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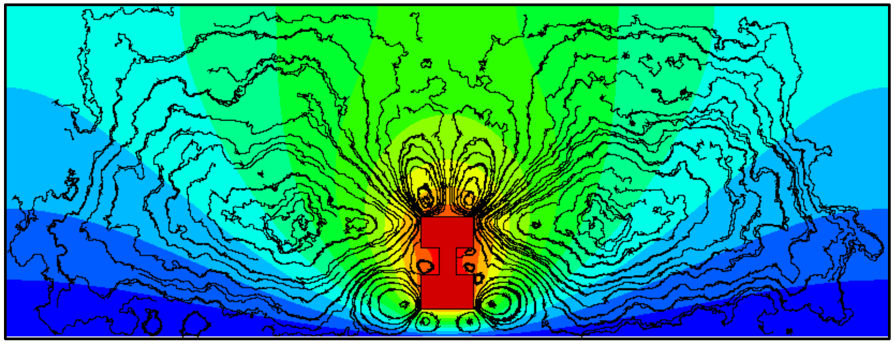

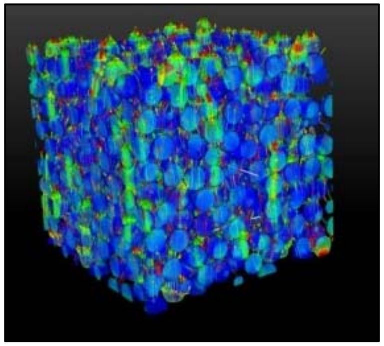

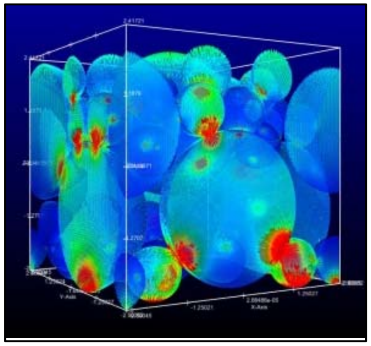

Uncertainty Quantification for Multiscale Thermal Transport Simulations

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June 2014

U.S. DEPARTMENT OF ENERGY NNSA

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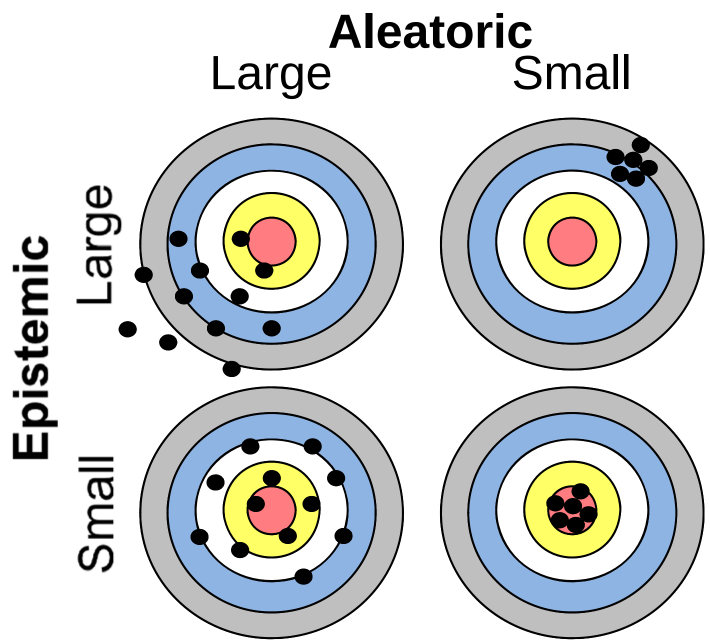
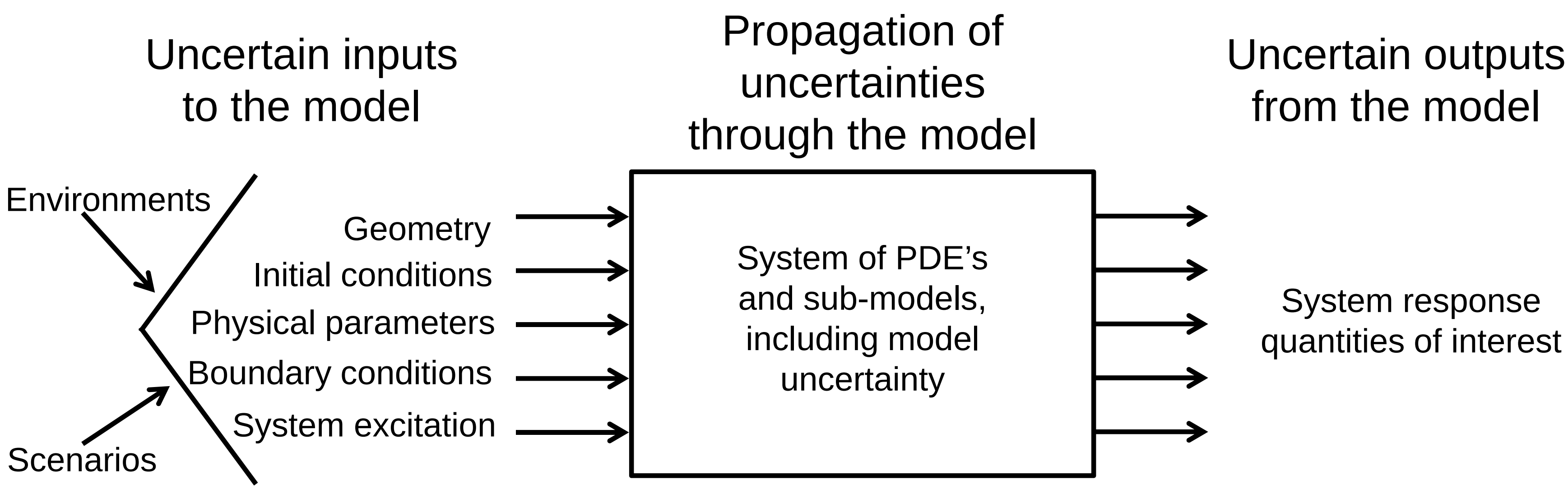
V&V and UQ

Verification ensures that the simulation mathematics and code are correctly computing the solution to the model equations.
Validation is the assessment of the accuracy of a computational simulation by comparison with experimental data.
Uncertainty Quantification assesses the statistical range by which a simulation result differs from the true value.
Aleatoric and Epistemic Uncertainties



Adapted from: Chernatynskiy, Phillpot, and LeSar, *Annu. Rev. Mater. Res.*, **43**, pp. 157-182, 2013.

