (CVPR) workshop paper (peer reviewed)

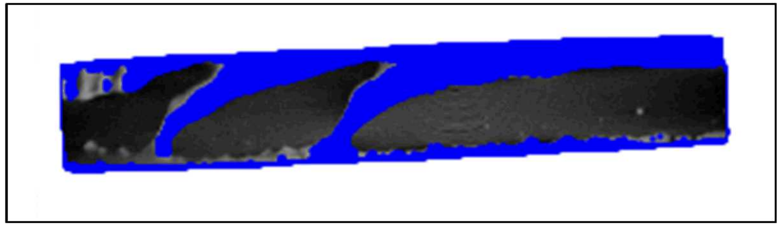
UQ enables anomaly detection

- Potential impact: Meticulous labels not required for usable segmentations

CT scan of laser welded material



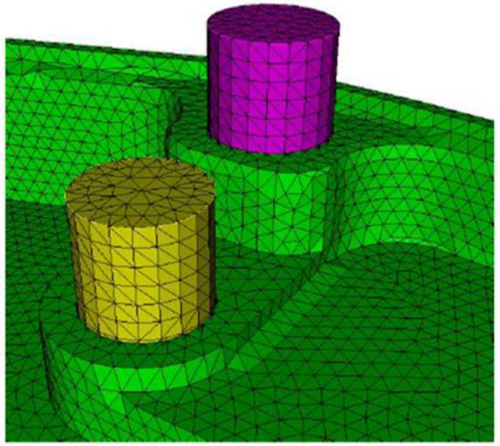
Anomalous features highlighted by uncertainty quantification



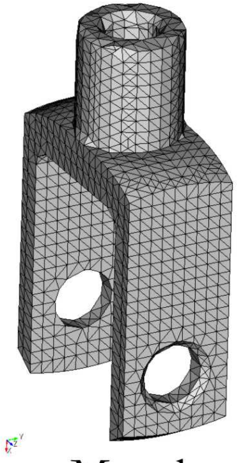
UQ techniques being incorporated into production-level segmentation efforts for Sandia's Digital Twin project

Automated tetrahedral meshing overview

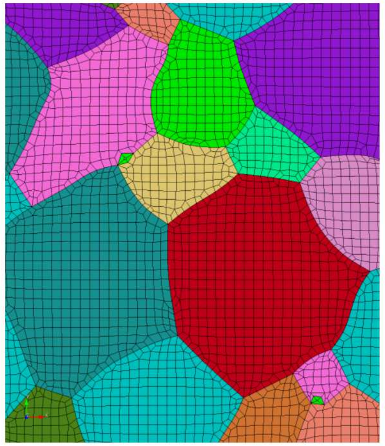
Meshing challenges
- Many materials
- Sharp features
- Mesh quality
- Mesh count



MeshGems



Morph

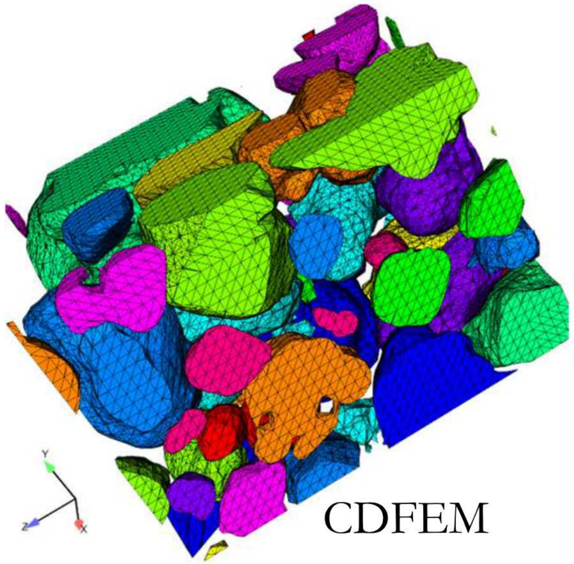


Sculpt

Imaging → Segmentation / Cleanup from Machine Learning → Sculpt → Possible Sculpt to Mesh Geometry to MeshGems

Imaging → Segmentation / Cleanup from Machine Learning → Poor Quality Mesh from CDFEM → Mesh Improvement via Omega_h

Imaging → Segmentation / Cleanup from Machine Learning → Good Quality Mesh from CDFEM with Snap-to-interface



