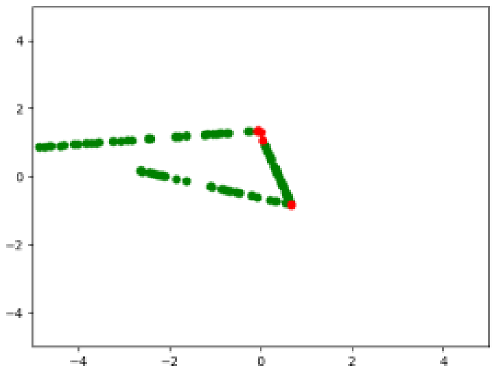
Paper #33784

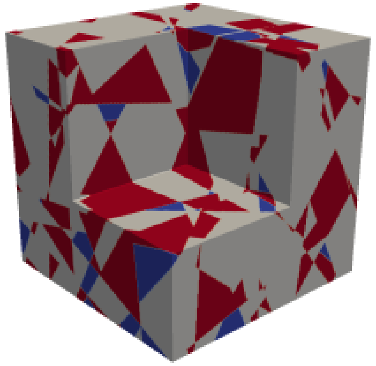
SAND2021-12157C

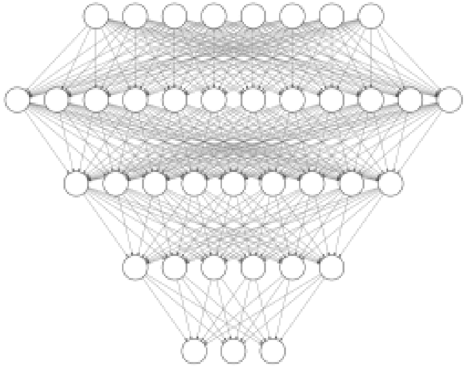
Sandia National Laboratories

LDRD
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Using Deep Neural Networks to Predict Material Types in Conditional Point Sampling Applied to Markovian Mixture Models







U.S. DEPARTMENT OF ENERGY
NNSA

PRESENTED BY

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Co-authors: Aaron Olson, Gabriel Popoola, Dan Bolintineanu, Theron Rodgers, and Emily Vu

SAND 2021-XXXXX

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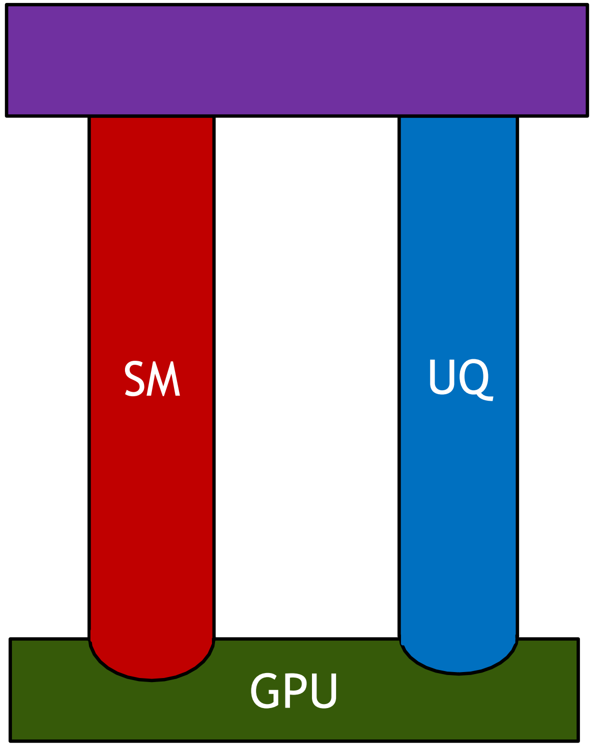
Overview: Next-Generation Monte Carlo Project

Develop efficient, embedded stochastic media (SM) and uncertainty quantification (UQ) Monte Carlo transport methods for the GPU.



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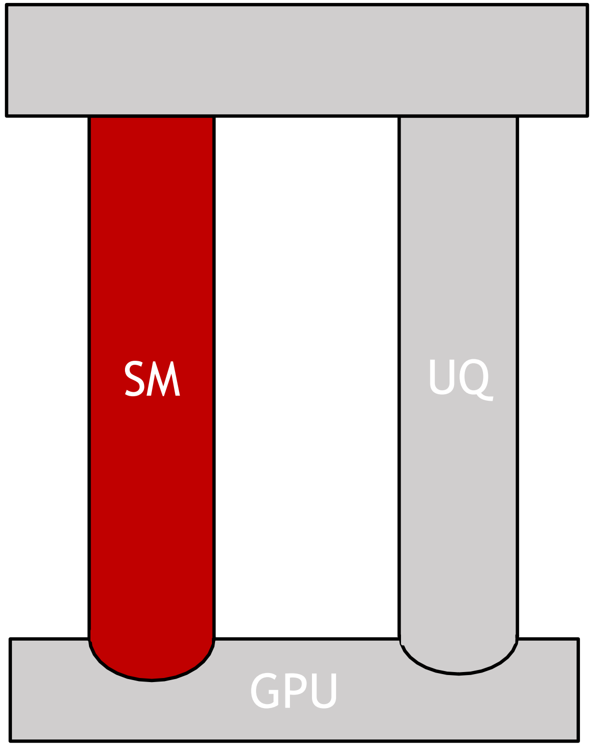


Overview: Conditional Point Sampling (CoPS)

Conditional Point Sampling (CoPS) - Monte Carlo stochastic media transport algorithm

- High accuracy in 1D and 3D for Markovian
- Can compute variance/PDFs of output
- M&C 2021 work:

CoPS for generalized mixing

CoPS memory/runtime efficiency

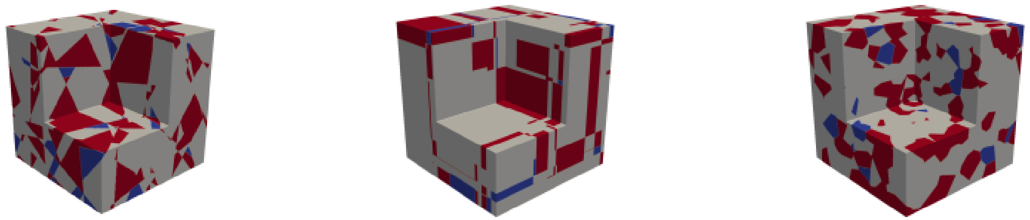
CoPS on the GPU

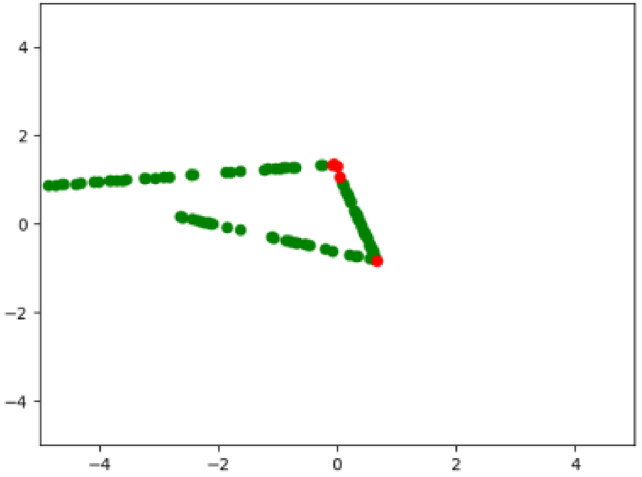
Radiation Transport Through Stochastic Media

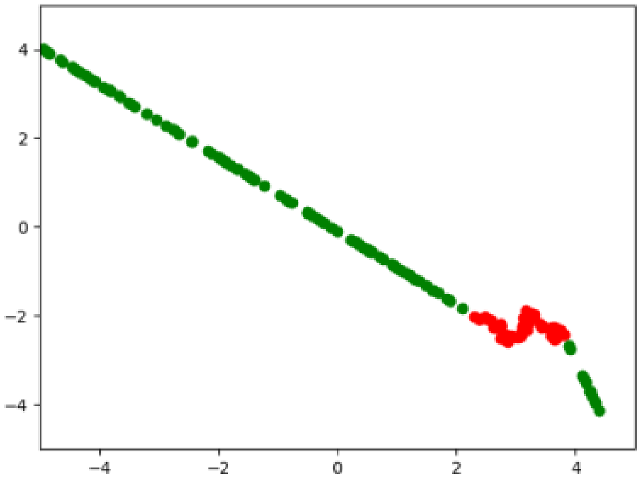
Radiation interacts with different materials in varying ways:

- Abundant, thin absorber
- Rare, heavy scatterer

How will radiation interact with a volume composed of a certain set of materials in a specific distribution and configuration?



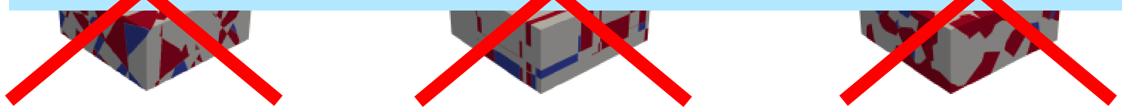


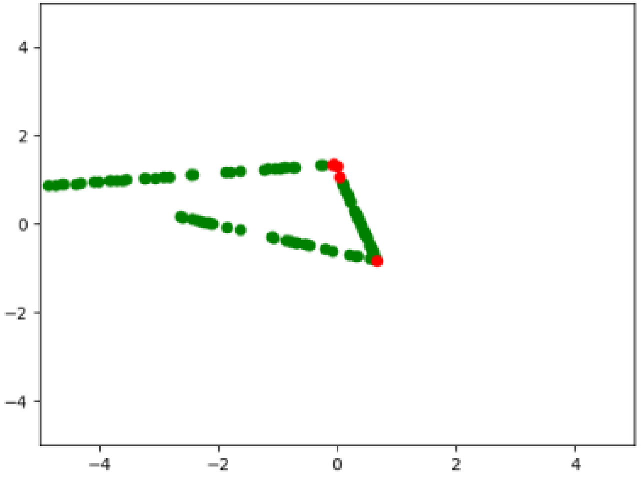


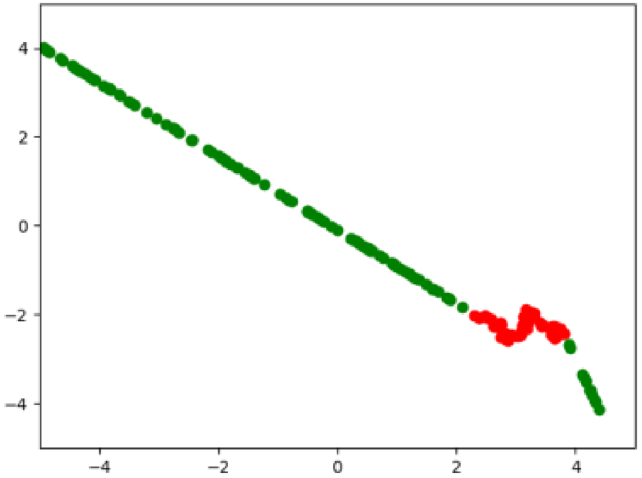
Predicting/Assessing Radiation Transport

- Manufacturing volumes and performing physical tests
  - Manufacturing costs, material availability, and equipment requirements can be prohibitive
- Numerical simulation
  - Effective, but can be computationally intensive
- Conditional Point Sampling (CoPS) utilizes a conditional probability function (CPF) that can be used as a substitute for running a full numerical simulation.

~~CoPS is a faster and more efficient way to predict radiation transport for stochastic materials.~~







