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PURDUE UNIVERSITY

Energy and Transport Sciences Laboratory

Uncertainty in 3D Image-Based Effective Property Simulations using Bayesian Convolutional Neural Networks

Chance Norris[1*], Tyler LaBonte[2], Carianne Martinez[2], Scott A. Roberts[3], and Partha P. Mukherjee[1]

[1]School of Mechanical Engineering, Purdue University, West Lafayette, IN 47907

[2]Applied Machine Intel & App Engineering, Sandia National Laboratories, Albuquerque, NM 87185

[3]Engineering Sciences Center, Sandia National Laboratories, Albuquerque, NM 87185

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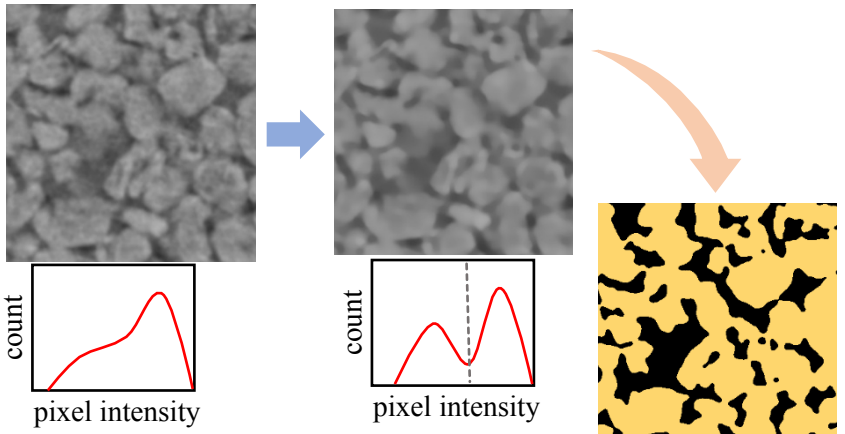
Motivation

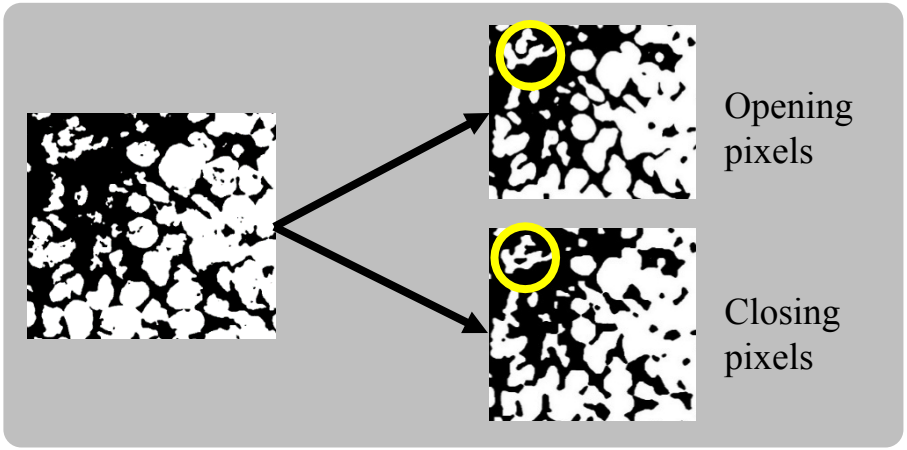
Thresholding/Segmentation

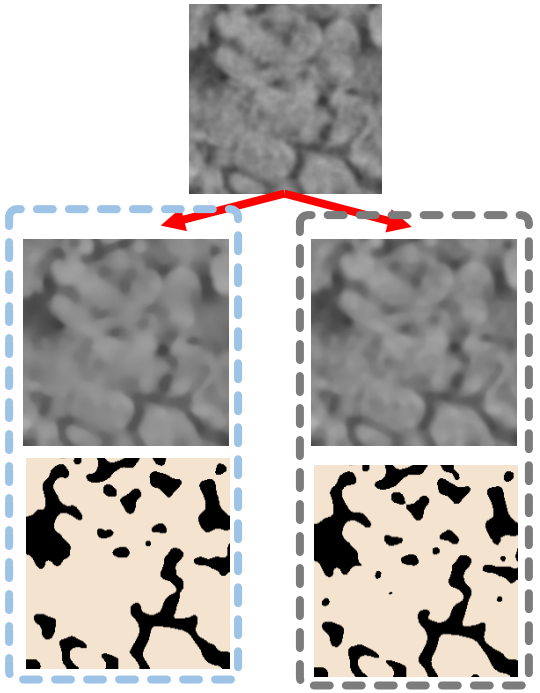
- Greyscale to binary images
- Image processing is used to gain bimodal pixel distribution prior to segmentation.



Subjectiveness of Segmentation

- Segmentation is fraught with subjectiveness.
- This process is also time consuming.

