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Meshing with Uncertainty

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Sandia Interdisciplinary Machine Learning Research (SIMLR) Team

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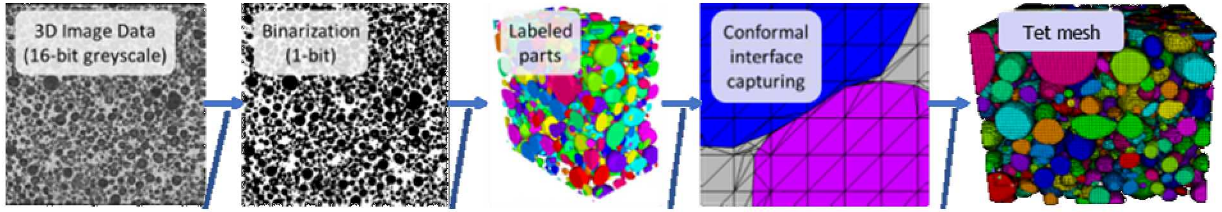
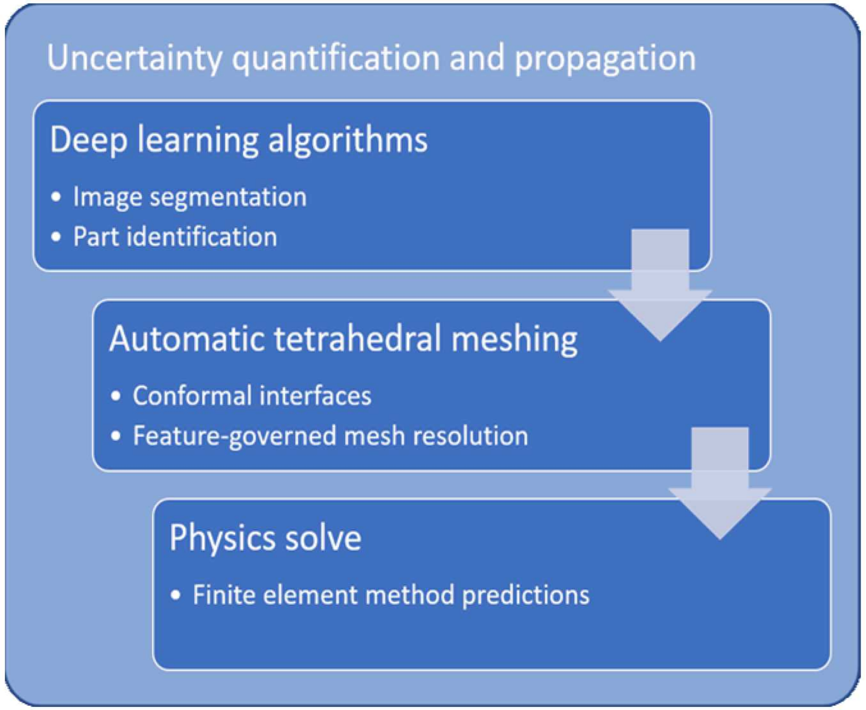
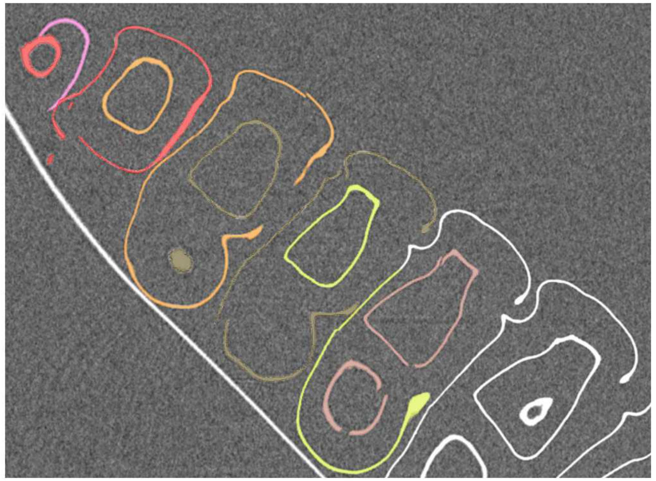
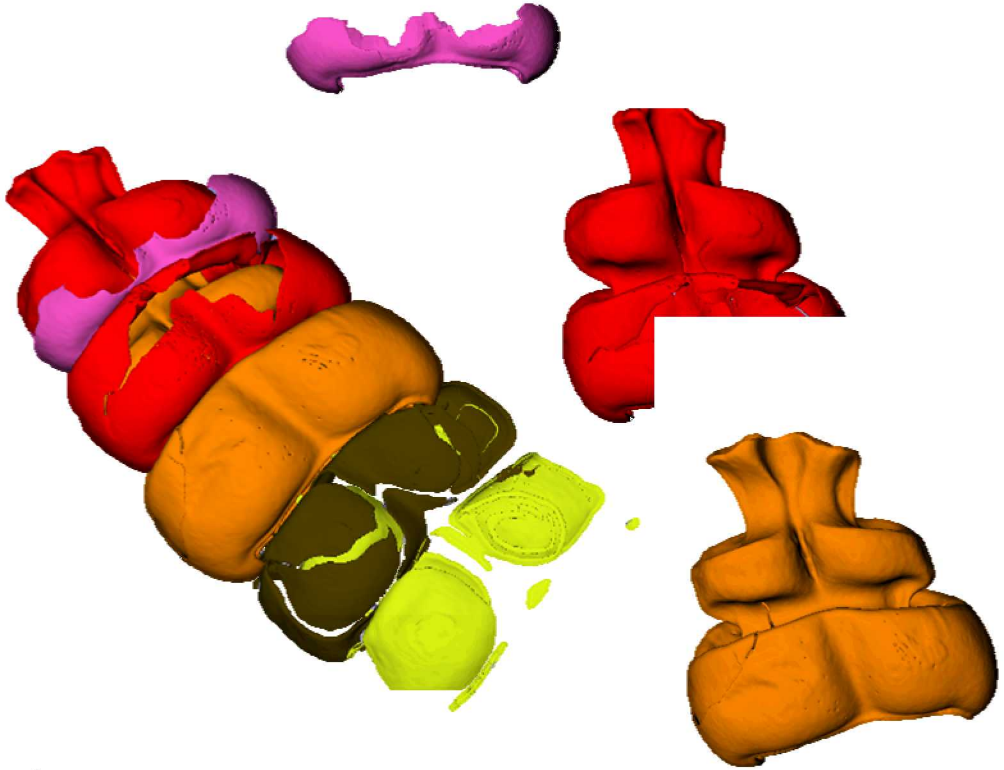
A lofty goal: Propagating uncertainty all the way through