Uncertainty Quantification (UQ)

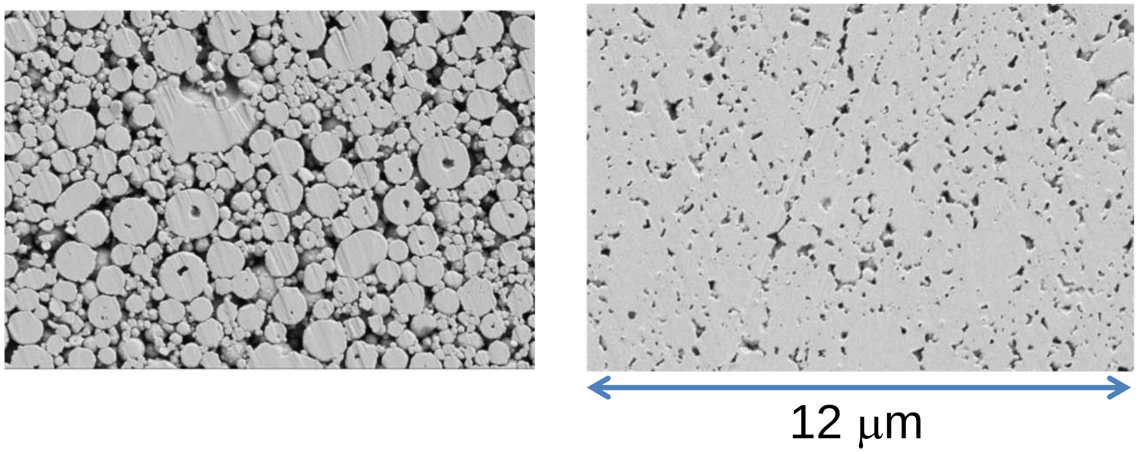


Classification of Uncertainty

- Aleatory – the inherent variation in a quantity that, given sufficient samples of the stochastic process, can be characterized via a probability density function
- Epistemic – uncertainty due to a lack of knowledge by the modelers, analysts conducting the analysis, or experimentalists in validation

Roy and Oberkampf, *Computational Methods in Applied Mechanics and Engineering*, **200**, pp. 2131-2144, 2011.

Thermal Transport in Powder Explosives



Local hot spots very important in powder explosives – need to know variability.

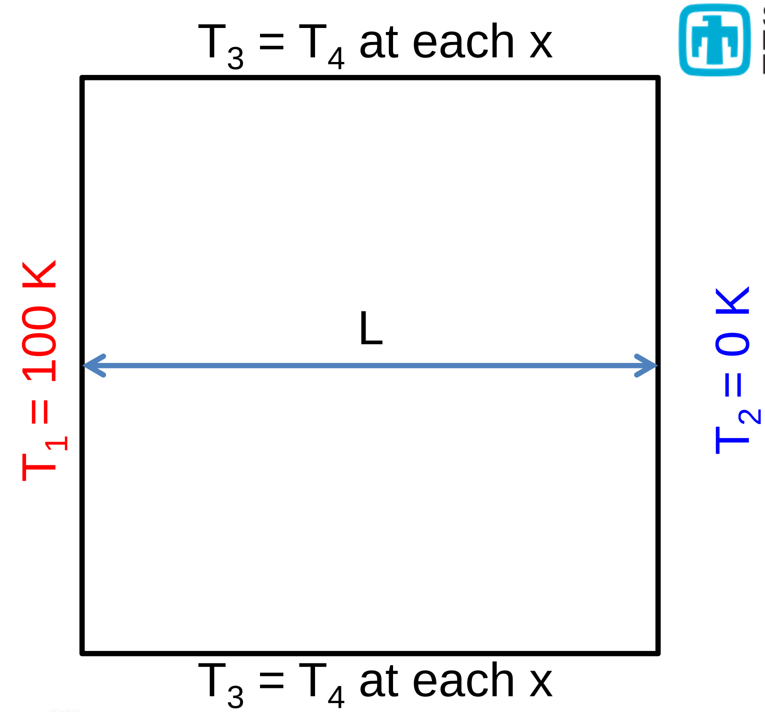
How does the microstructure affect the uncertainty in thermal transport simulations for heterogeneous materials?