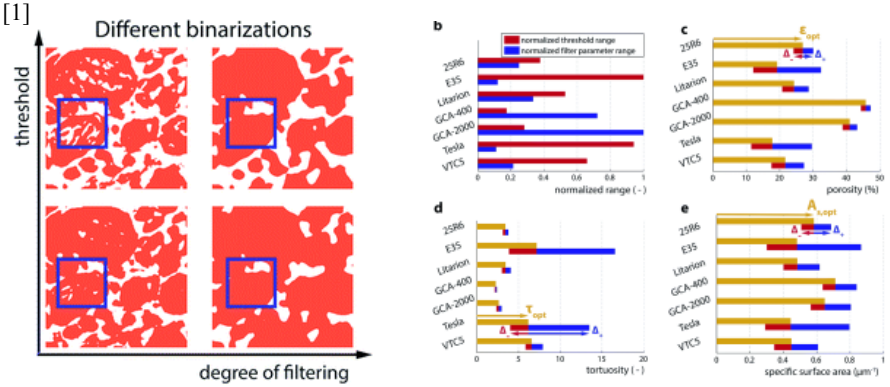




Background

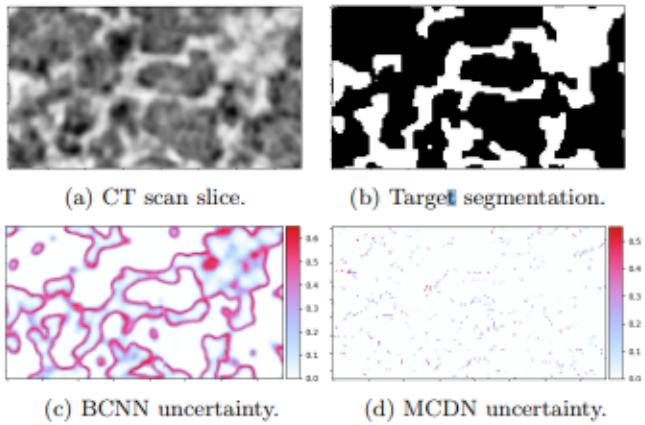
- Wood et. al. varied thresholding and filtering parameters.
- Looked at effective property changes.

[1]



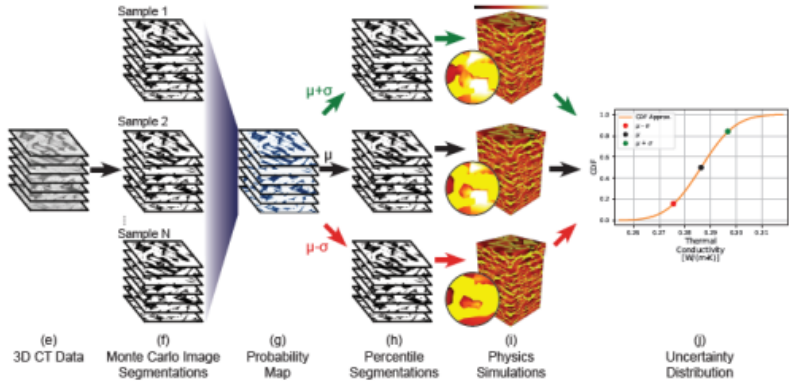
- LaBonte et al. probed uncertainty via BCNN and MCDN.

[2]



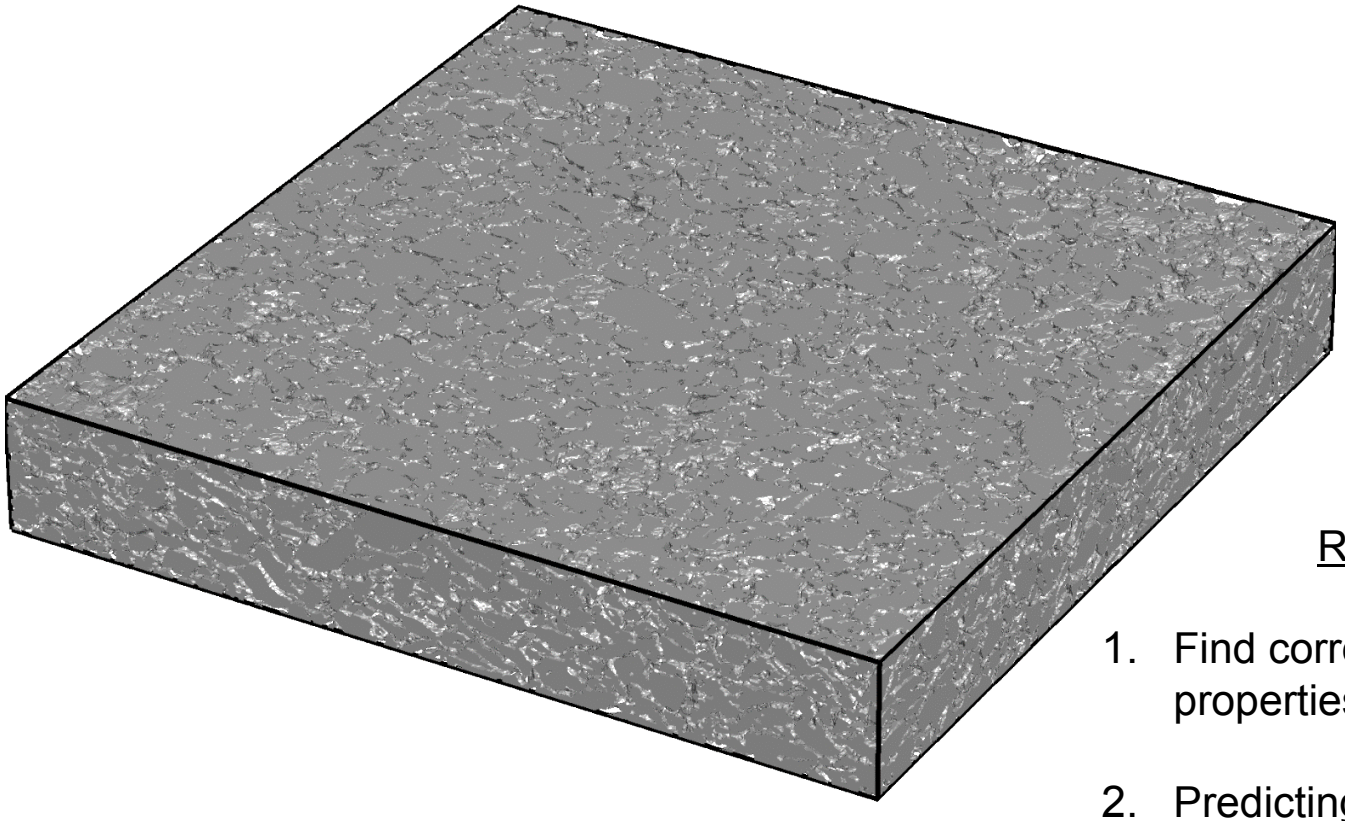
- Krygier et al. used percentile segmentations to propagate segmentation uncertainty to physical quantities.

