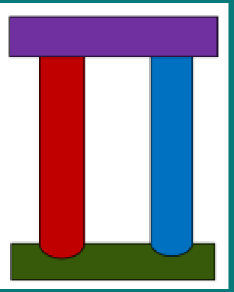
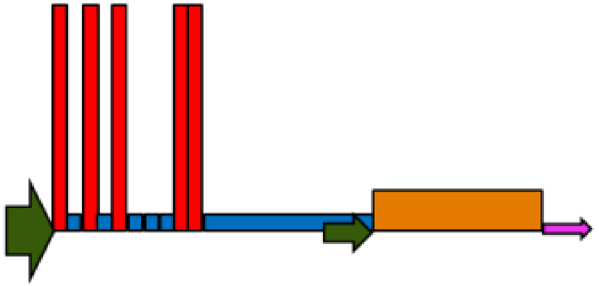
SAND2021-0911PE

LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Next Generation Uncertainty Quantification and Stochastic Media Monte Carlo Transport Methods





PRESENTED BY

Aaron Olson

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

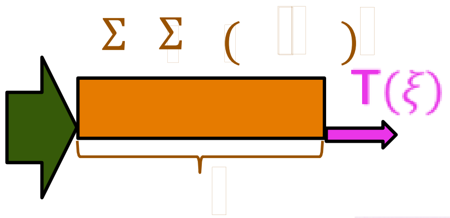
LDRD Summary

Develop efficient uncertainty quantification (UQ) and stochastic media (SM) Mixed Monte Carlo Sampling (MMCS) transport methods for the GPU

Topic Area: Uncertainty Quantification/Stochastic Media

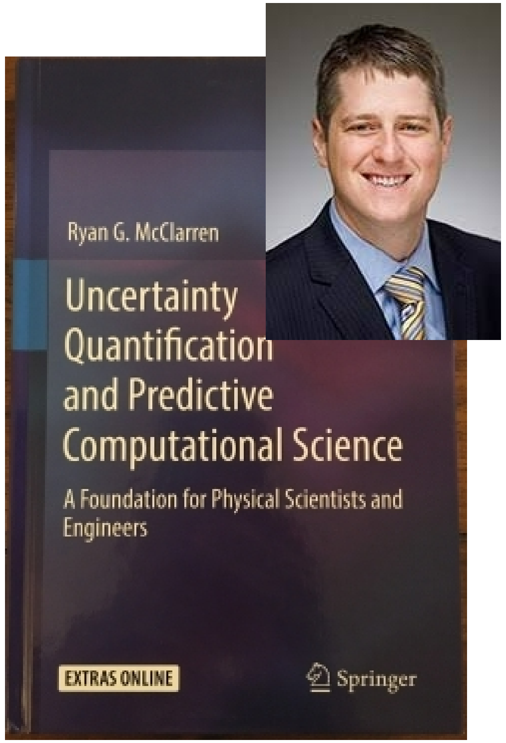
Develop efficient uncertainty quantification (UQ) and stochastic media (SM) Mixed Monte Carlo Sampling (MMCS) transport methods for the GPU