- Hypothesis: We can develop an automated and credible image-to-mesh technology that can demonstrate the physics impact of per-unit variability on material, component, or system performance
- 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:
  1. Automatic CT segmentation via Machine Learning (ML)
  2. Automatic conformal tetrahedral mesh creation (ATM)
  3. Uncertainty quantification and propagation (UQ)









Using ML to save time and effort while improving accuracy

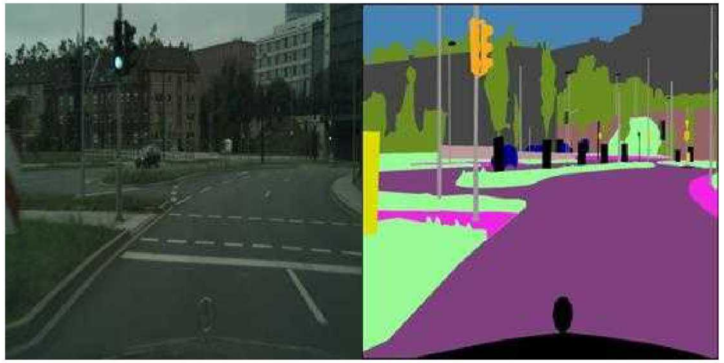
CT SEGMENTATION

Segmentation is a classic computer vision problem

- Image segmentation is well studied
  - Small files
  - Large training sets

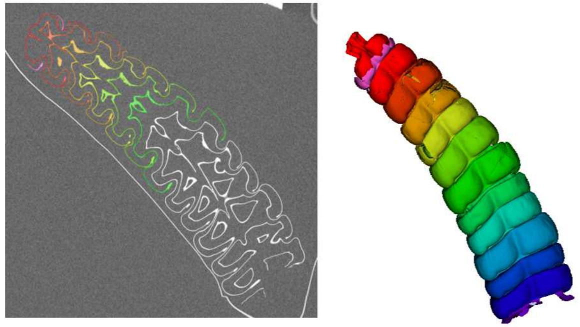
- Volumetric segmentation is different
  - Big data
  - Class imbalance (lots of background)
  - Small training sets with “bad” human labels
  - Humans can’t label billions of voxels without taking big shortcuts

- Medical researchers are leading this work toward Deep Learning solutions



https://www.cityscapes-dataset.com/

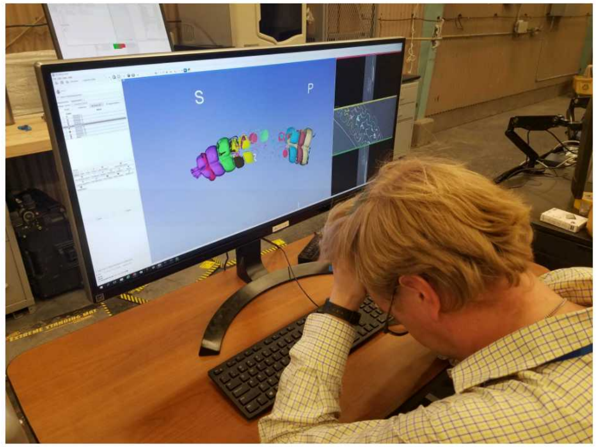
Cityscape
(~1e5 pixels)

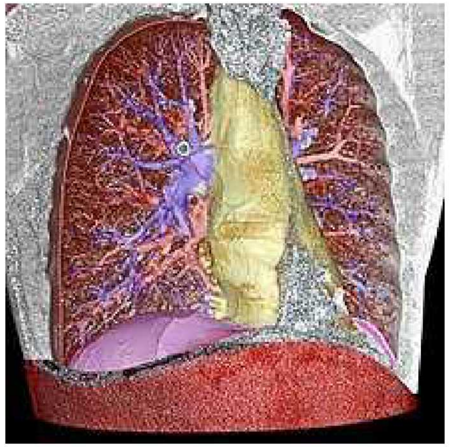


Rattlesnake Tail
(~1e9 voxels)