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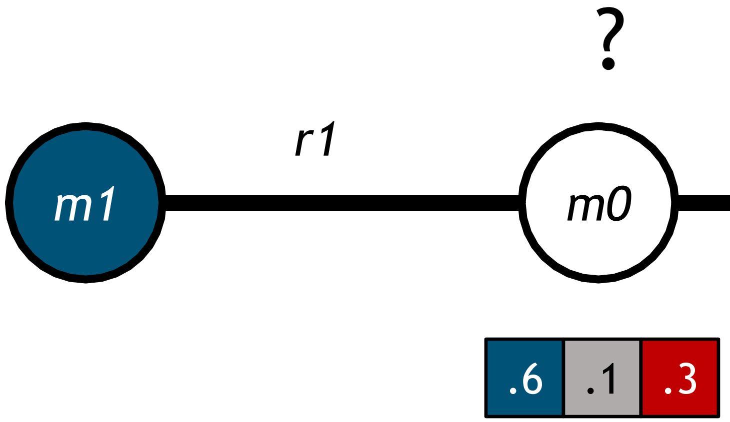
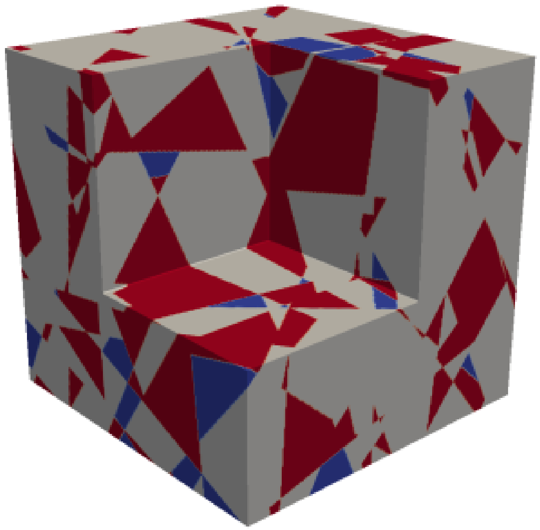
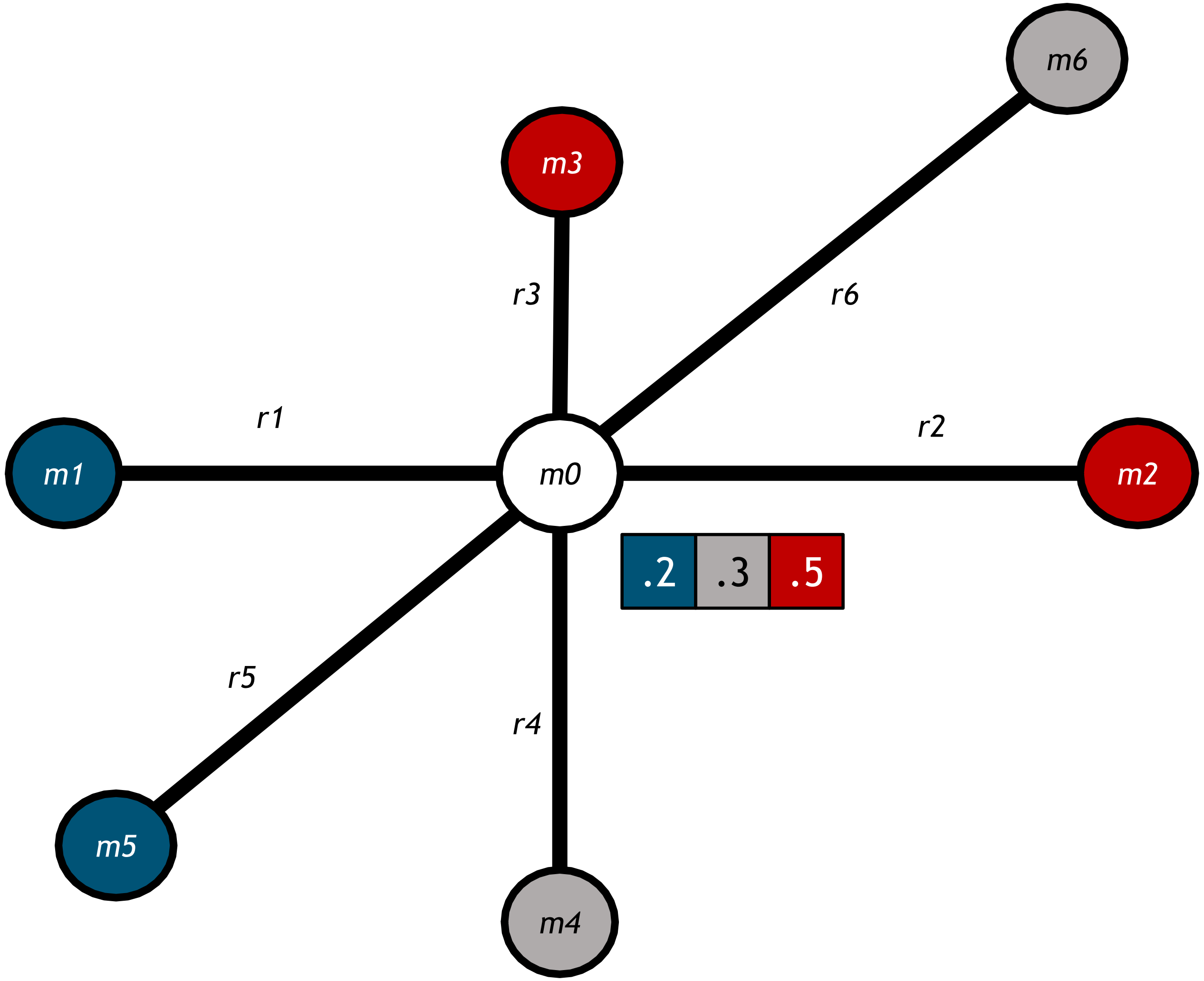
CoPS

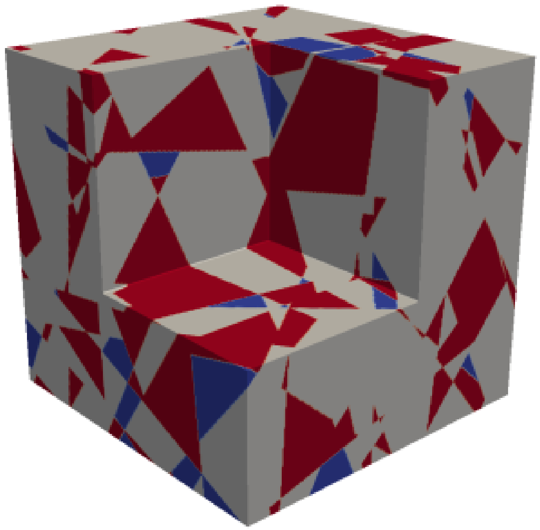
Determining Material Probabilities in 1-D





Determining Material Probabilities in 3-D





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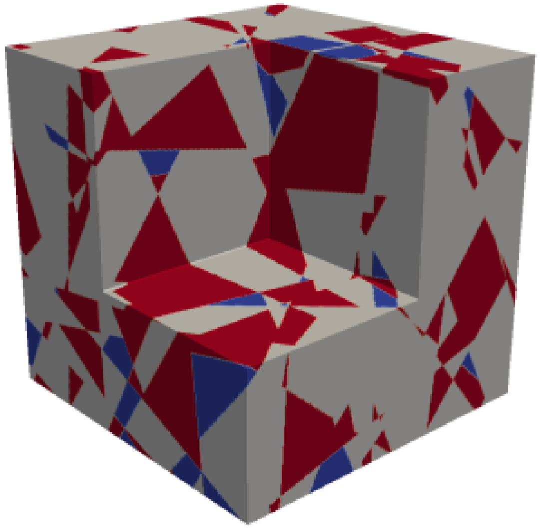
CoPS

Strengths and Limitations of CoPS CPFs

- Has been shown to be effective for Markovian.
  - Analytical CoPS solutions have been derived.
  - *CoPS3PO* produces errorless probability estimates for Markovian mixtures in certain sampling configurations.