UQ – quantify effects of input uncertainty on outputs

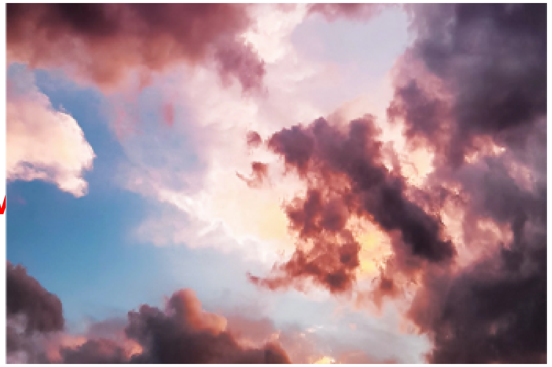


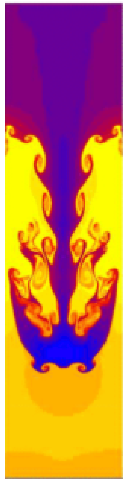
$$T = e^{-r\Sigma_t}$$

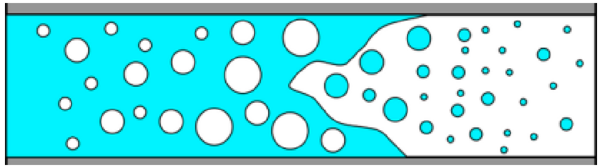
$$T(\xi) = e^{-r\Sigma_t(\xi)}$$

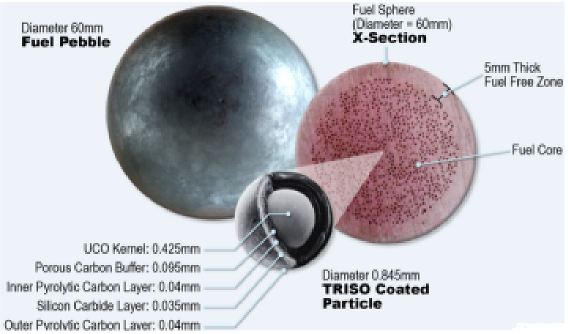


SM – structures only know statistically

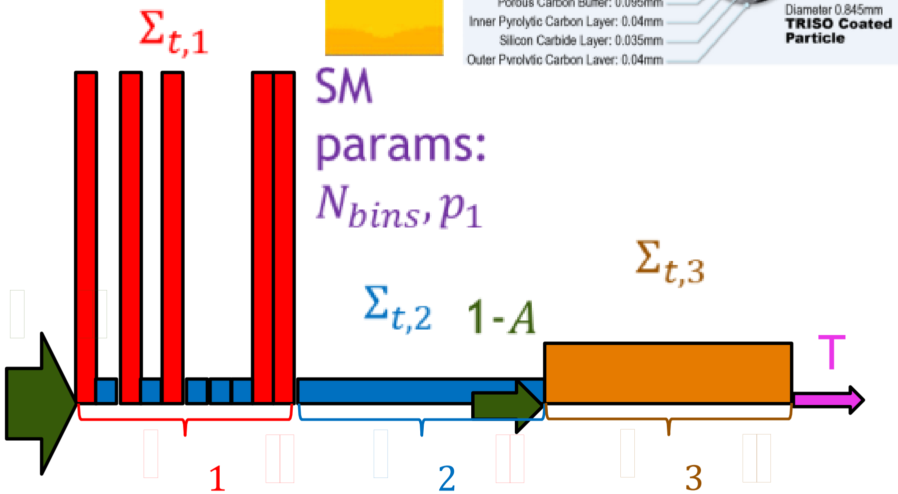








Combined – treat SM as uncertainty source



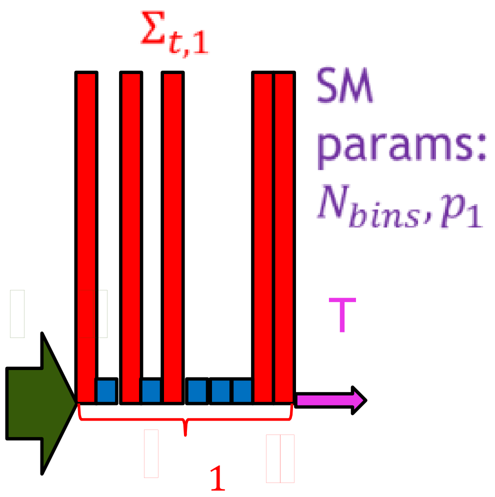
SM params: N_{bins}, p_1

Uncertainty sources:

- Boundary conditions
- Coefficients
- Geometry
- Stochastic mixing
- SM hyperparameters

Foundational Concept: Mixed Monte Carlo Sampling Efficiency

Develop efficient uncertainty quantification (UQ) and stochastic media (SM) Mixed Monte Carlo Sampling (MMCS) transport methods for the GPU