CT Segmentation is hard for humans

- CT scans must be labeled by component for simulations





https://en.wikipedia.org/wiki/Image_segmentation

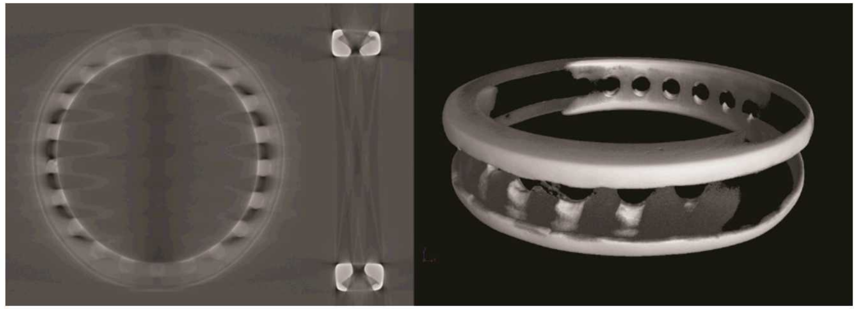
Labeling by hand does not scale

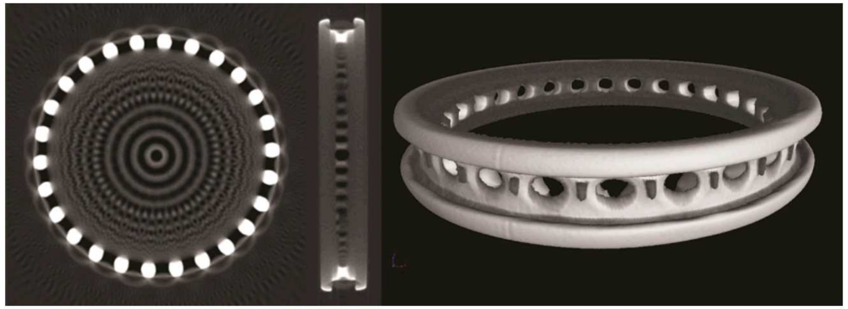
Deep Learning algorithms

- Find each component of the object by material
- Find any anomalies
- Pass this to a usable form for numerical simulations

Automated Segmentation presents challenges

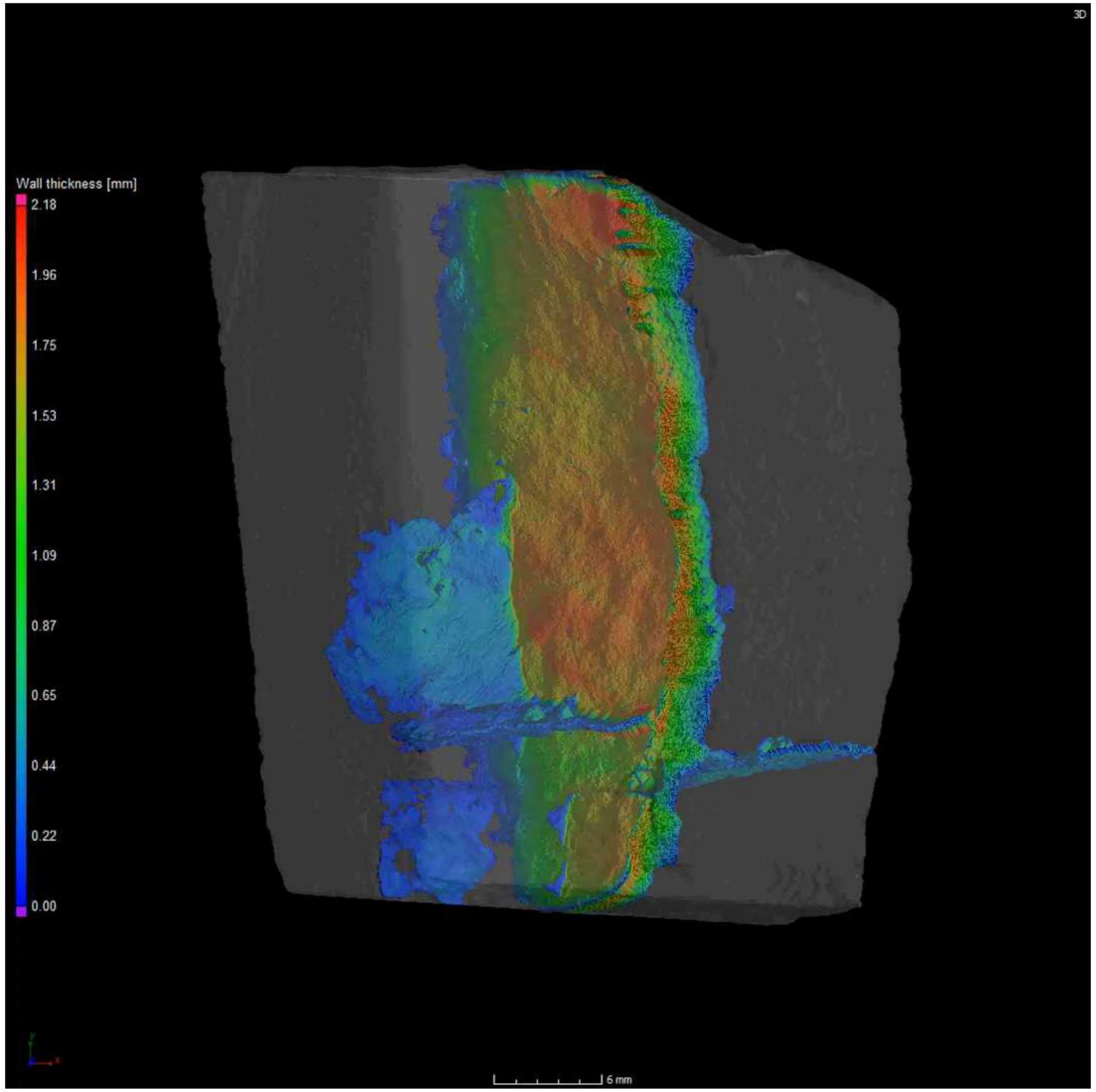
- CT scans are large
  - Medical literature: 128x128x64
  - Ours: ~1000x larger
  - Soon: ~10000x larger
- Class Imbalance
  - Empty space often dominates the scan
- Artifacts and noise
  - Difficult to separate materials of similar density
  - Shadow effects