- Innovative analysis was required to create a CoPS CPF for Markovian mixtures.

- Creating analytical CoPS CPF for other types of mixtures and sampling configurations may be hard to scale (if possible at all).

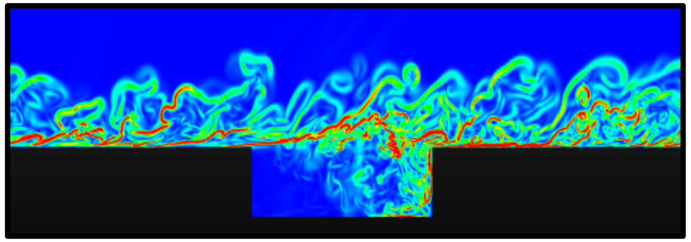


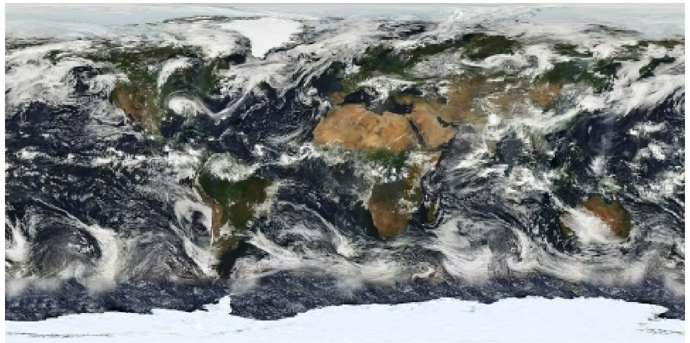
Is there a way to more easily develop accurate CPFs for generalized mixture models and sampling configurations?

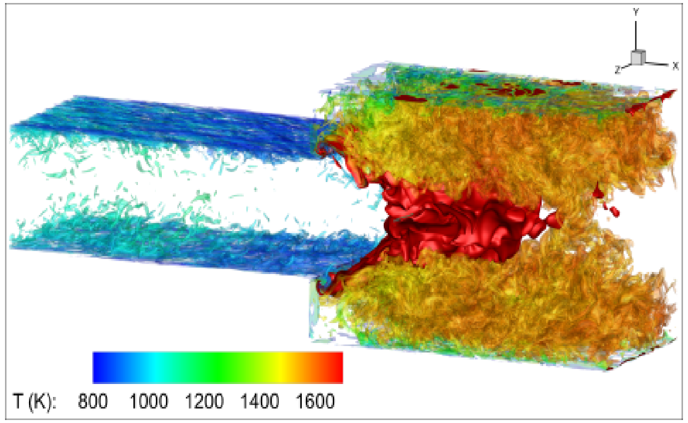
Using Artificial Intelligence to Extract CPFs from Material Data

- Artificial intelligence (AI) techniques can extract latent rules/information from large datasets.
- Utilized successfully in many scientific fields.
- We propose to use AI to extract CPFs in a data-driven manner, rather than analytically.

AI-based CPF development will provide scalable radiation transport prediction across mixture models and sampling configurations.







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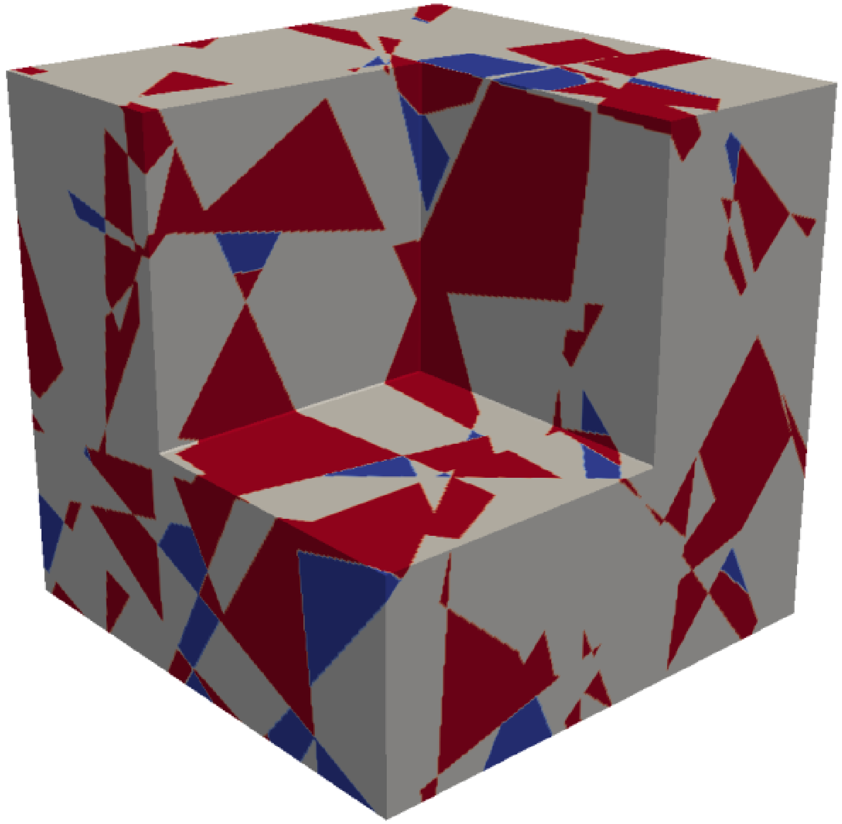
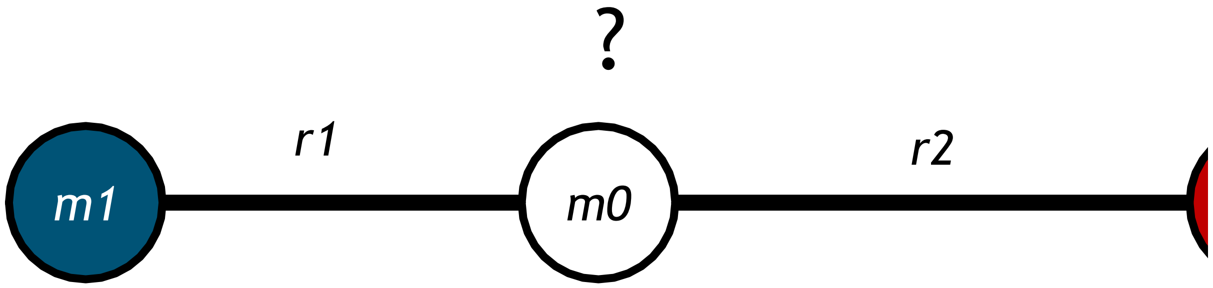
CoPS