Monte Carlo sampling, Monte Carlo transport

Optimize number of

- Samples
- Histories/sample

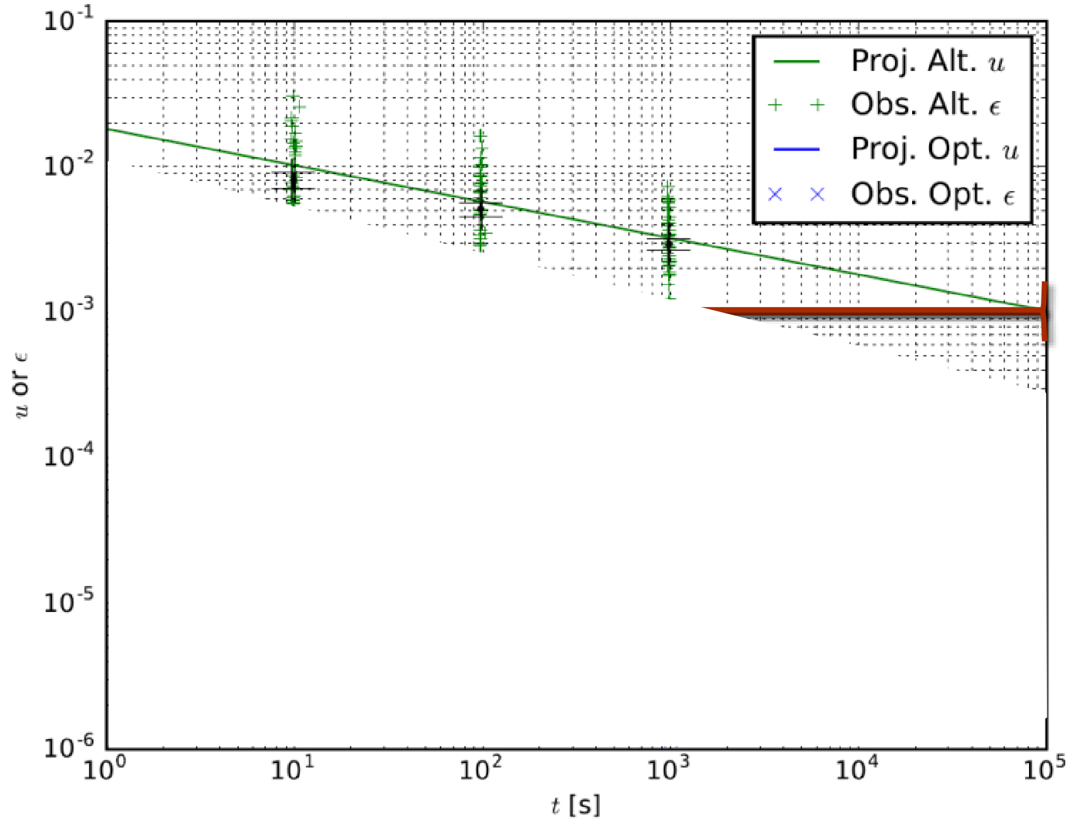
An Optimal-Cost Monte Carlo Approach to Stochastic Media Transport Calculations

Aaron J. Olson* and Brian C. Franke*

$$N = \frac{\sigma_{MC}}{\sigma_{RS}} \frac{\sqrt{C_{RS}}}{\sqrt{C_{MC}}}$$

Set N

Converge w/ R



=

$$\lim_{R\to\infty} u_{alt} = \sigma_{RS} C_{MC}^{1/4} t^{-1/4}$$

Optimal

$$u_{tot} = \left(\sqrt{C_{RS}}\sigma_{RS} + \sqrt{C_{MC}}\sigma_{MC}\right) t^{-1/2}$$