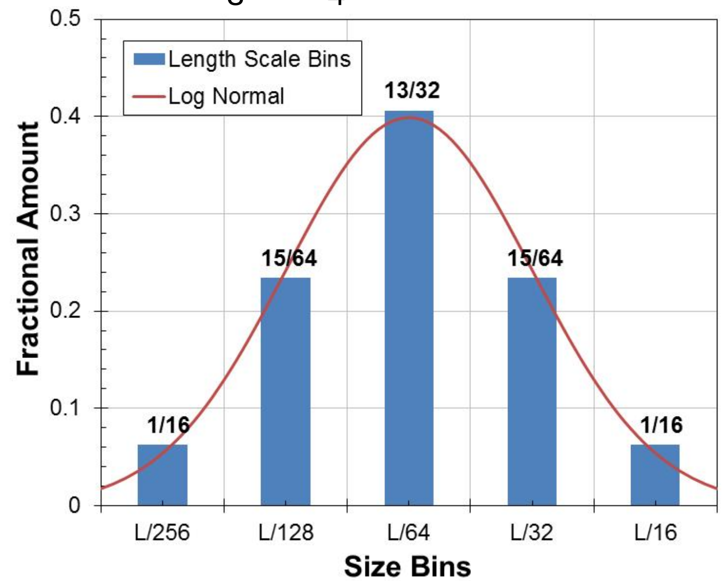
Simulations

- Steady state simulations

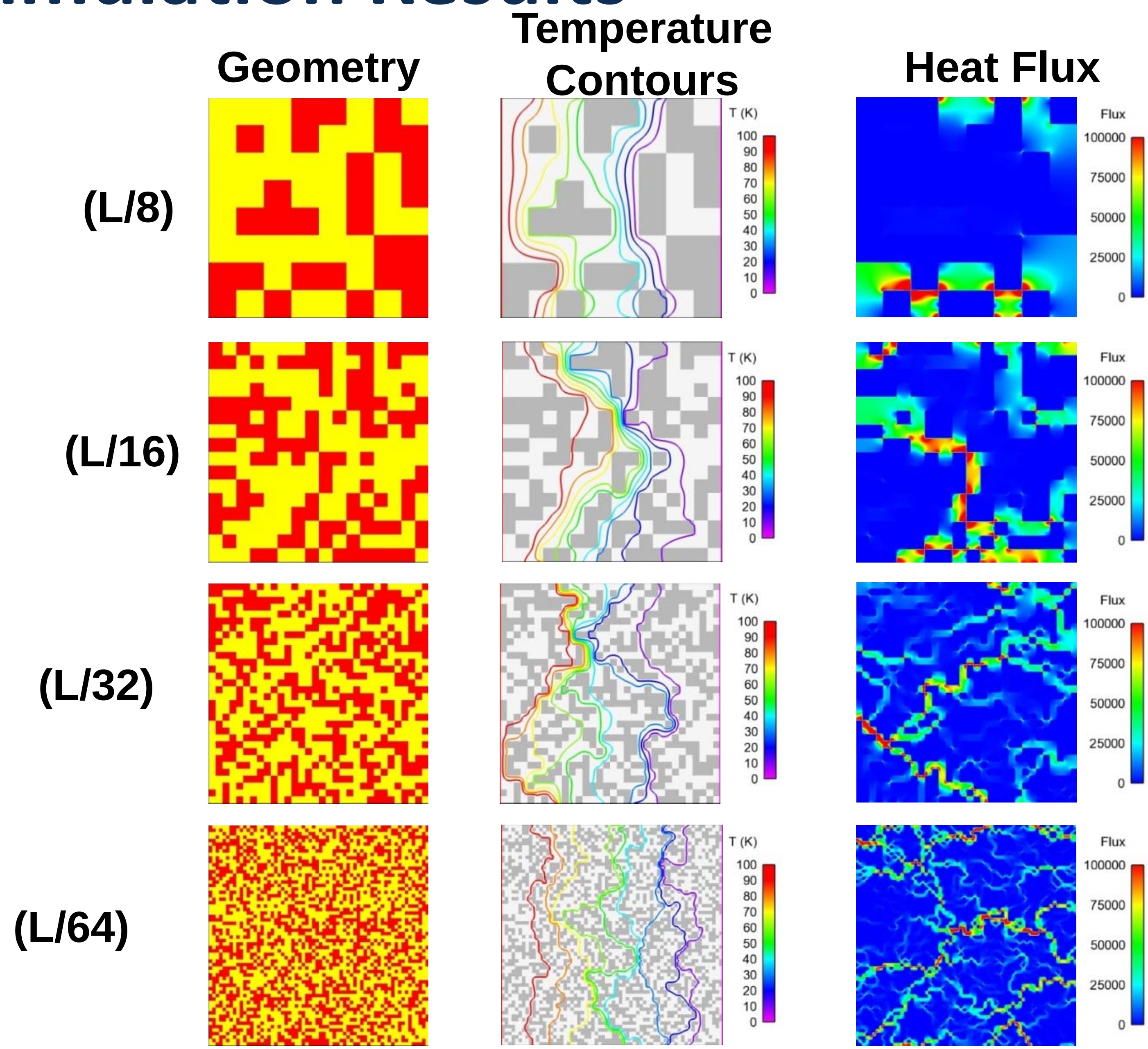
$$T(x) = T_1\left(1 - \frac{x}{L}\right)$$

- L = 5.12 cm, grid 512x512 elements, grid size is 0.01 cm
- Material A: high density, high thermal conductivity
- Material B: low density, low thermal conductivity
- Feature sizes varied from L/8 to L/256, one log-normal mixture
- Volume fractions varied from all A to all B
- Used SNL's Sierra-Aria code