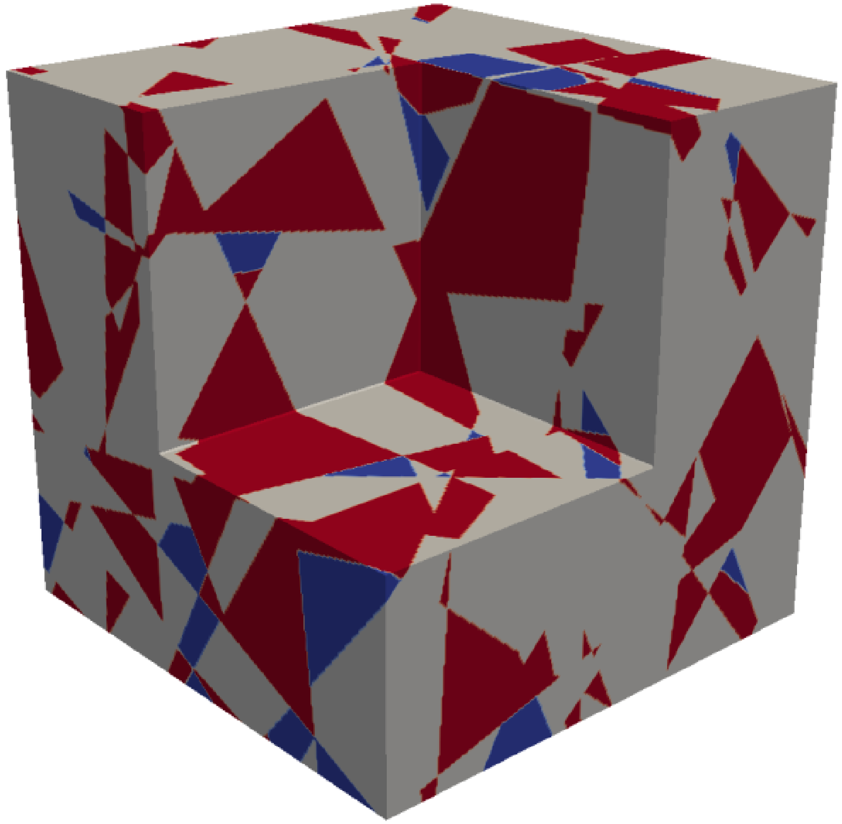
Material Realization Data

- Ternary Markovian mixtures
- 5 different realizations, created with the following parameters:
  - Λ_C = 20.8 grid points
  - Material abundances
    - p_0 = 6%
    - p_1 = 65%
    - p_2 = 29%
- 300^3 grid
  - 27,000,000 grid points
  - 90,000 (0.3%) for training
  - 30,000 (0.1%) for testing



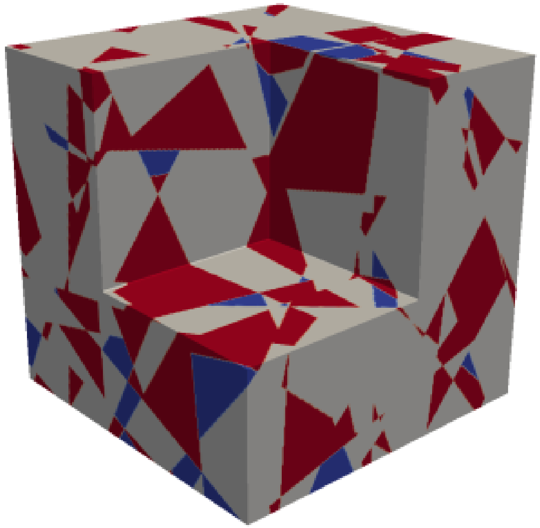
Data Representation for 1-D sampling





Example	m_0	m_1	r_1	m_2	r_2
1	0	1	7	0	5
2	2	2	12	1	13

Data Representation (One-Hot Encoding)