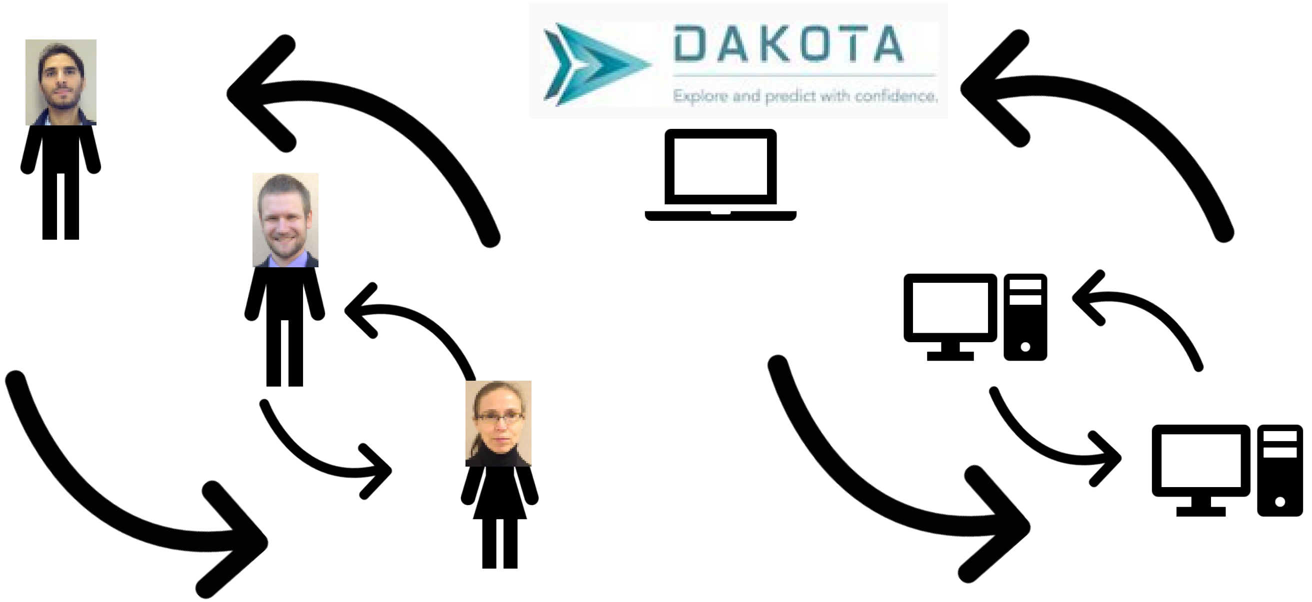
- As long as cost of taking sample (C_{RS}) small, massive savings possible with histories per sample (N) small
- MMCS: Monte Carlo sampling in uncertainty space and in solver with frequent resampling of

LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Foundational Concept: Mixed Monte Carlo Sampling Embedding

Develop efficient uncertainty quantification (UQ) and stochastic media (SM) Mixed Monte Carlo Sampling (MMCS) transport methods for the GPU

Current UQ workflow (external linkage)



Targeted UQ workflow (embedding)

Initial MMCS Methods: CoPS and EVADE

Develop efficient uncertainty quantification (UQ) and stochastic media (SM) Mixed Monte Carlo Sampling (MMCS) transport methods for the GPU

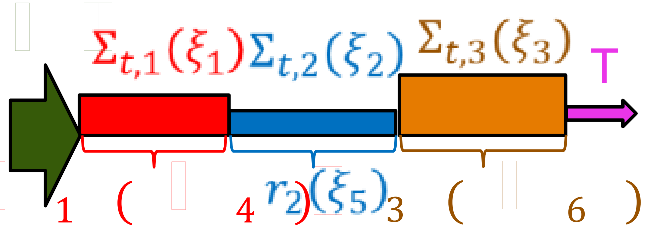
Embedded Variance Deconvolution (EVADE): Parse parameter-driven variance from solver variance

Calculation of Parametric Variance using Variance Deconvolution

Aaron J. Olson*

Get w/ N=1 Est. w/ N>1

= −



N = 10⁴, 10^3 = 2

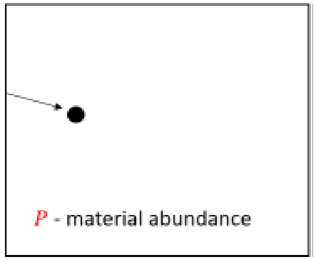
	Semi-an.	VADE	EVADE
	0.010069	0.11029	0.1001(2)
$\langle \epsilon_{V_P} \rangle$		0.00525	0.00053