[3]



[1] Pietsch, P., Ebner, M., Marone, F., … M. S.-S. E. & & 2018, undefined. Determining the uncertainty in microstructural parameters extracted from tomographic data. *pubs.rsc.org*.
[2] LaBonte ,…, 'We Know Where We Don't Know: #D Bayesian CNNs for Credible Geometric Uncertainty', 2020, https://arxiv.org/abs/1910.10793
[3] Krygier, Michael,…,'Quantifying the Unknown: Impact of Segmentation Uncertainty on Image-Based Simulations', Nature Communications, 2021, https://arxiv.org/abs/2012.09913

Objective



Research Questions

1. Find correlations between effective properties/image quality.
2. Predicting uncertainty through image quality
3. Uncertainty propagation through geometric uncertainties
4. Microstructural influences on uncertainty propagation.

Muller, S. et. al. *Journal of The Electrochemical Society,* **2018**, 165(2), A339-A344.

Electrode Images

Numbered Electrodes			
Ia	IIa	IIIa	IVa
Ib	IIb	IIIb	IVb
Ic	IIc	IIIc	IVc

Where a, b and c denotes three samples taken from one commercial sheet

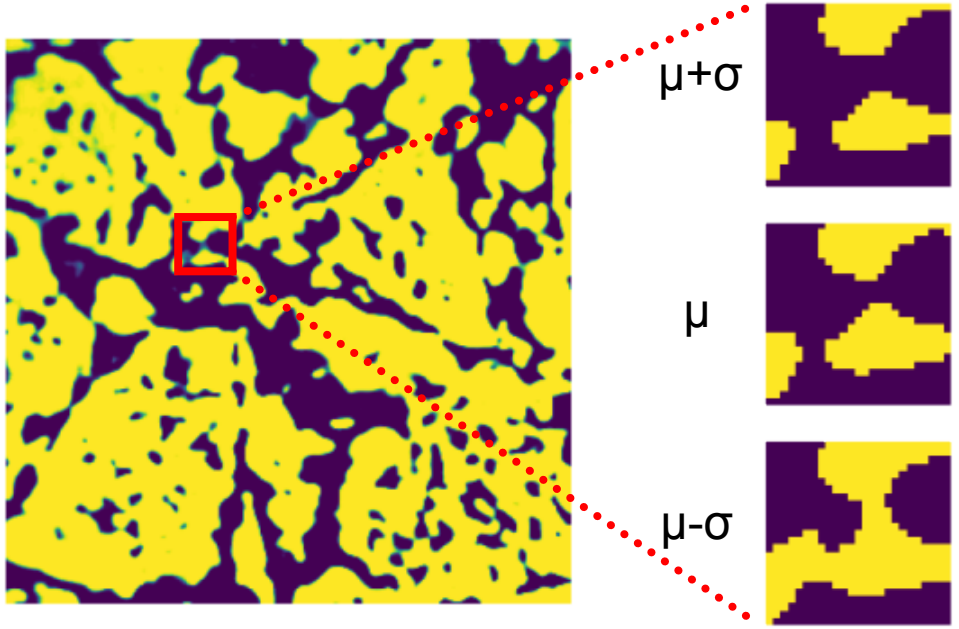
Named Electrodes					
Litarion	Tesla	SamsungE35	Samsung 25R6	GCA400	GCA2000

Named electrodes have 2x the resolution per voxel than the numbered.