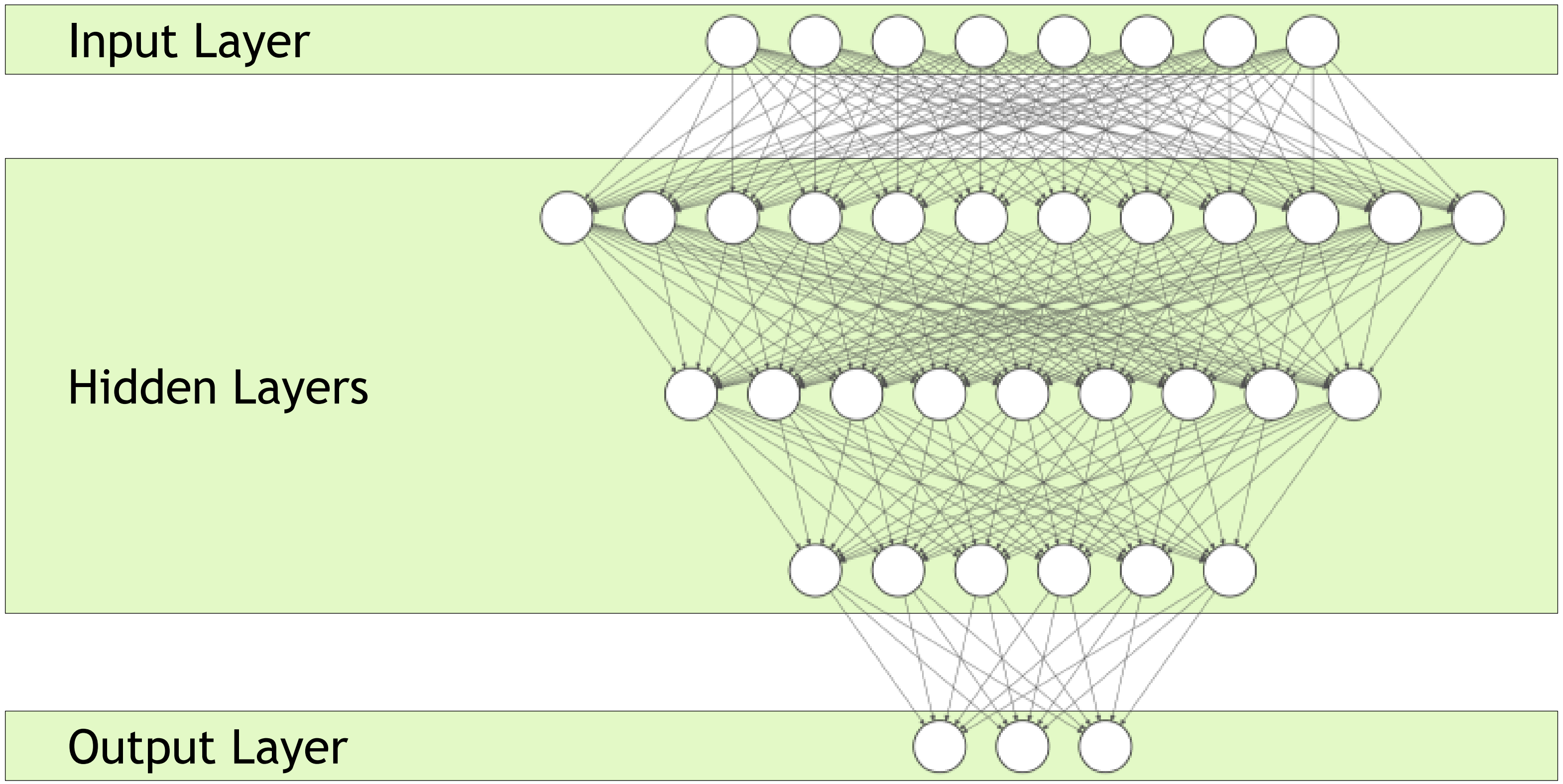


Example	m_0	m_1	r_1	m_2	r_2
1	0	1	7	0	5
2	2	2	12	1	13

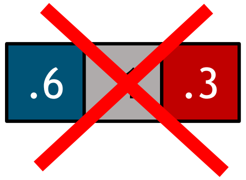
Exan	$n_{1,2}$	r_1	$m_{2,0}$	$m_{2,1}$	$m_{2,2}$	r_2
1	0	7	1	0	0	5
2	1	12	0	1	0	13

Neural Network Architecture

$m_{1,0}$	$m_{1,1}$	$m_{1,2}$	r_1	$m_{2,0}$	$m_{2,1}$	$m_{2,2}$	r_2
0	1	0	7	1	0	0	5
0	0	1	12	0	1	0	13



$m_{0,0}$	$m_{0,1}$	$m_{0,2}$
1	0	0
0	0	1



Implemented in Keras/Tensorflow

Layers: [8,*12,9,6*,3]

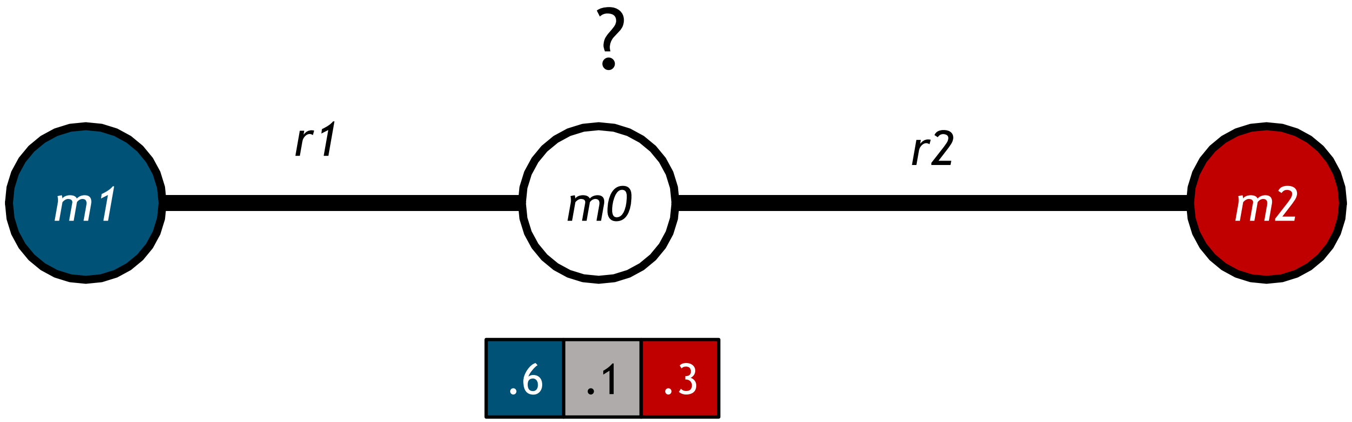
Optimizer : NAdam

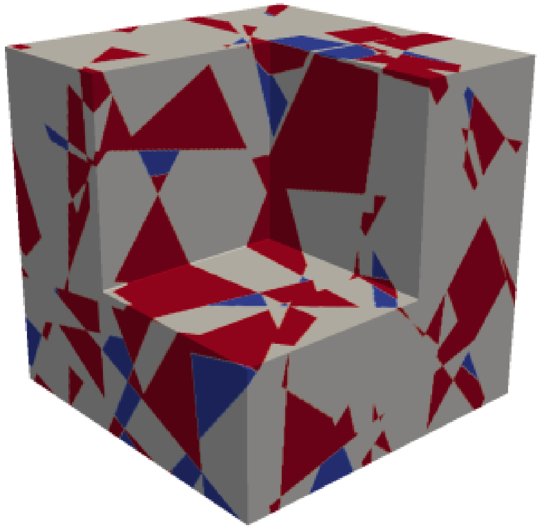
Activations (Hidden): ReLU

Activations (Output): Linear

Designed model was robust to mild changes in parameterization.