Simulation Results



f_A=0.4375
f_B=0.5625

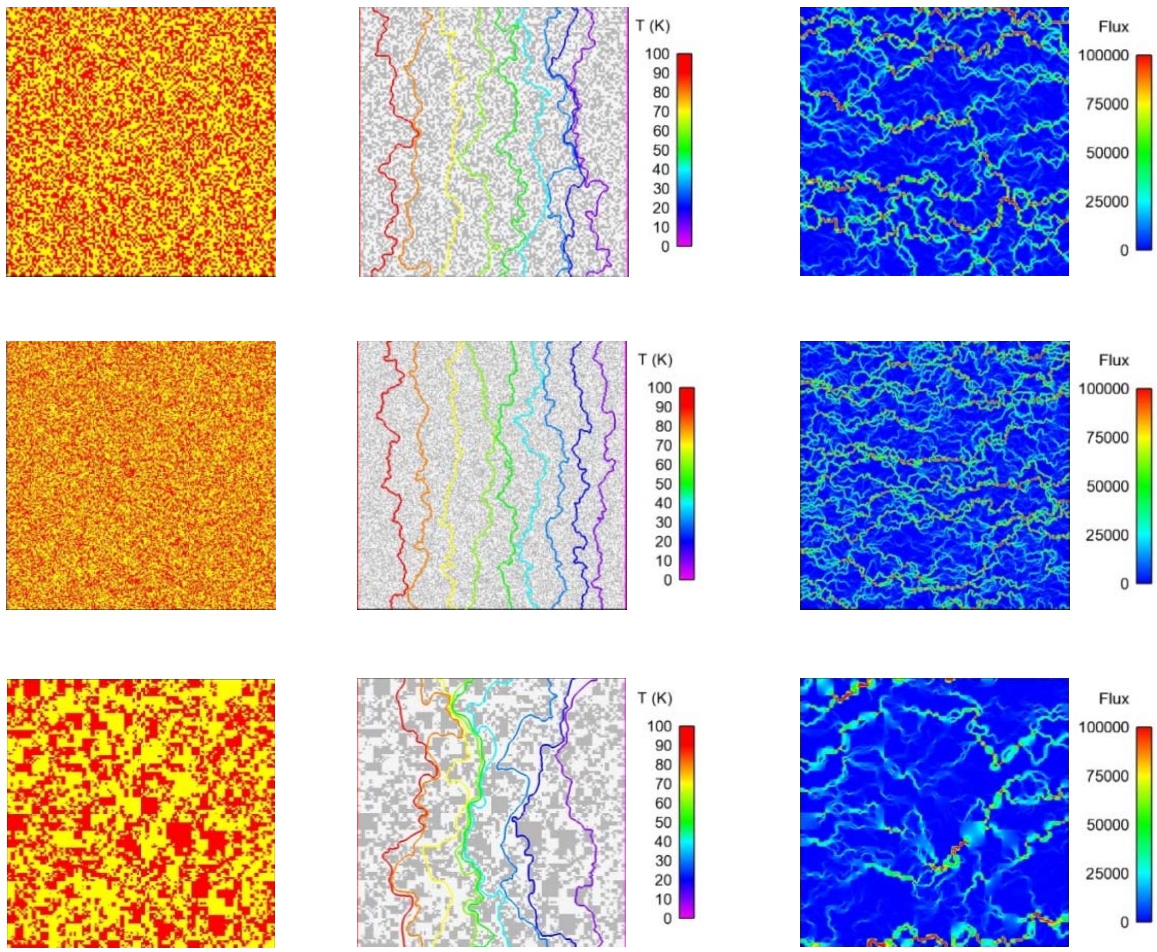
Simulation Results

Geometry | Temperature Contours | Heat Flux

(L/128)

(L/256)

(Log-normal mixture)



f_A=0.4375
f_B=0.5625

Temperature and Standard Deviation

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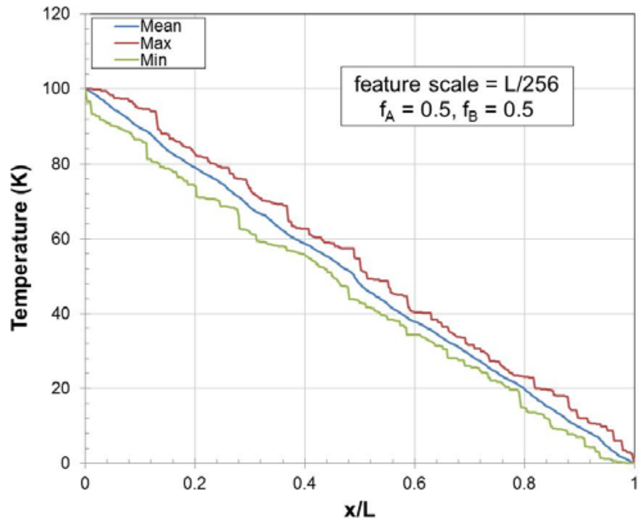
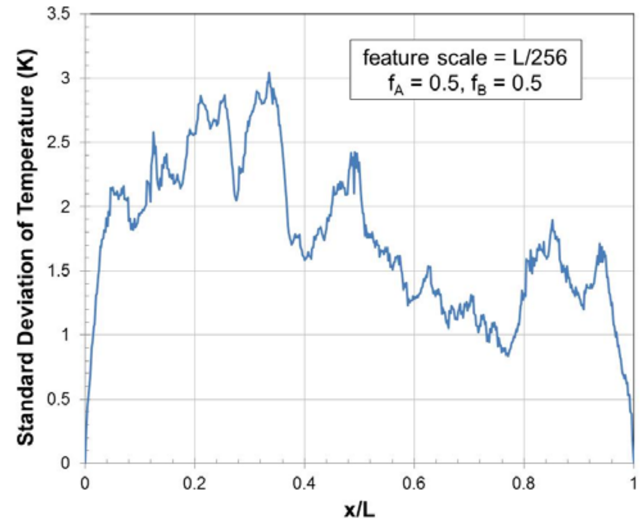
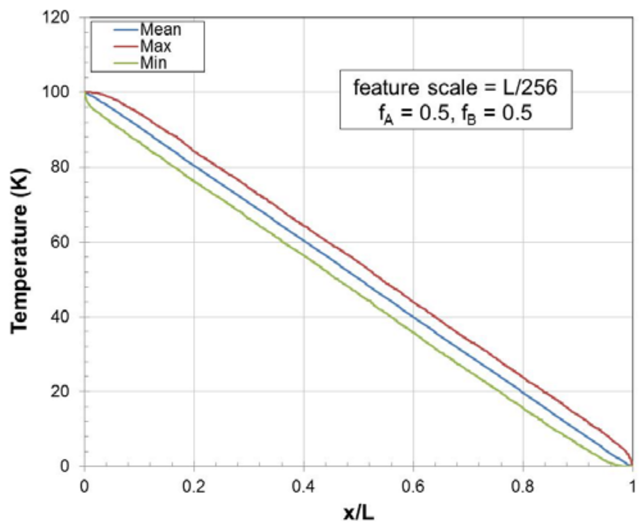
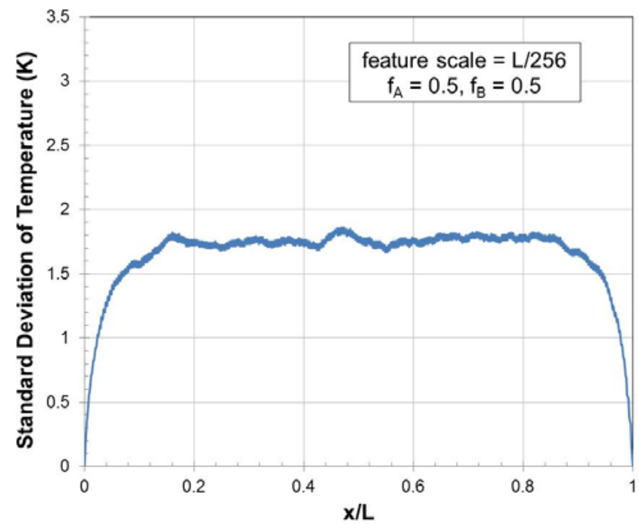
1 realization