Mitigating Challenges

- CT scans are large
  - Used chunks of the volume
  - Optimized our model for GPU memory usage on GPU cluster
- Class Imbalance
  - Adjusted loss function that guides training
- Artifacts and noise
  - Selected Convolutional Neural Network (CNN) architecture with strength in shape recognition



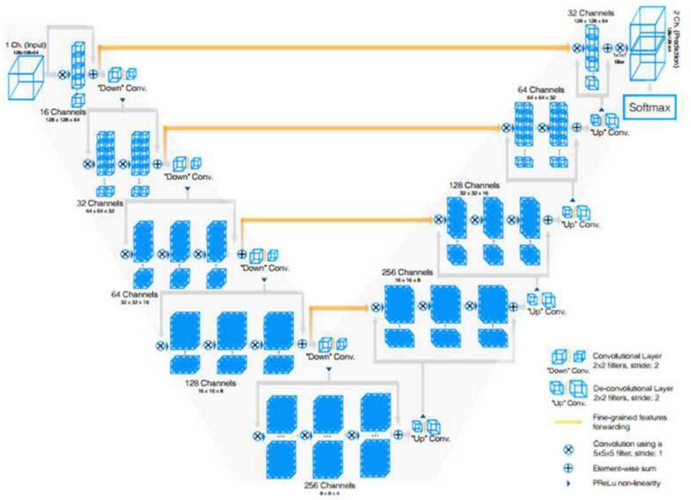
Deep learning is big data and large networks

- *"Deep learning is the first class of algorithms that is scalable... performance just keeps getting better as you feed them more data"*

Andrew Ng, Founder of Google Brain

- U-net, a big advance in biomedical segmentation
  - Olaf Ronneberger, Philipp Fischer, Thomas Brox , "U-Net: Convolutional Networks for Biomedical Image Segmentation", in Medical Image Computing and Computer-Assisted Intervention (MICCAI), Springer, LNCS, Vol.9351: 234--241, 2015

- V-net follows as a natural extension
  - F. Milletari, N. Navab, and S. A. Ahmadi, "V-net: Fully convolutional neural networks for volumetric medical image segmentation," in 2016 Fourth International Conference on 3D Vision (3DV), Oct 2016, pp.565–571

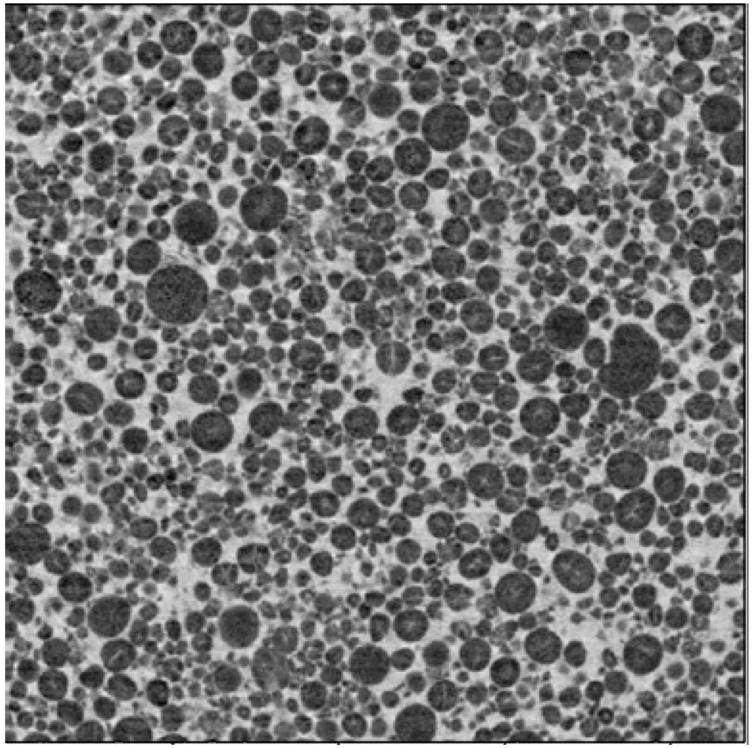


V-Net architecture for segmenting volumetric data (2016)

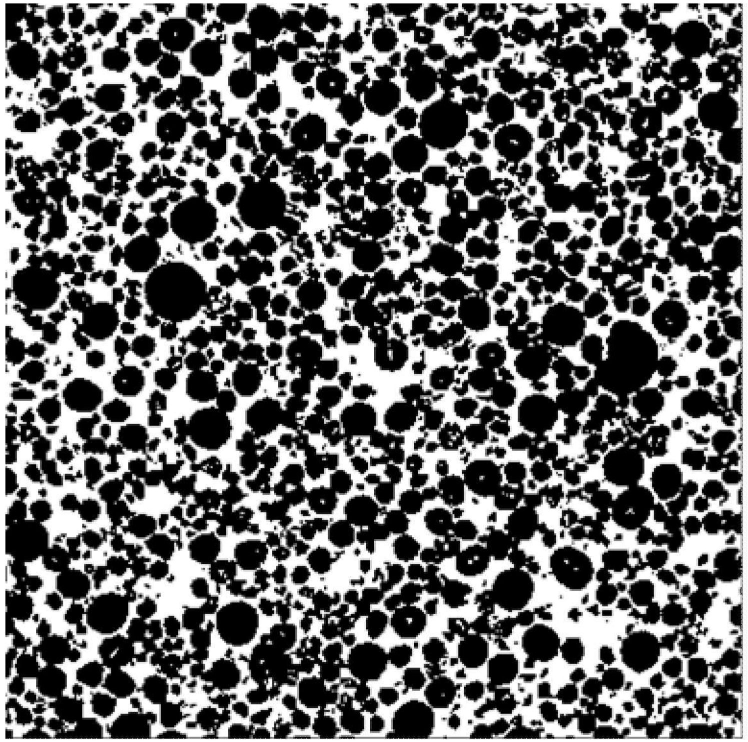
We started with a V-Net and made improvements as necessary