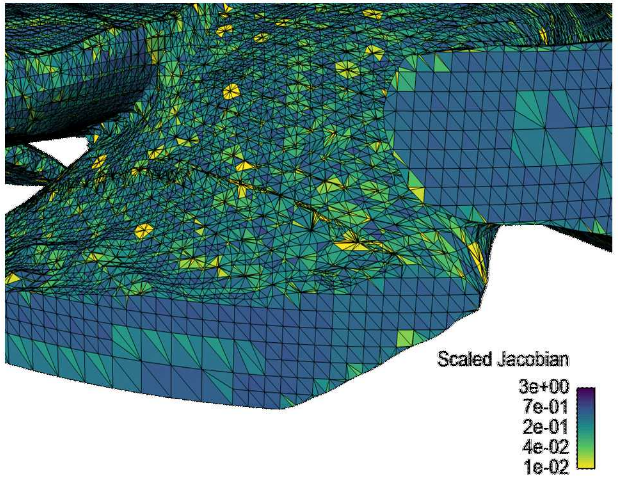
CDFEM

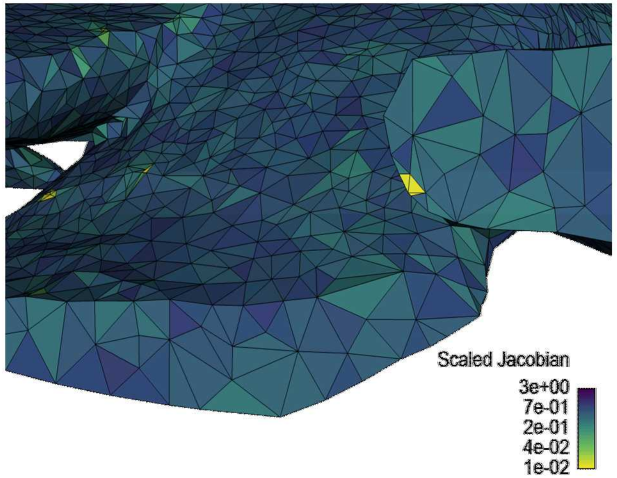
Many approaches under development, likely different algorithms needed for different problems