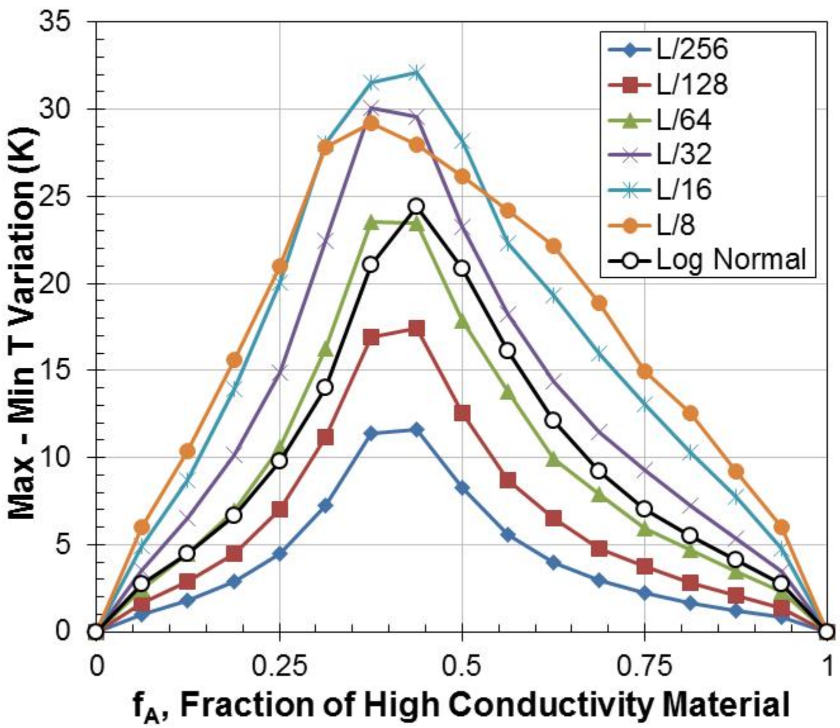


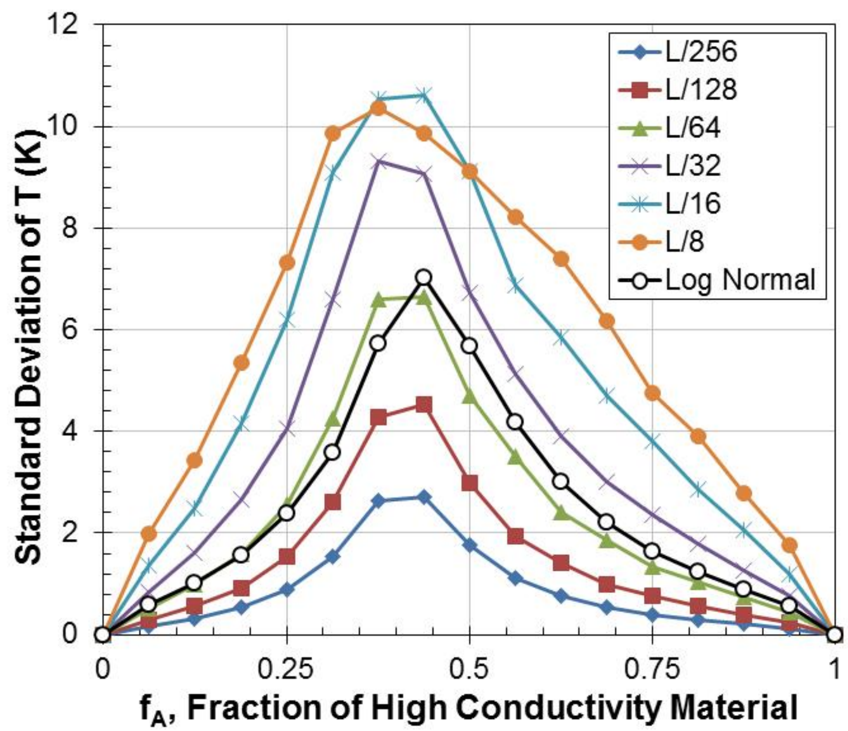
100 realizations





Variation as a Function of Volume Fraction and Feature Length Scale





Effective Medium Theory Expressions

Symmetric $$f_A \frac{(\lambda_A - \lambda_{mix})}{(\lambda_A + (d-1)\lambda_{mix})} + f_B \frac{(\lambda_B - \lambda_{mix})}{(\lambda_B + (d-1)\lambda_{mix})} = 0$$

Asymmetric $$\frac{(\lambda_{mix} - \lambda_A)^d}{\lambda_{mix}} = \frac{(1 - f_A)^d (\lambda_B - \lambda_A)^d}{\lambda_B}$$

Asymmetric $$\frac{(\lambda_{mix} - \lambda_B)^d}{\lambda_{mix}} = \frac{(1 - f_B)^d (\lambda_A - \lambda_B)^d}{\lambda_A}$$