Volumetric battery segmentation achieves high accuracy compared to human labels

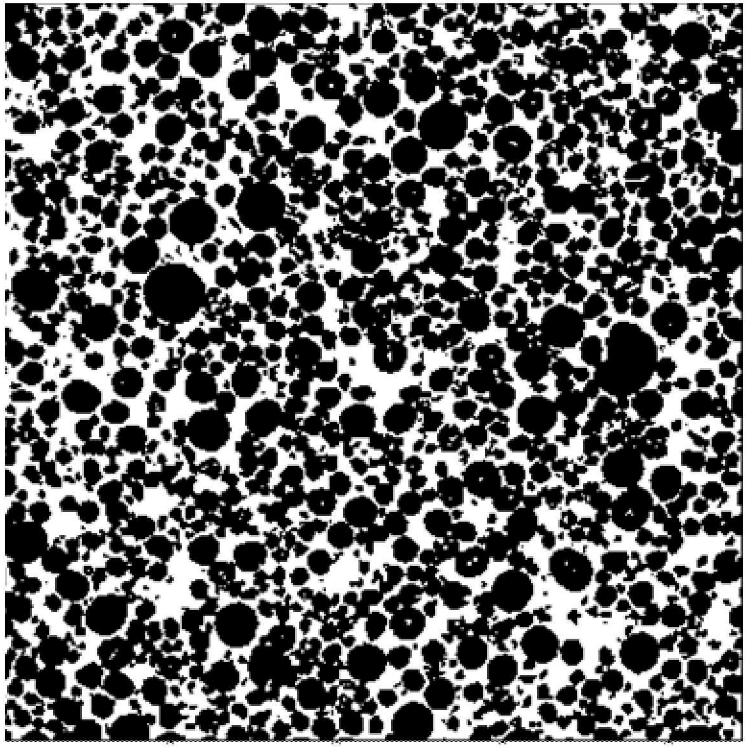
Slice of 3D Image



Human label



ML prediction



Averaged 99.7% accuracy over held out test set

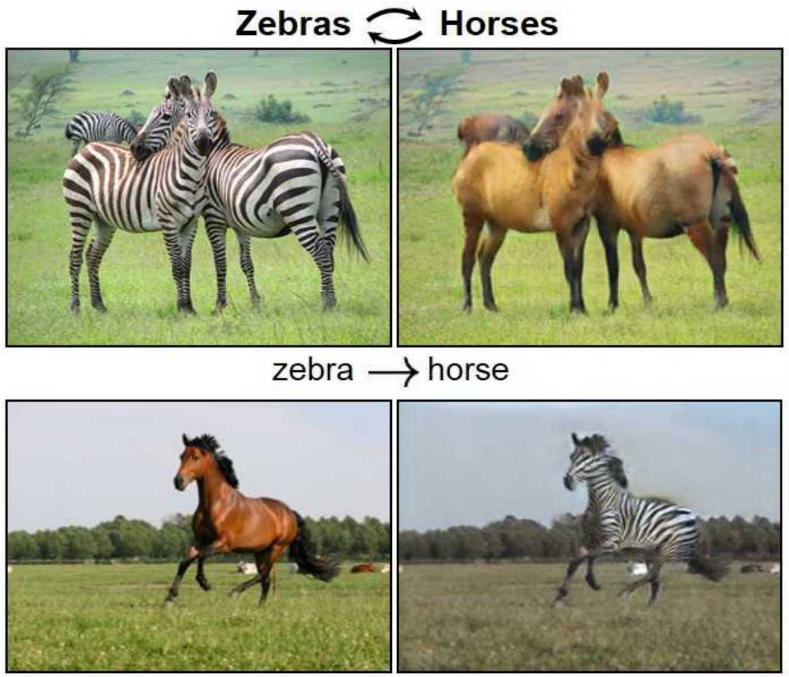
https://github.com/junyanz/pytorch-CycleGAN-and-pix2pix

Using CycleGAN for automatic segmentation

SEMI-SUPERVISED LEARNING

CycleGAN translates images between domains

Zhu, J. Y., Park, T., Isola, P., & Efros, A. A. (2017). Unpaired image-to-image translation using cycle-consistent adversarial networks. arXiv preprint.