Experiments with 1-D Samples





- CoPS3PO provides Truth material probabilities
- CoPS2 provides high-quality baseline

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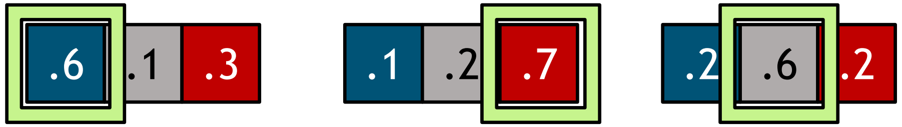
DNN Produced Accurate Material Predictions in 1-D

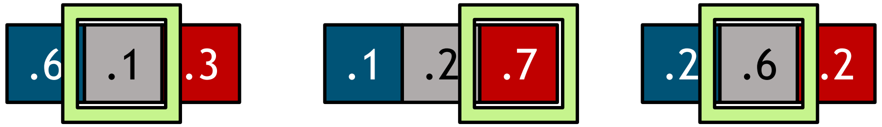
Higher accuracy values indicate better prediction performance.

Accuracy Basis: Highest Probability



Method	Real 0	Real 1	Real 2	Real 3	Real 4	Average
Truth	77.8	79.2	84.1	82.4	75.0	79.7
CoPS2	80.4	81.9	86.6	84.5	77.9	82.3
DNN	**83.9**	**86.5**	**89.6**	**87.1**	**81.9**	**85.8**

Accuracy Basis: Random Probabilistic Selection



Method	Real 0	Real 1	Real 2	Real 3	Real 4	Average
Truth	73.2	75.4	80.1	77.8	70.5	75.4
CoPS2	69.1	70.2	73.0	71.7	67.3	70.3
DNN	**76.4**	**78.7**	**84.9**	**80.7**	**72.3**	**78.6**

DNN CPFs were more accurate for predicting the material types than CoPS2 and the actual truth values.

DNN Produced CPFs Close to Truth Values in 1-D

Jensen-Shannon Divergence from Truth Values

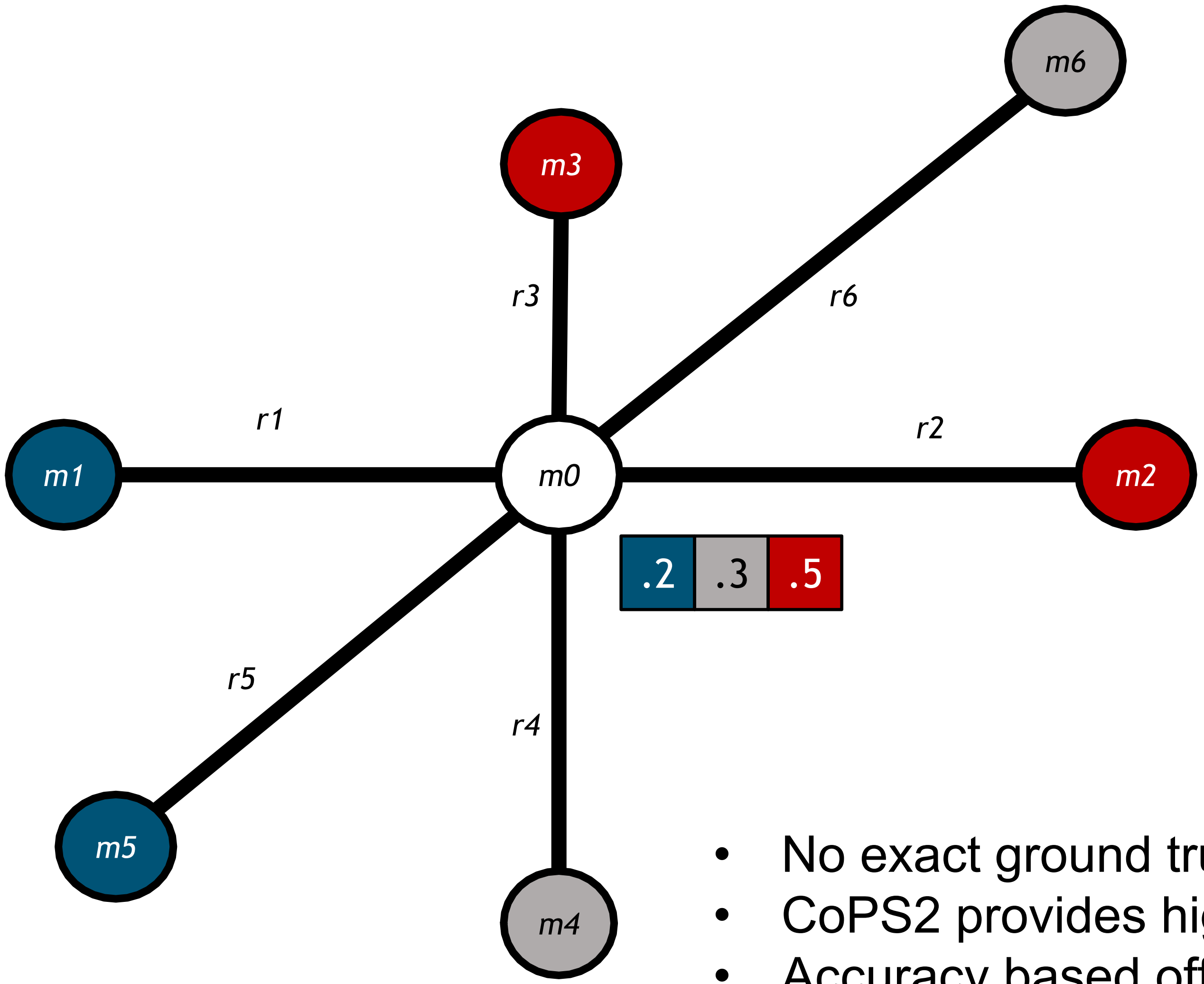
Method	Real 0	Real 1	Real 2	Real 3	Real 4	Average
CoPS2	**.147**	**.146**	.154	.151	**.147**	.149
DNN	.169	.153	**.112**	**.129**	.166	**.146**

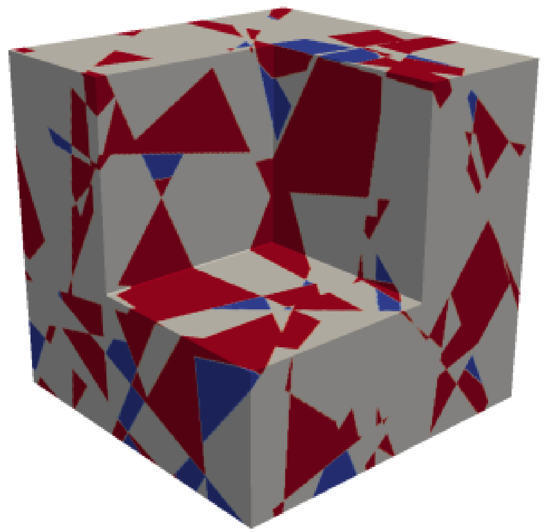
Lower divergence values indicate CPFs that are closer to the Truth Values.