Parallel $$\lambda_{mix} = f_A \lambda_A + f_B \lambda_B$$

Series $$\lambda_{mix} = \frac{1}{f_A/\lambda_A + f_B/\lambda_B}$$

Effective Thermal Conductivity as a Function of Fraction of the Material A

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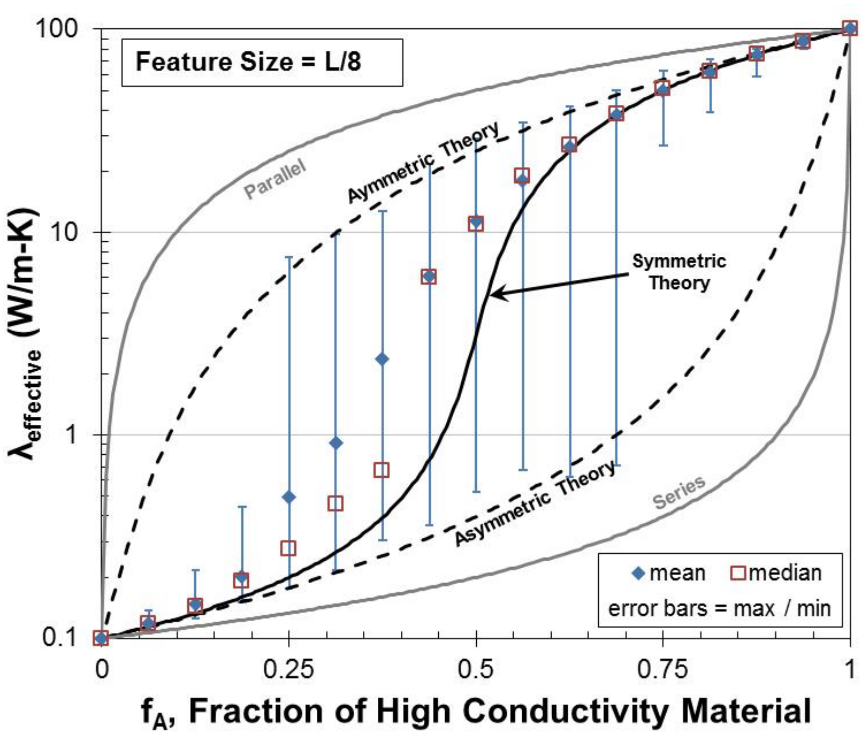
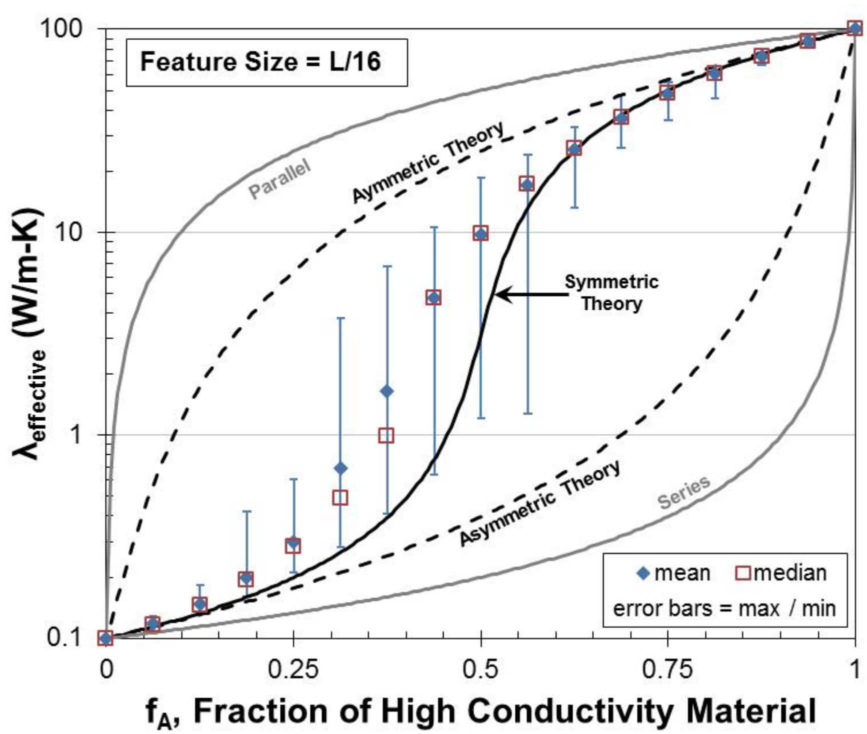
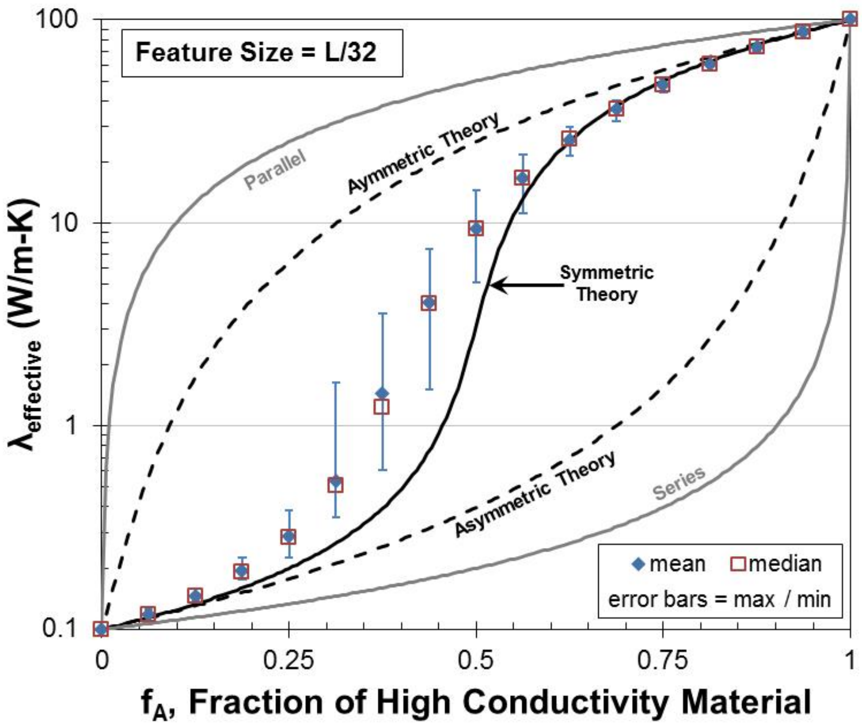
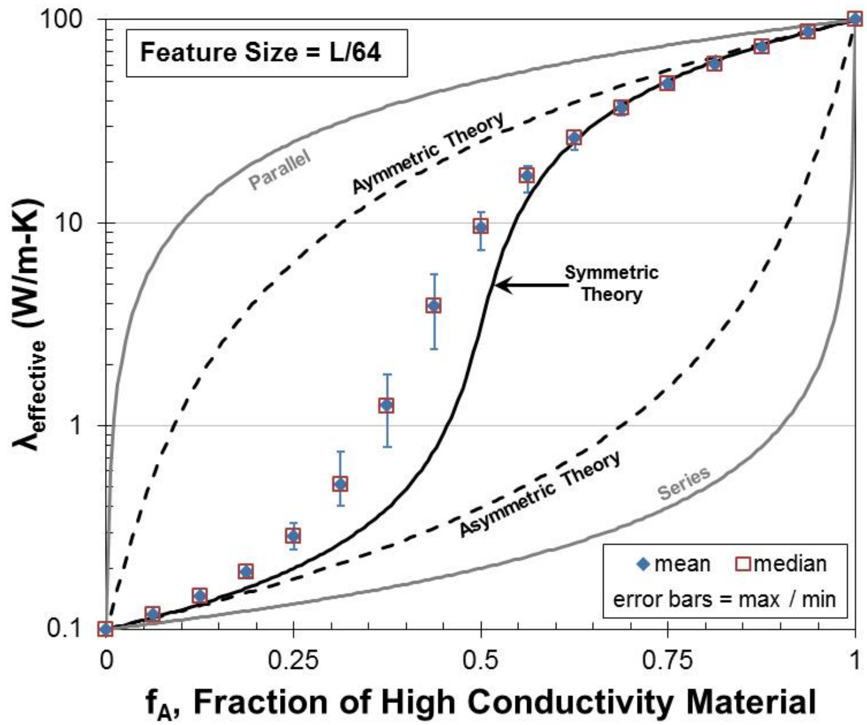