All electrode data is open source provided by Vanessa Wood's group from ETH Zurich

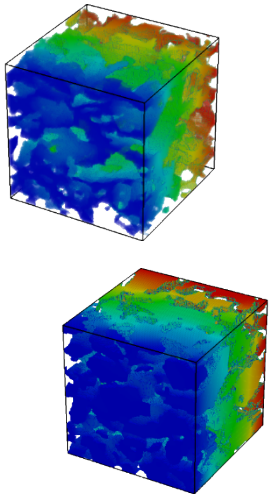
*Muller, S. et. al. *Journal of The Electrochemical Society,* **2018**, 165(2), A339-A344. and Pietsch, P. et al. Sustainable Energy and Fuels, **2018**, 2(3), 598-605

Structural Acquisition and Physics Quantities



Percentile segmentations were created through probability maps via the BCNN.

A total of 11 percentile segmentations were used.

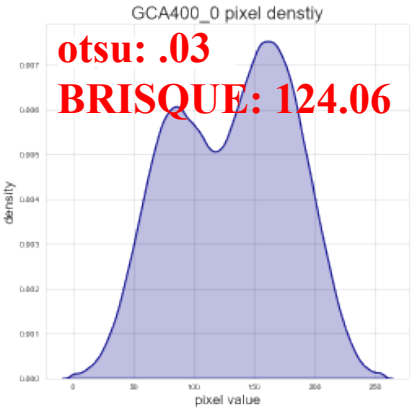


Tortuosity/Conductivity

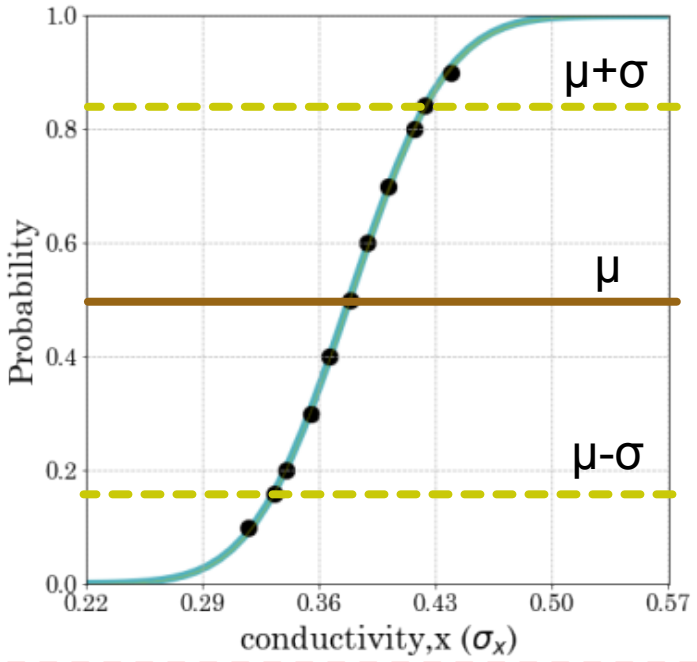
Tells how the pore/particle phase is interconnected, respectively.

Image Quality

OTSU intervariance and BRISQUE scores were used.