On average, DNN CPFs were as close to the actual truth values as CoPS2.

However, DNNs produce much wider variance than CoPS2.

Experiments with 3-D Samples





- No exact ground truth material probabilities
- CoPS2 provides high-quality baseline
- Accuracy based off of Random Probabilistic Selection

DNN Produced Accurate Material Predictions in 3-D

Accuracy Basis: Random Probabilistic Selection

Method	Real 0	Real 1	Real 2	Real 3	Real 4	Average
CoPS2	80.5	80.0	83.4	81.0	79.5	80.9
DNN	**87.8**	**87.3**	**91.1**	**87.4**	**86.0**	**87.9**

Higher accuracy values indicate better prediction performance.

DNN CPFs were more accurate for predicting the material types than CoPS2.

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CoPS

DNN Inter-Realization Accuracies are Stable

Method	Real 0	Real 1	Real 2	Real 3	Real 4
Intra-Realization Inferencing	**87.8**	**87.3**	**91.1**	**87.4**	**86.0**
Inter-Realization Minimum	86.6	86.5	90.4	85.9	84.3
Inter-Realization Maximum	87.4	**87.3**	90.7	**87.4**	85.7
Inter-Realization Average	87.1	86.9	90.6	86.9	85.2

Higher values indicate better prediction performance.

DNN accuracies do not deviate greatly, even across different material realizations.

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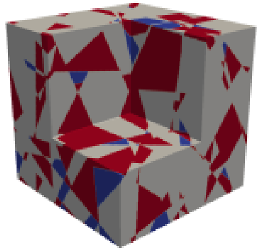
CoPS

Conclusions

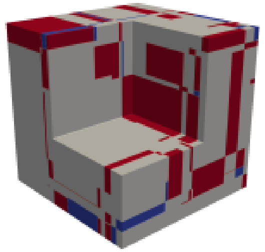
- DNNs were successful in deriving accurate CPFs for the 1-D and 3-D cases for Markovian by extracting latent information from material mixture realizations.

This research represents significant progress towards efficient and accurate development of CoPS CPFs for radiation transport in stochastic media using AI.

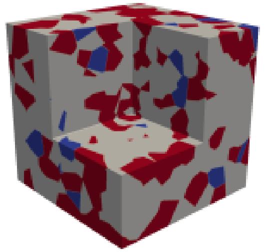
- We are expanding this methodology to generalized mixing types (e.g., Box-Poisson, Voronoi, etc.)



Markovian

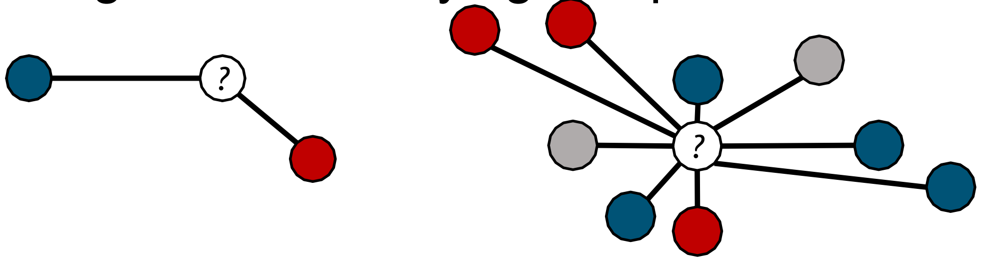


Box-Poisson



Voronoi

- We are extracting CPFs for varying sample densities and configurations.



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Develop efficient, embedded stochastic media (SM) and uncertainty quantification (UQ) Monte Carlo transport methods for the GPU.

CLS/LRP for three+ materials

Vu, Paper #33712
Transport in Stochastic Media I

Markovian three+ materials

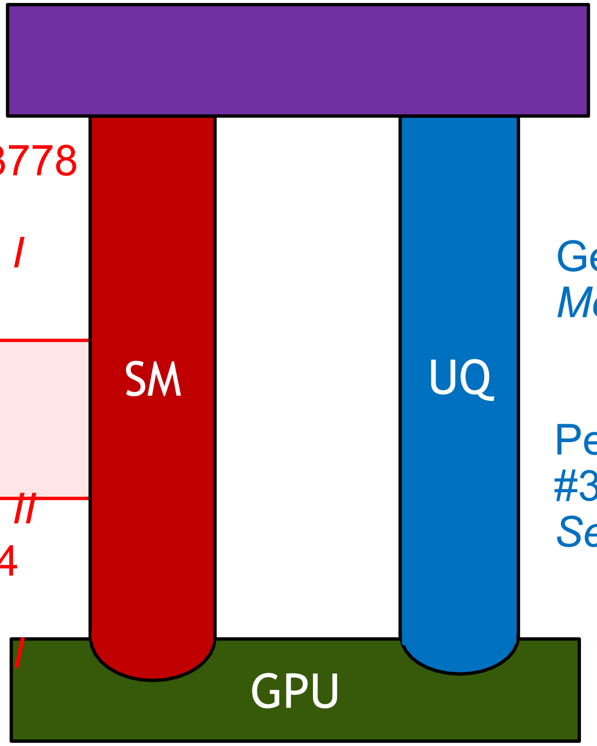
Olson, Paper #33778
Transport in Stochastic Media I

CoPS **for generalized mixing**

Davis, Paper #33784
Transport in Stochastic Media II

CoPS **memory/runtime efficiency**

Vu, Paper #33614
Transport in Stochastic Media I



Geraci, Paper #33671
Monte Carlo Methods

PCE surrogate models

Petticrew, Paper #33657
Sensitivity Analysis

Global sensitivity analysis

CoPS **on the GPU**

Kersting, Paper #33673
Monte Carlo Algorithms

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