Effective Thermal Conductivity as a Function of Fraction of the Material A





Effective Thermal Conductivity as a Function of Fraction of the Material A

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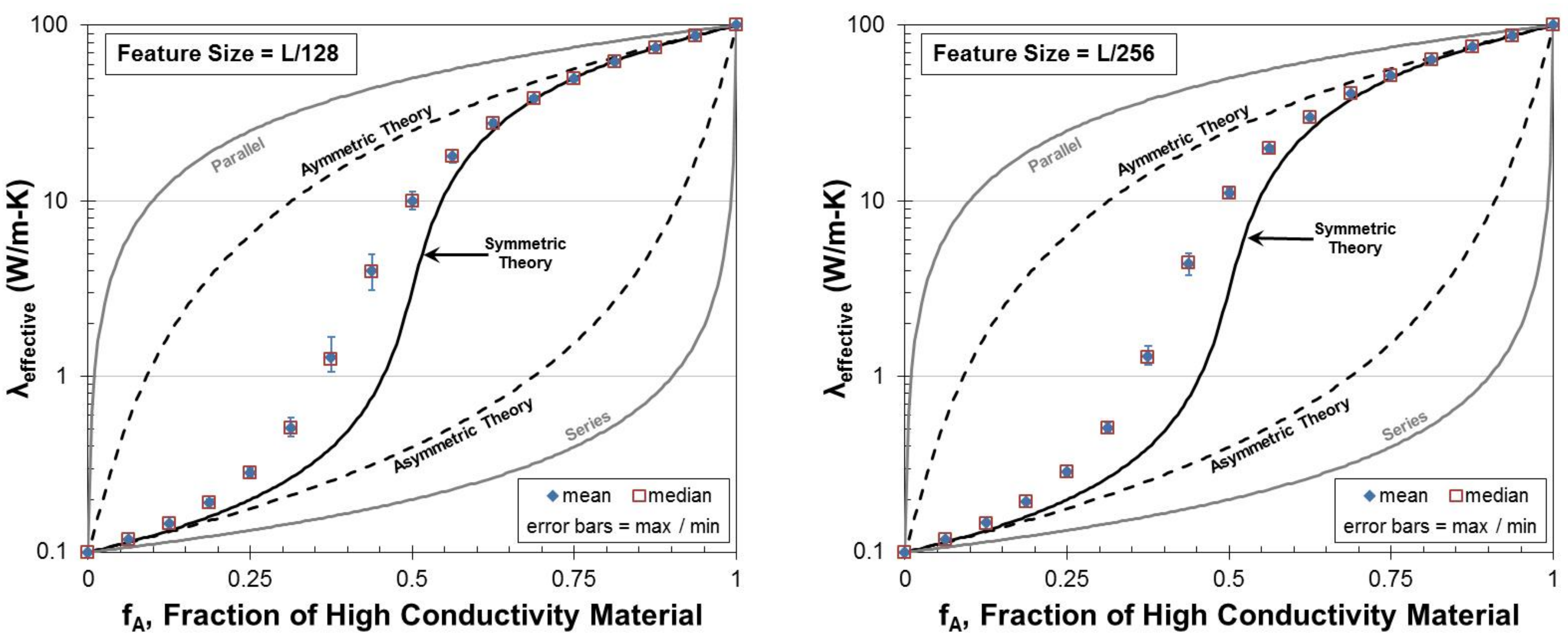