Learns two functions:

F(x) = Horse to zebra

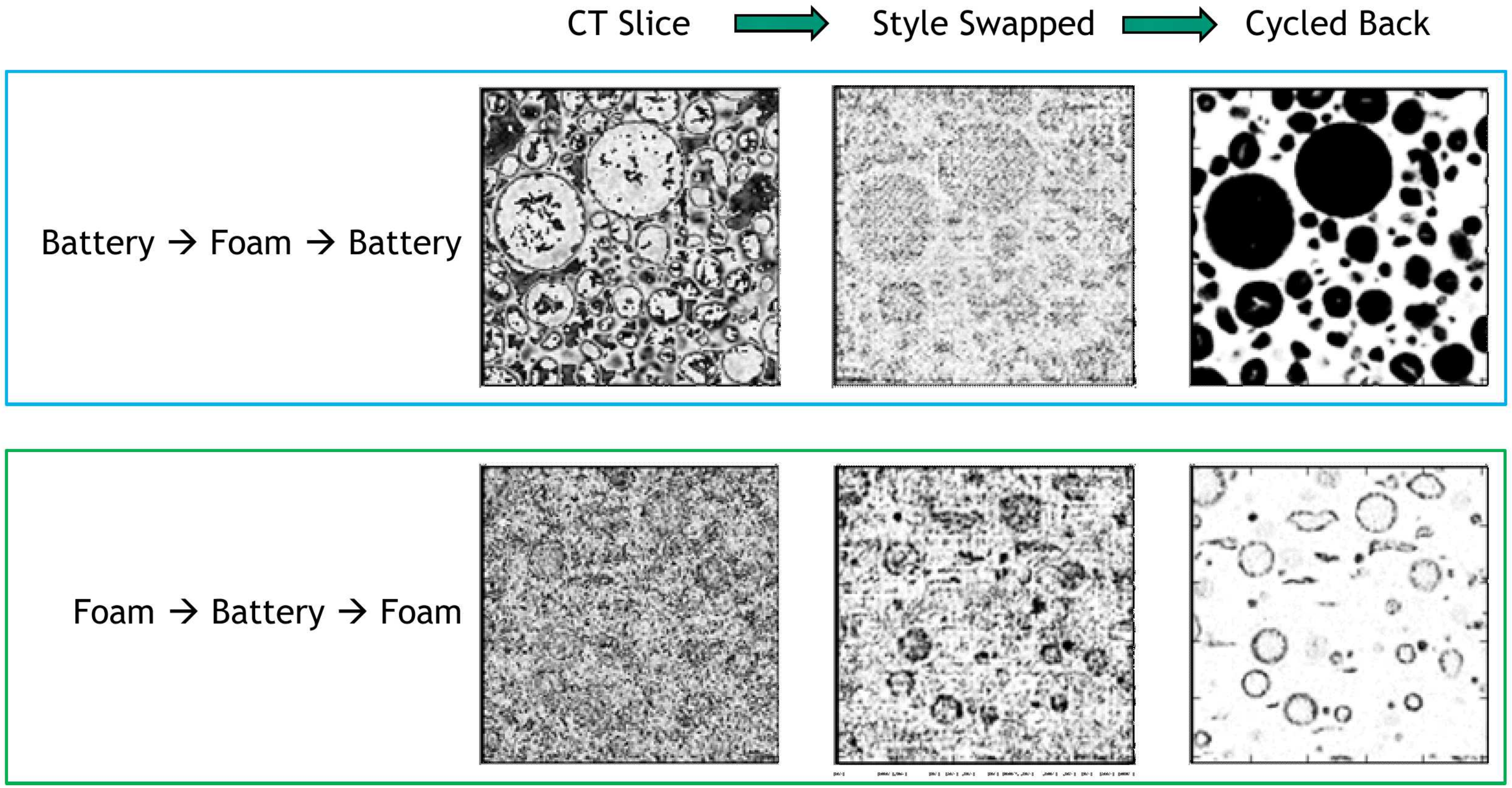
G(x) = Zebra to horse

Cycles back to starting point to learn without paired examples

F(G(x)) = x

Generative adversarial networks are powerful new models that are widely applicable

Batteries to Foam — Leveraging existing datasets via CycleGAN



CycleGAN provides a rough segmentation of both battery and foam

Domain Adaptation could reduce supervised labeling cost

Repurpose labels from one domain (battery) to another domain (foam)

- CycleGAN transforms foam CTs into the “style” of battery labels
- Semi-supervised