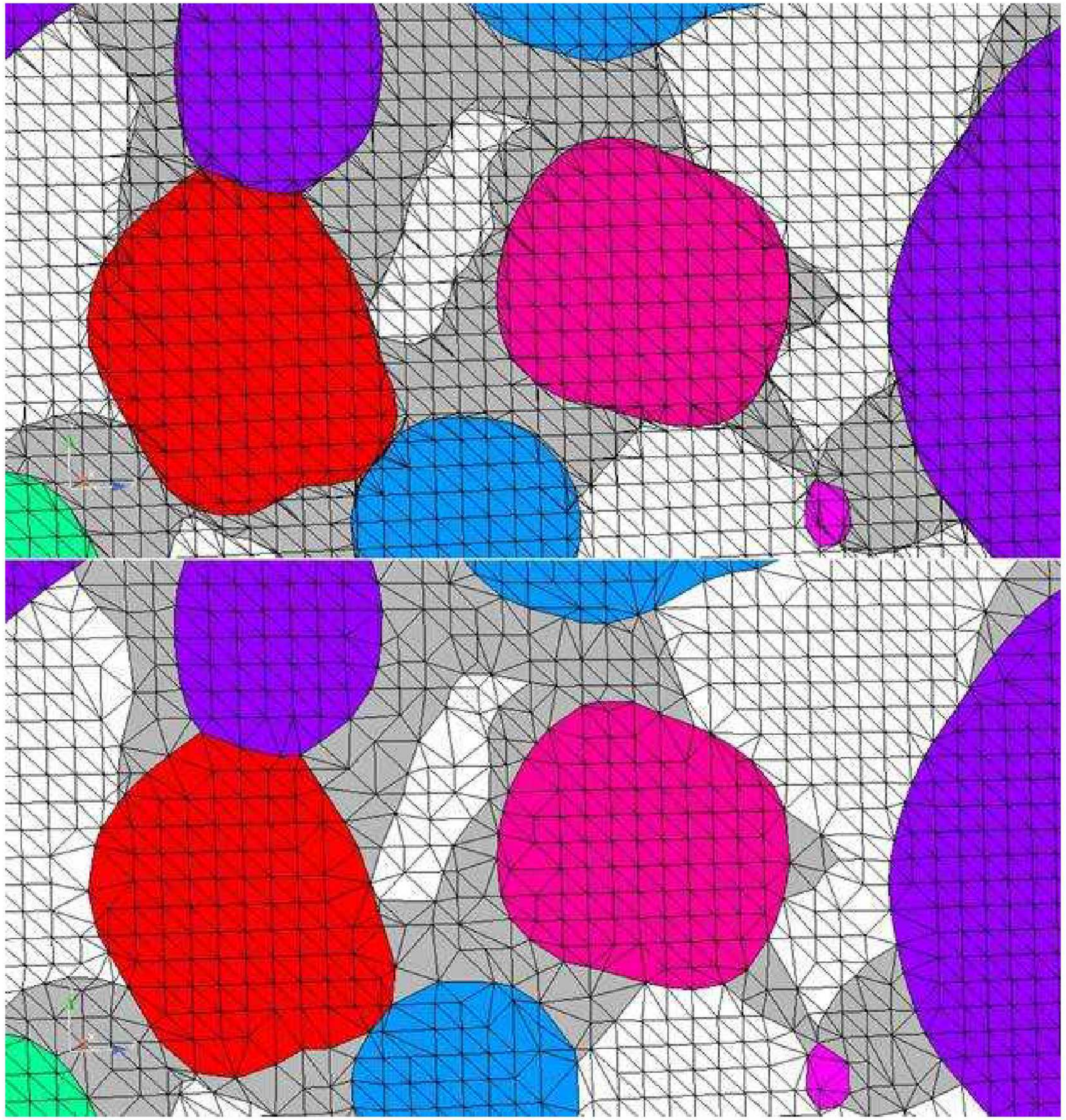
Mesh improvement strategies

Developed "morph" to improve element quality in CDFEM-generated meshes

- Maintains surface description while (re)moving internal nodes and edges to improve quality
- Works on any exodus/STK mesh
- Available as "improve_mesh" in Sierra 4.52