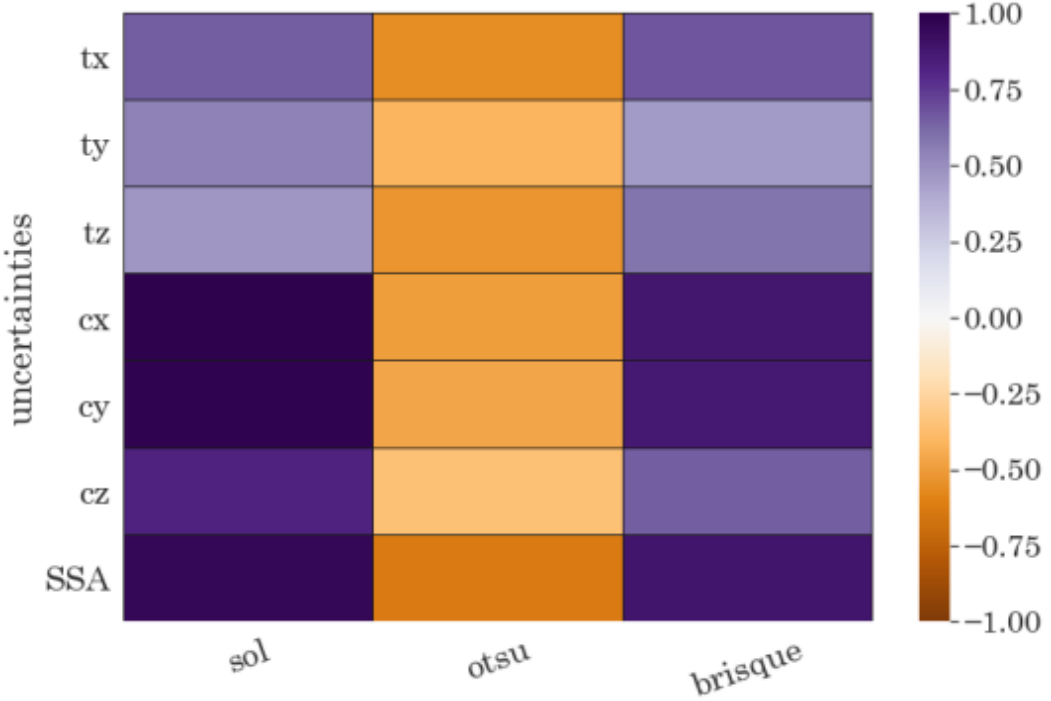


Property Correlations



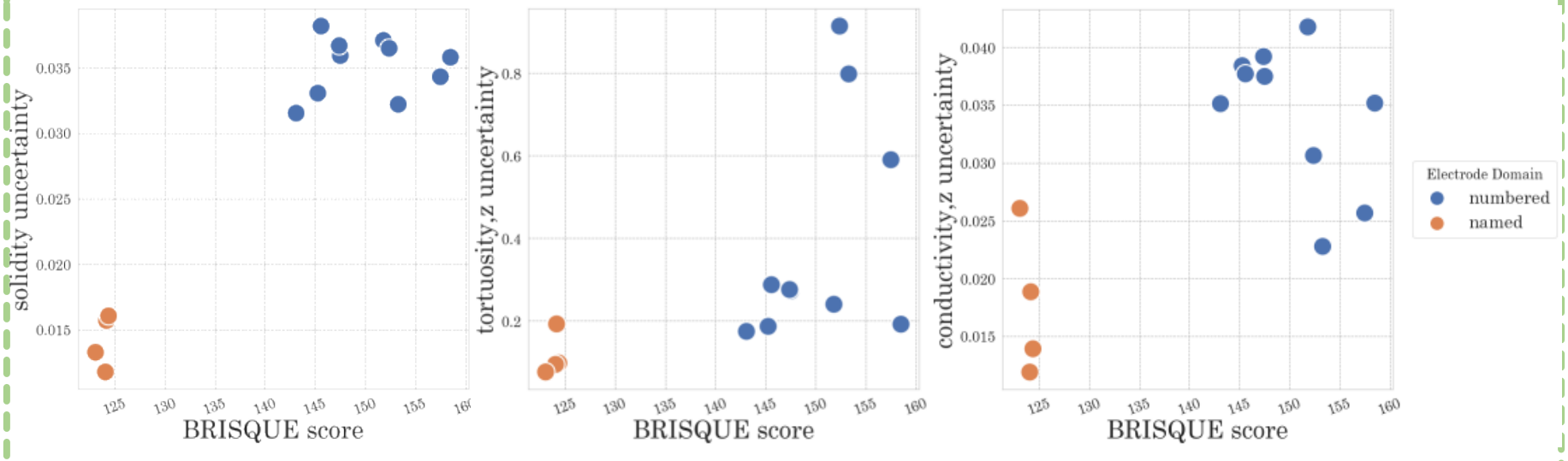
- All effective properties show a gaussian distribution
- By evaluation we can get the mean and standard deviation

Uncertainty Correlation Matrix



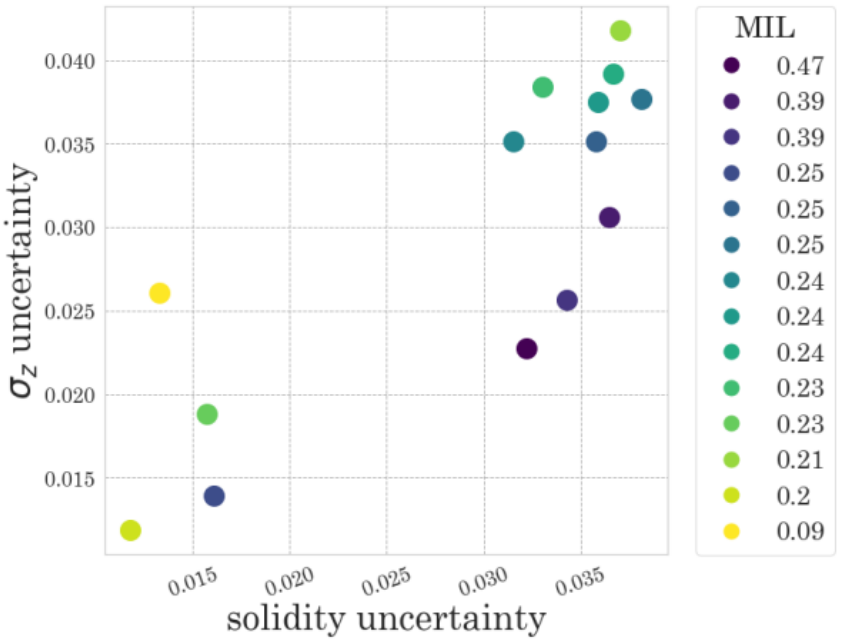
- Higher correlations between conductivity.
- Tortuosity is more dependent on structural morphology.