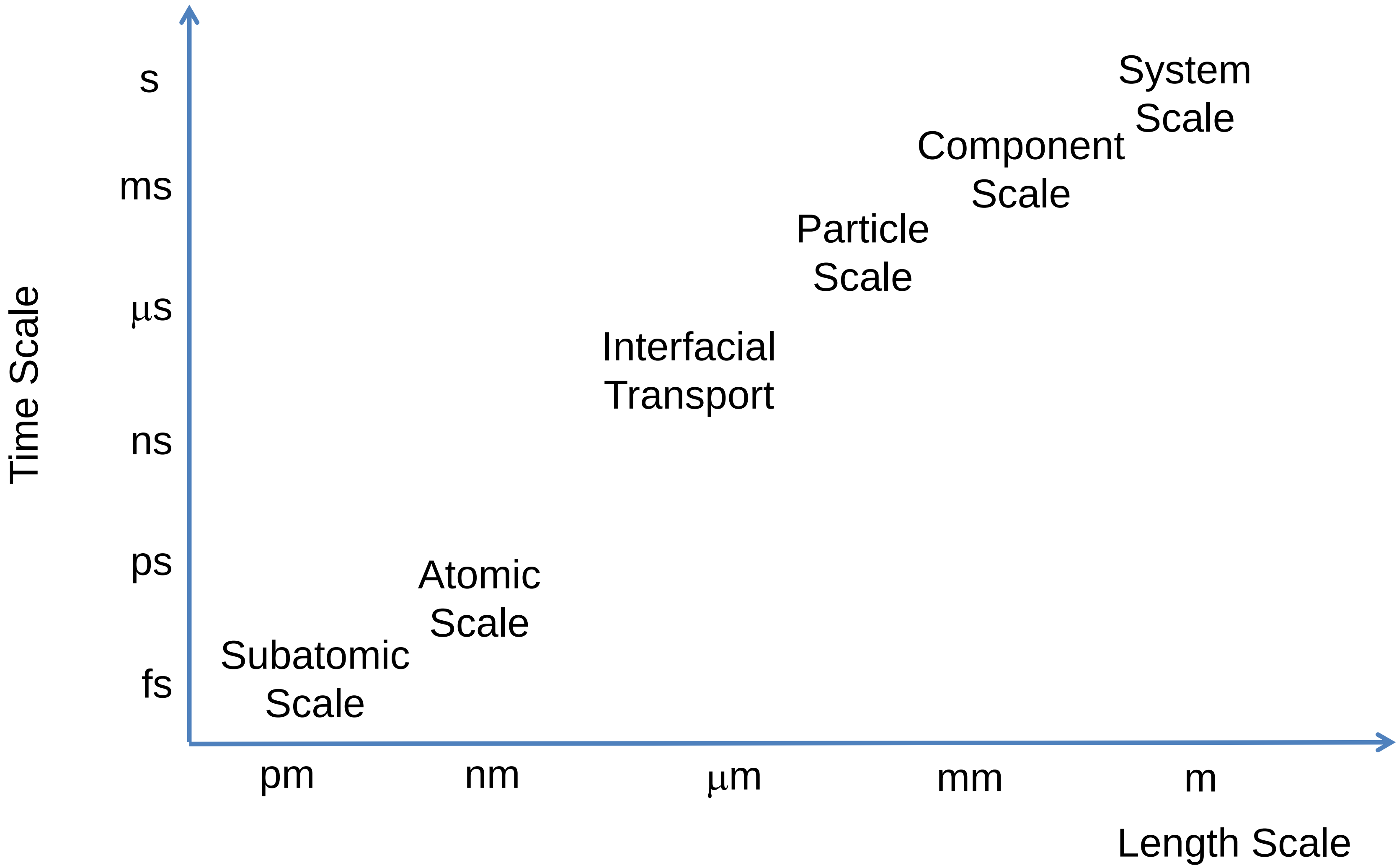
Summary

- Uncertainty quantification techniques suitable for multiscale heat transfer simulations are needed.
- Steady state heat transfer simulations of a two component provide insight into the aleatoric uncertainty inherent in heterogeneous materials.
- A peak in the uncertainty was observed near the percolation threshold of $f_A \sim 0.4$ and decreased by a factor of 2 from the peak for f_A's greater than 0.75 or less than 0.25.
- Uncertainties in max.-min. T's are around 30K for coarser structures: L/8, L/16, and L/32, and as much as 10K for the finest feature of L/256.
- Statistical representations are needed for the aleatoric uncertainty in heterogeneous materials that can be retained and passed between scales.

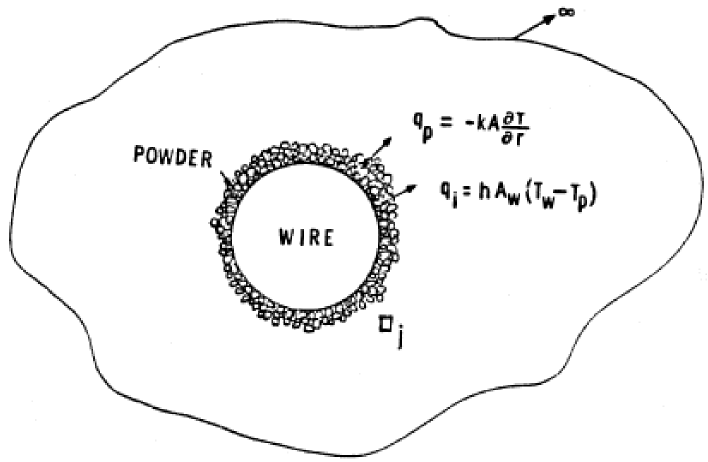
Acknowledgments

- Sandia National Laboratories Laboratory Directed Research and Development (LDRD) funding.

Multiscale Modeling

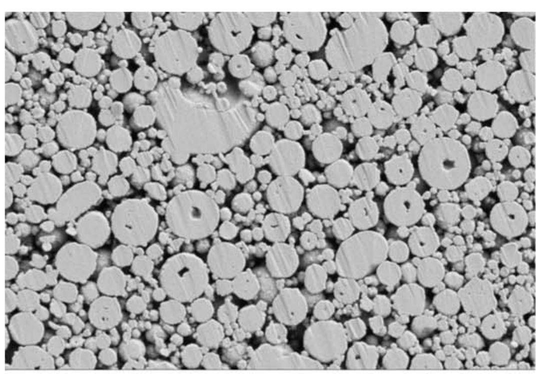


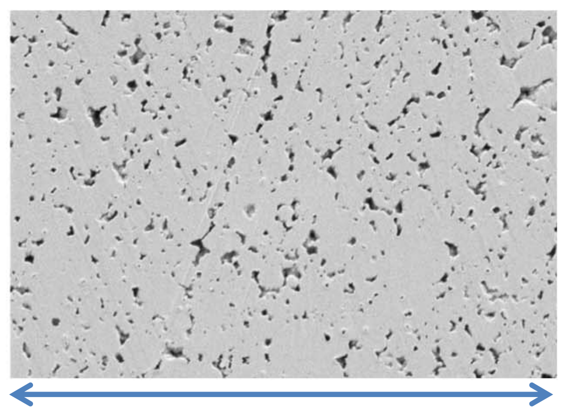
Transport in Heterogeneous Powders



$$\iint_V (i^2R)_j\,dV = \iint_V \left(\rho C_p \frac{\partial T}{\partial t}\right)_j dV + \int_S \vec{q}\cdot d\vec{S}$$

HEAT GENERATION RATE	INTERNAL ENERGY INCREASE RATE	HEAT LOSS TO SURROUNDINGS





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