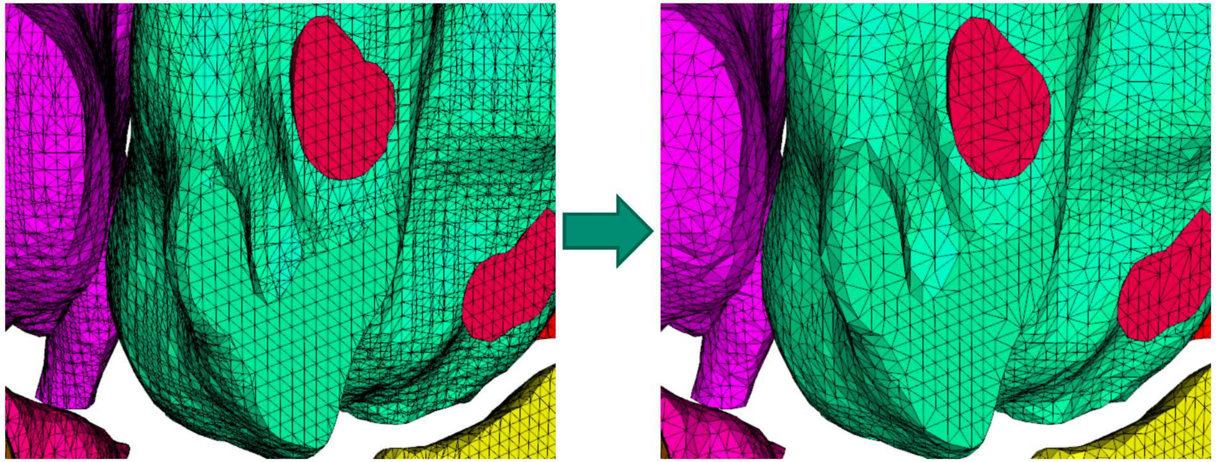




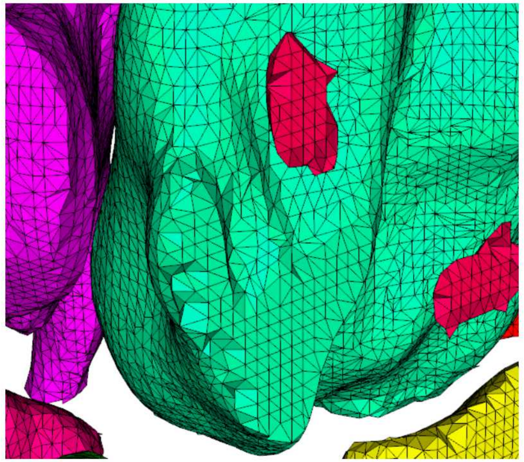


Pathway towards generating mesh quality suitable for solid mechanics analyses

Newly developed tools for credible microstructure meshing



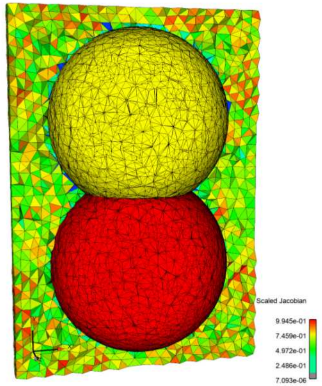
Developed *Emend* for CDFEM mesh improvement



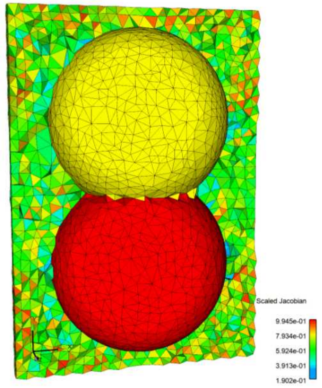
Extend *Morph* for microstructure modeling

Ongoing work: Automatic sharp feature capture from microstructure data

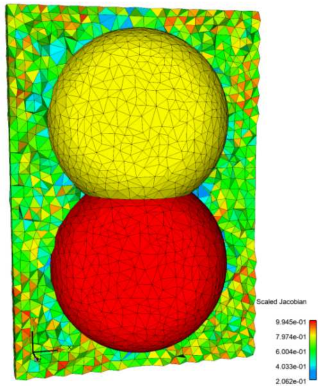
CDFEM: Sharp Feature with Exceedingly Low Quality



Morph: Guaranteed Quality But No Sharp Feature Capture Due to STL Input

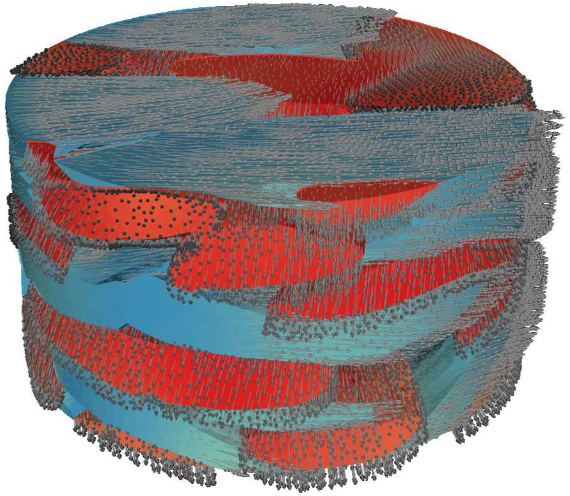


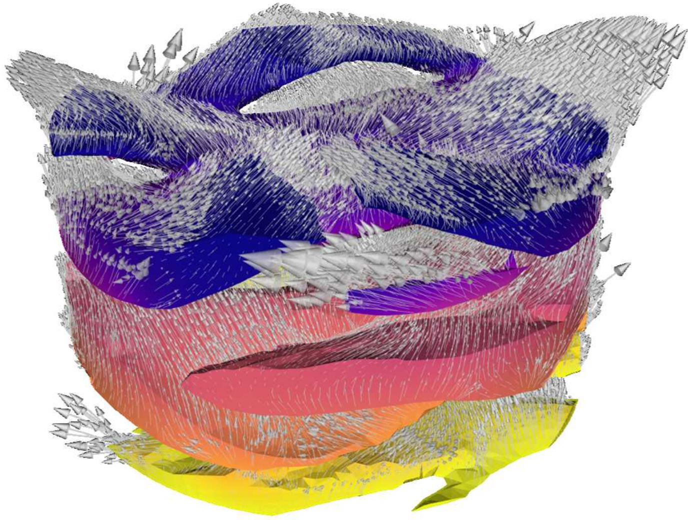
Desired: Guaranteed Quality While Retaining Sharp Microstructural Features