Image-Quality Correlation

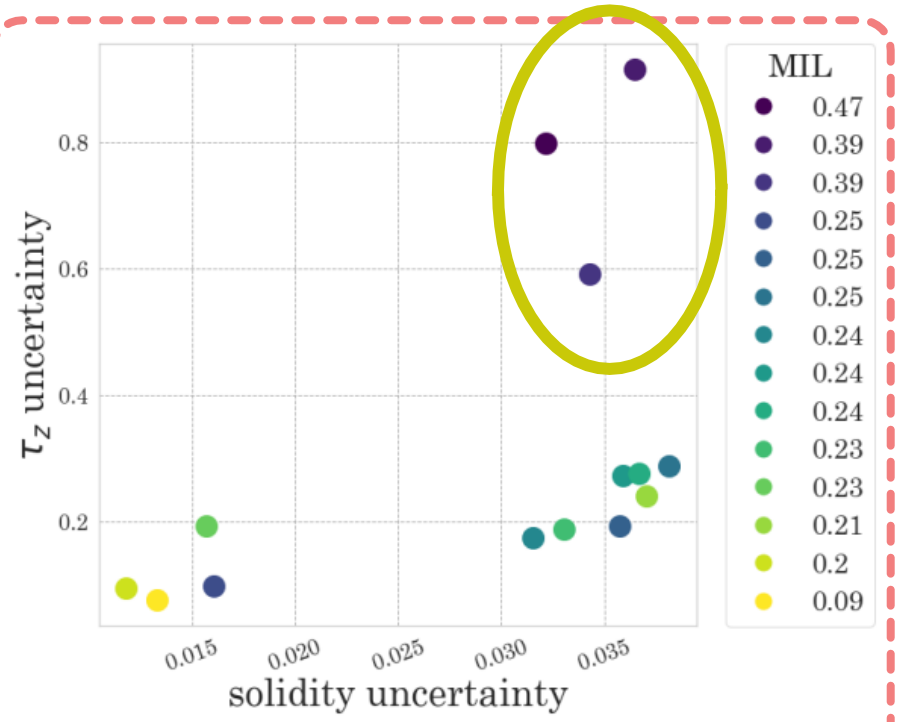


- Lower BRISQUE score the clearer the image.
- Named and numbered electrodes are grouped.
- Based on resolution or other factors dependent on imaging process.

Geometric Uncertainty Correlations



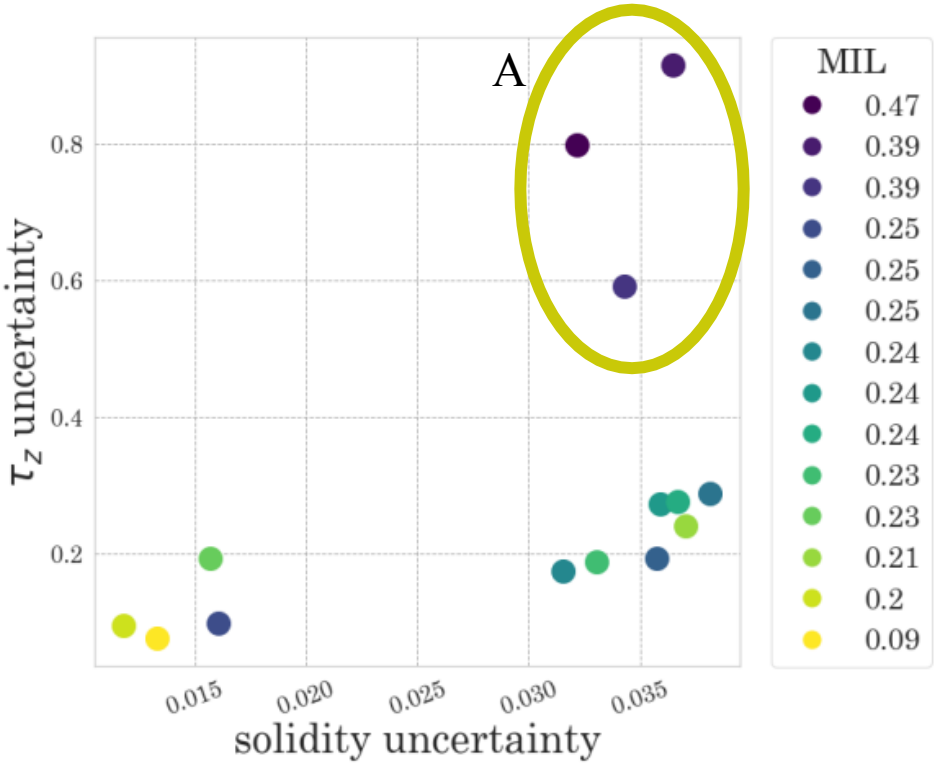
- Larger solidity uncertainties result in larger conductivity uncertainties.
- Independent of structural anisotropy