Hand-labeled small slices from 7 CT scans of foam

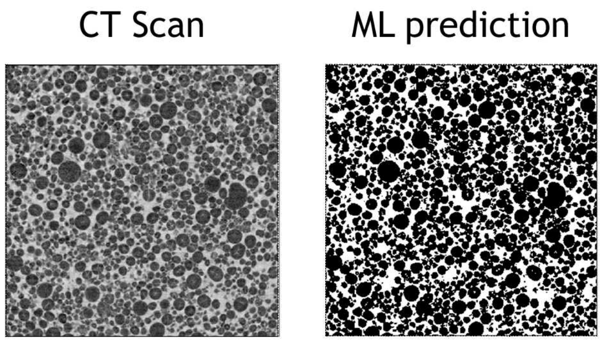
Used 2 labels to select stopping point

Inferred over remaining 5 volumes

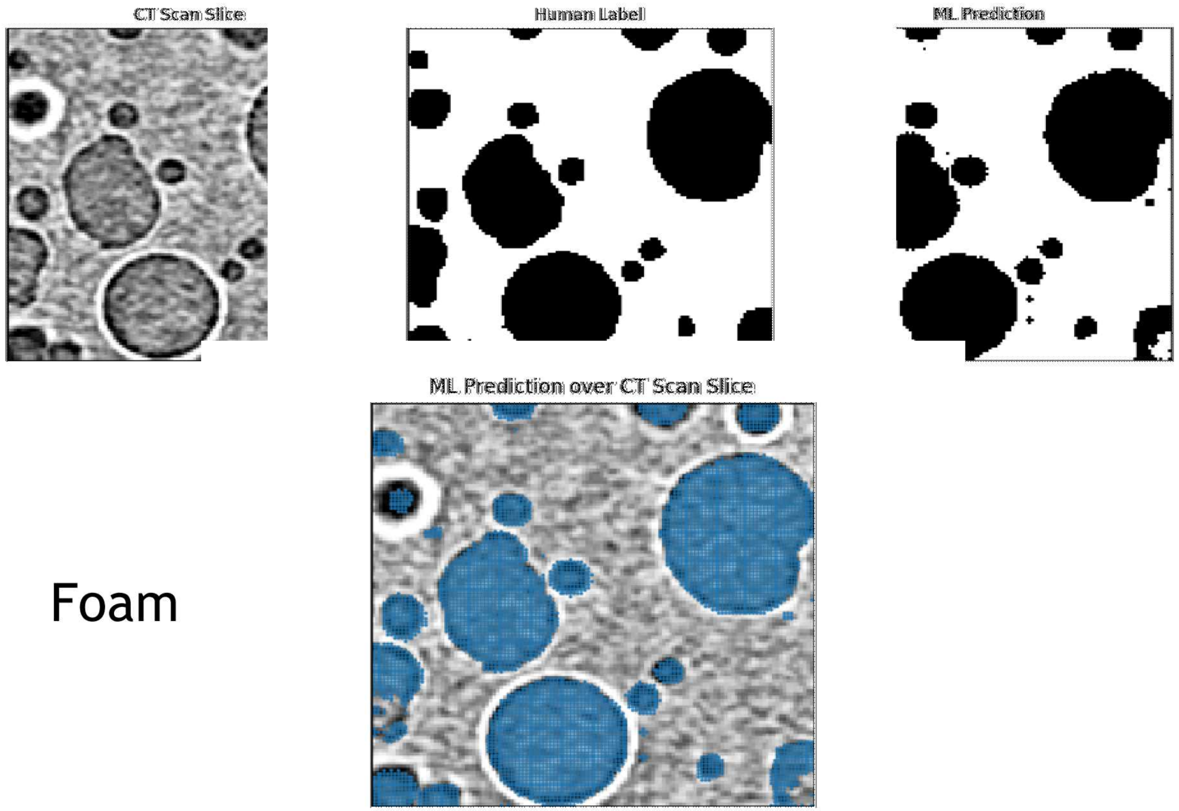
Post-process (fill in gaps) with standard CV methods