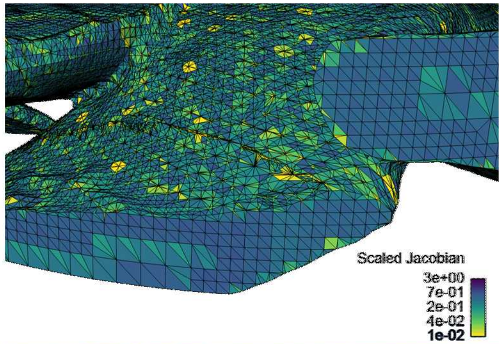


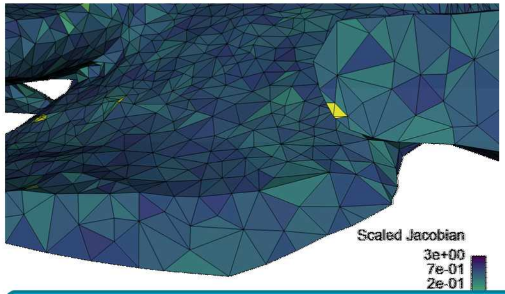
Advancing state-of-the art in high-quality, automatic tetrahedral mesh generation on complex assemblies

Anisotropic segmentation and meshing of TPS coupons

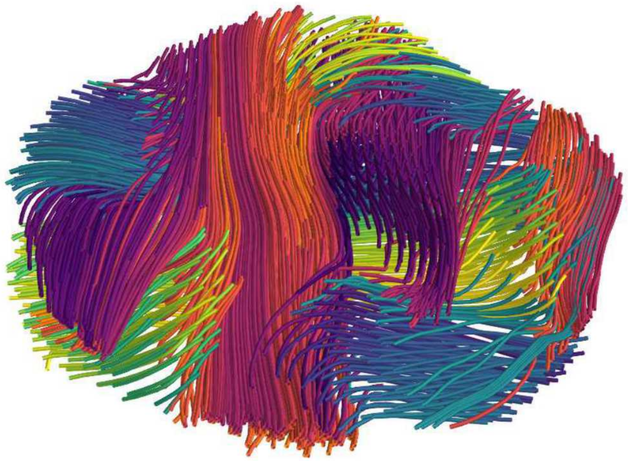








Use tow texture to calculate orientation and separate weave



Emend improves minimum element quality 4 orders of magnitude, maintaining topology

	Element Count	Average Scaled Jacobian	Min Scaled Jacobian	Effective Cond.
CDFEM	4959942	0.4644	1.456e-9	4.706
Emend	478940	0.5464	1.235e-5	4.837

First high-quality meshed TPS coupon from image to simulation using fully automatic workflow

Coordinating programs

Previous

- Battery degradation LDRD (2014-2016)
- Battery mesoscale modeling DOE/EERE/VTO (2016-2019)

Ongoing

- C-SWARM PSAAP Center at Notre Dame (Matous)
- Detonators W78 (Erikson)
- Machine learning for mesh generation (Shead/Owen)
- Sandia Injury Biomechanics Laboratory (Hovey)
- Foam / GMB encapsulation (Long, Kramer)
- Shaped charges (Korbin)
- Laser welds (Karlson)

Upcoming activities and challenges

Machine learning
- Instance segmentation (labeling) and learning of anisotropic directionality
- Surface meshing using graph neural networks (GNNs)
- Surface, edge, and vertex detection

Meshing
- Algorithmically automate surface meshing
- Meshing of sharp features from STL files in morph
- Additional control of topology change and element quality in emend

Uncertainty quantification and propagation
- Propagate image uncertainty through to mesh and physics simulation
- Identify uncertainty from surface and volume meshing and propagate

Relevant Publications

C. Martinez *et al.*, "Segmentation Certainty Through Uncertainty: Uncertainty-Refined Binary Volumetric Segmentation Under Multifactor Domain Shift," CVPR Workshops (2019). Online

S. A. Roberts *et al.*, "A verified conformal decomposition finite element method for implicit, many-material geometries," J. Comp. Phys., 375 (2018) 352-367. DOI: 10.1016/j.jcp.2018.08.022

S. A. Roberts *et al.*, "Insights into lithium-ion battery degradation and safety mechanisms from mesoscale simulations using experimentally-reconstructed mesostructures," J. Electrochem. En. Conv. Stor., 13 (2016) 031005. DOI: 10.1115/1.4034410

S. A. Roberts *et al.*, "A Framework for Three-Dimensional Mesoscale Modeling of Anisotropic Swelling and Mechanical Deformation in Lithium-Ion Electrodes," J. Electrochem. Soc., 161 (2014) F3052-F3059. DOI: 10.1149/2.0081411jes

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