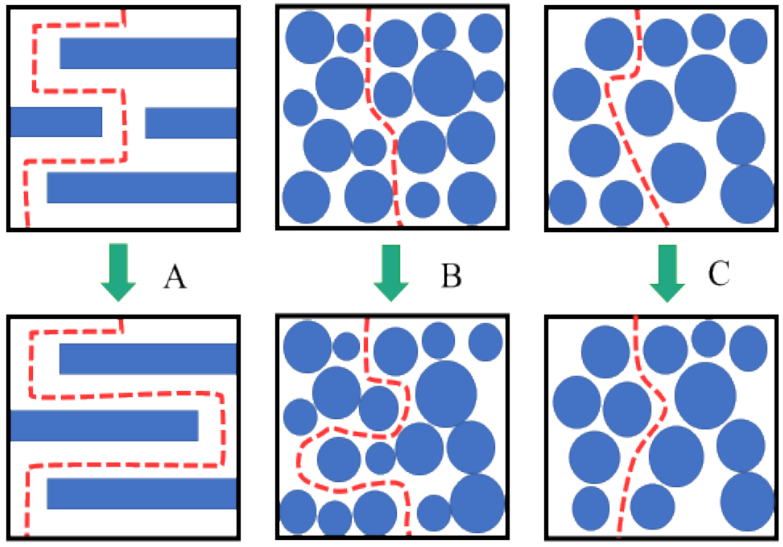


- Larger solidity uncertainties result in larger conductivity uncertainties.
- Highly anisotropic structures resulting in higher uncertainties.

Microstructural Influences

- Tortuosity is more sensitive to morphology changes than solidity changes.
- Conductivity us less sensitive to morphology changes compared to solidity changes.

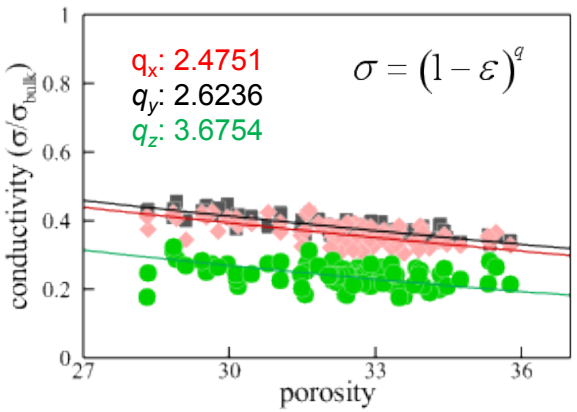




Geometric Uncertainty Propagation in Conductivity

Bruggeman Approximation

Conductivity can be fit to a Bruggeman approximation.



In the limit,

$\varepsilon \rightarrow 0\%$
$\sigma/\sigma_{bulk} \rightarrow 1$

$\varepsilon \rightarrow 100\%$
$\sigma/\sigma_{bulk} \rightarrow 0$

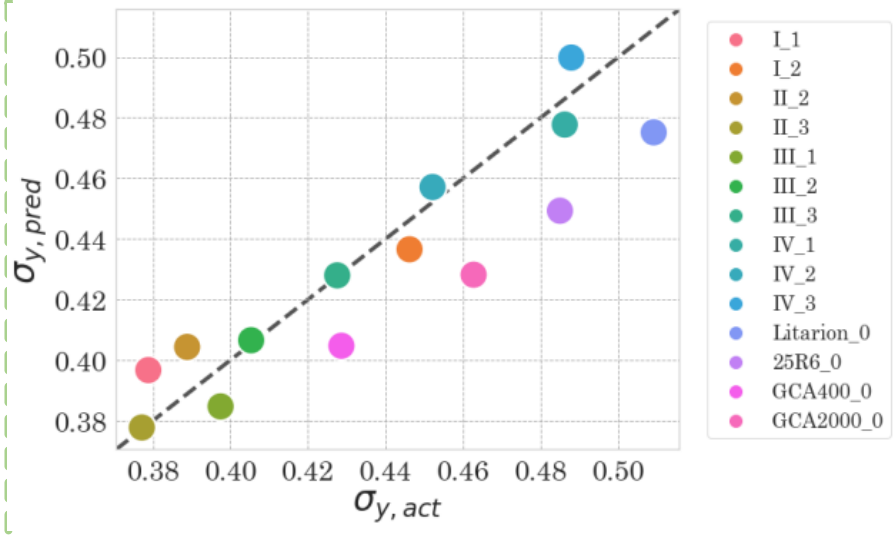
conductivity variability in IIc

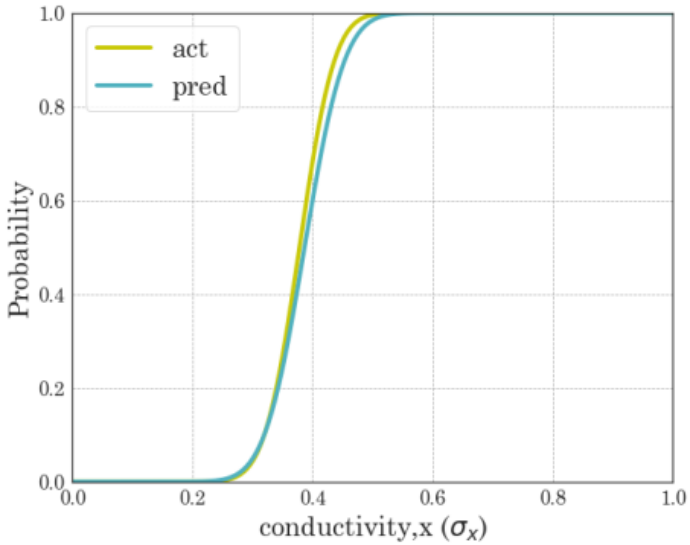
Uncertainty Propagation

Using the following identity of uncertainty propagation:

$$\delta F = |F'(x)|\delta x$$

$$\delta\sigma = |-qs^{q-1}|\delta s$$

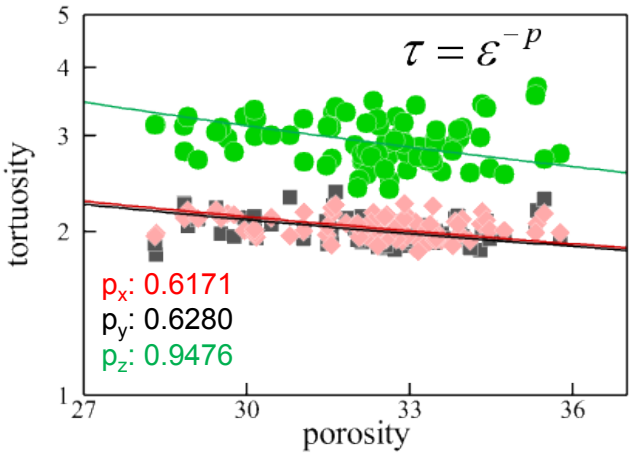




Geometric Uncertainty Propagation in Tortuosity

Bruggeman Approximation

Tortuosity can be fit to a Bruggeman approximation.



In the limit,
$\varepsilon \rightarrow 100\%$
$\tau \rightarrow 1$

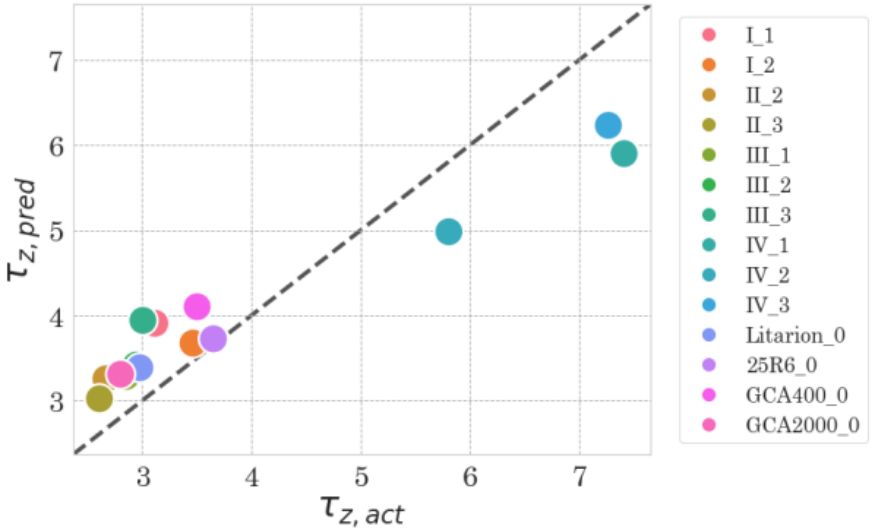
tortuosity variability in IIc

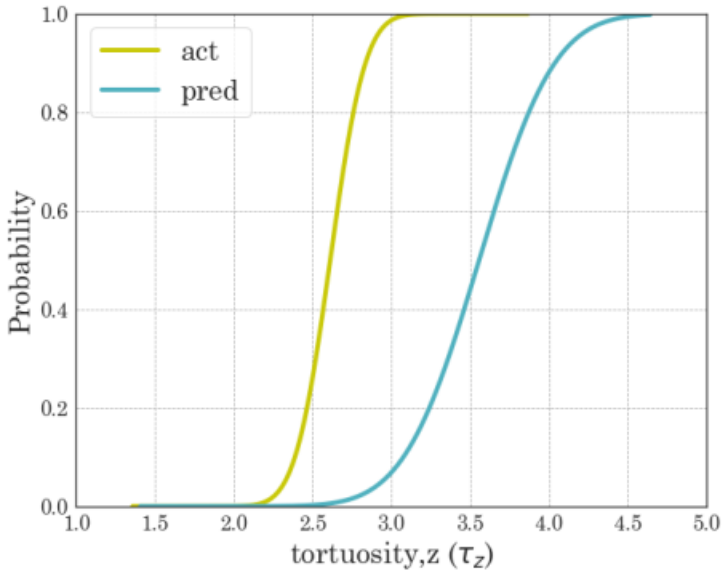
Uncertainty Propagation

Using the following identity of uncertainty propagation:

$$\delta F = |F'(x)|\delta x$$

$$\delta\tau = |-\mathrm{p}(1-s)^{-p-1}|\delta\mathrm{s}$$





Conclusion

- Correlations were found in image-quality- geometric, and physics quantity uncertainties.
- Image-quality was not able to be used for uncertainty propagation.
- Structural morphology impacted geometric uncertainty propagation to physics quantities.
- Using Bruggeman approximation, physics quantity uncertainties were predicted to a successful degree.

Acknowledgements

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Scott Roberts and team

Sandia National Laboratories