Average 94.8% accuracy when compared with human labeled slices

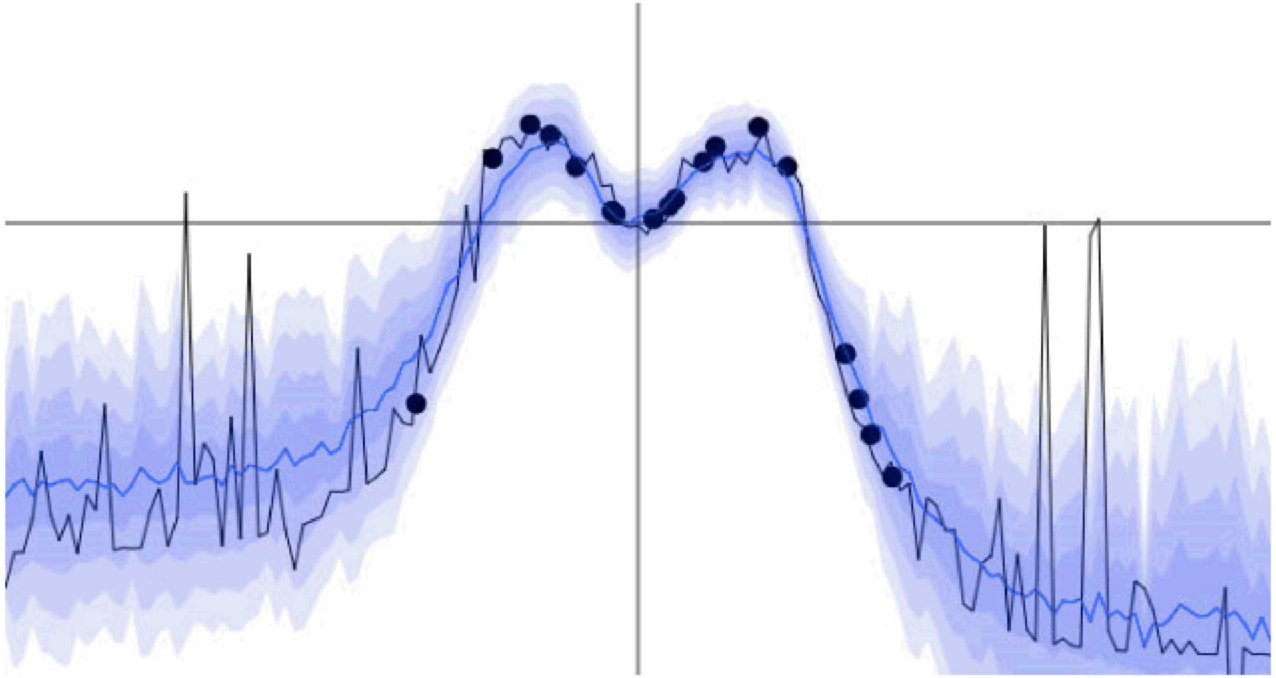
Battery



Foam



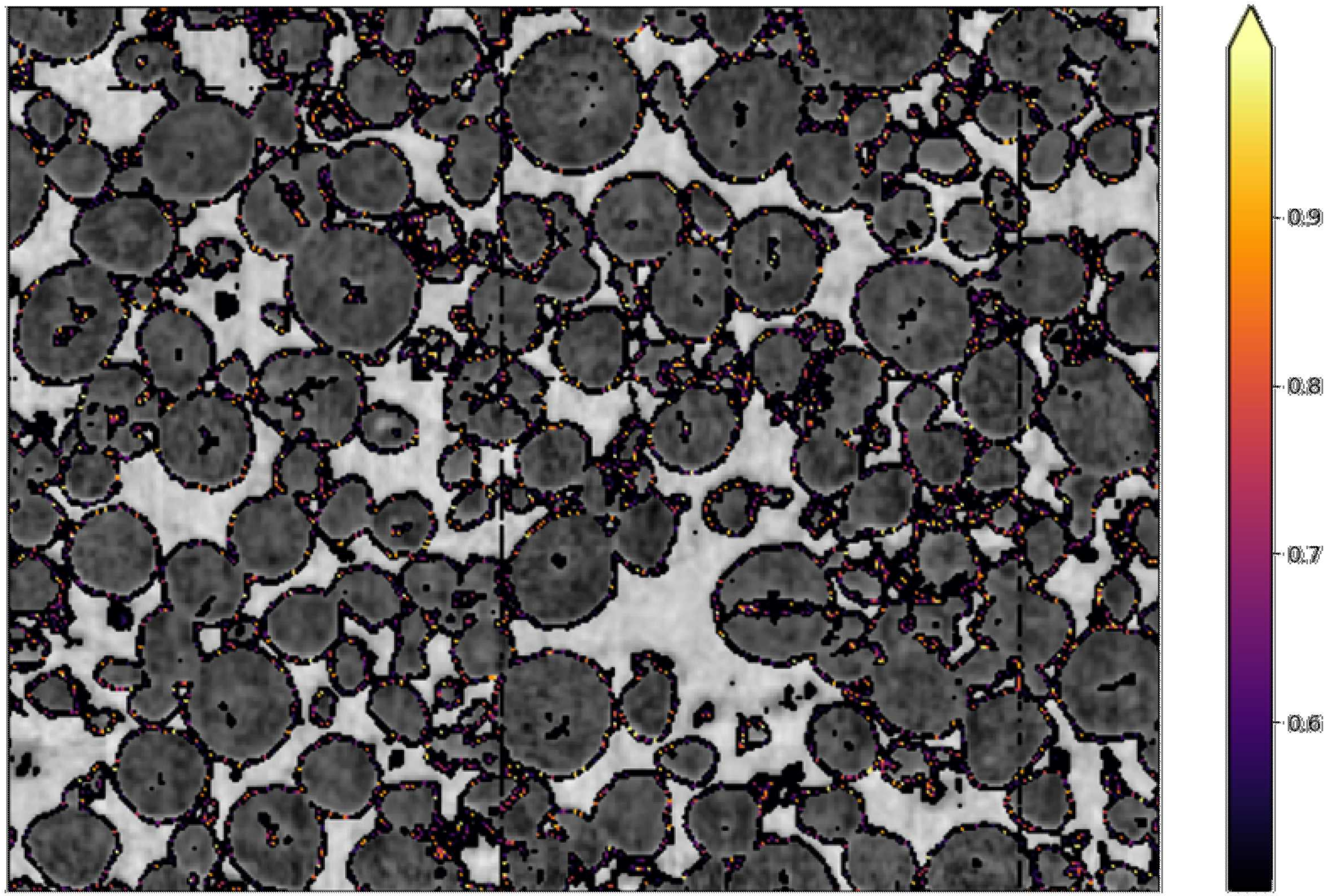
http://www.cs.ox.ac.uk/people/yarin.gal/website/blog_3d801aa532c1ce.html



Using dropout to estimate segmentation confidence

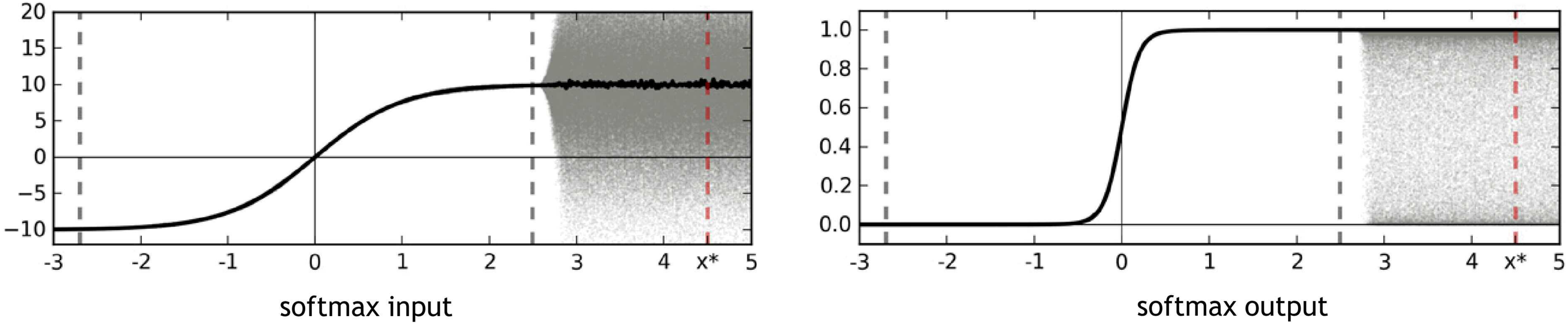
UNCERTAINTY QUANTIFICATION

Softmax uncertainty as a baseline



Standard neural network models do not provide error bars

- Softmax output is not always enough to determine model uncertainty



https://www.cs.ox.ac.uk/people/yarin.gal/website/blog_3d801aa532c1ce.html

- We can use dropout at inference time to approximate uncertainty
  - Gal, Yarin, and Zoubin Ghahramani. "Dropout as a Bayesian approximation: Representing model uncertainty in deep learning." international conference on machine learning. 2016.