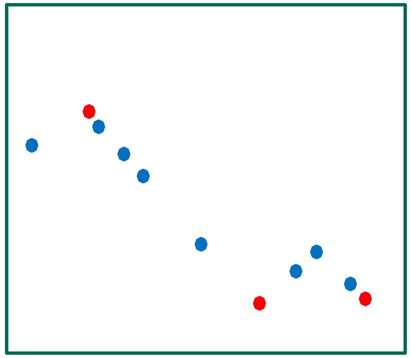
10X

Conditional Point Sampling (CoPS): Sample stochastic media mixing only at discrete points

Conditional Point Sampling: A Novel Monte Carlo Method for Radiation Transport in Stochastic Media

Emily H. Vu*† and Aaron J. Olson†





EVADE with CoPS for SM variance

An Extension of Conditional Point Sampling to Quantify Uncertainty Due to Material Mixing Randomness

Emily H. Vu[1,2] and Aaron J. Olson[2]

	V_P-reflectance		V_P-transmittance	
	Bench	CoPS	Bench	CoPS
Case 2a	0.082	0.0823(4)	0.0079	0.0079(3)

Next-Gen MC LDRD Overview

Develop efficient uncertainty quantification (UQ) and stochastic media (SM) Mixed Monte Carlo Sampling (MMCS) transport methods for the GPU

Four MMCS goals:

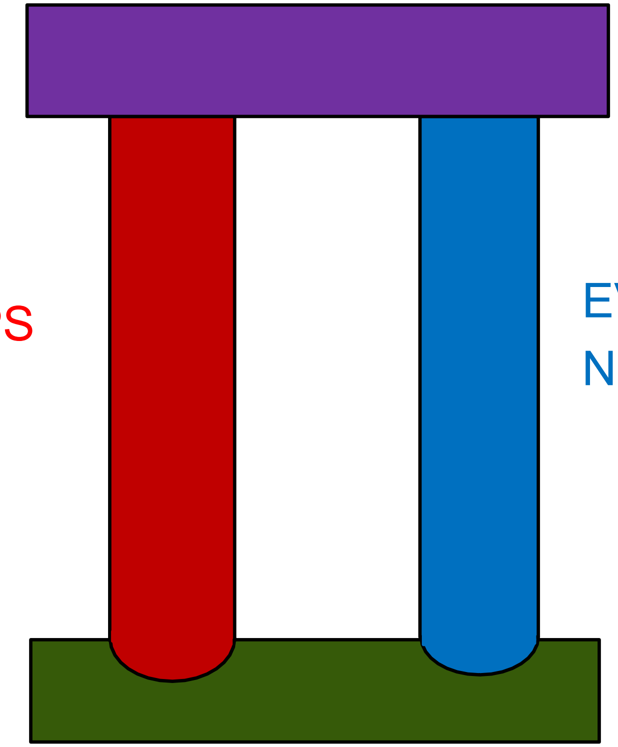
- Develop UQ methods
- Develop data-driven SM capabilities
- Adapt UQ tools to incorporate SM uncertainty
- Efficiently embed methods on the GPU

LDRD Key Questions:

- What is possible?
- What is practical?

LDRD : Fall 2019-Fall 2022
CEMeNT: Fall 2020-Fall 2025

CoPS



EVADE
New MMCS methods

CHEETAH-MC

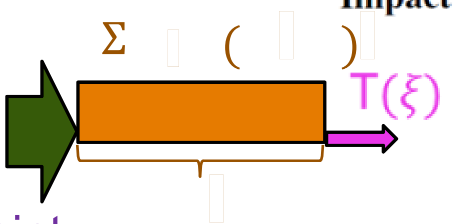
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Progress: MMCS Polynomial Chaos Expansion Tools

Develop efficient uncertainty quantification (UQ) and stochastic media (SM) Mixed Monte Carlo Sampling (MMCS) transport methods for the GPU

Four MMCS goals:

- Develop UQ methods
- Develop data-driven SM capabilities
- Adapt UQ tools to incorporate SM uncertainty
- Efficiently embed methods on the GPU



$$T(\xi) = e^{-r\Sigma_t(\xi)}$$

Impact of sampling strategies in the polynomial chaos surrogate construction for Monte Carlo transport applications

Gianluca Geraci[1] and Aaron J. Olson[1]

MMCS savings, small N_η:

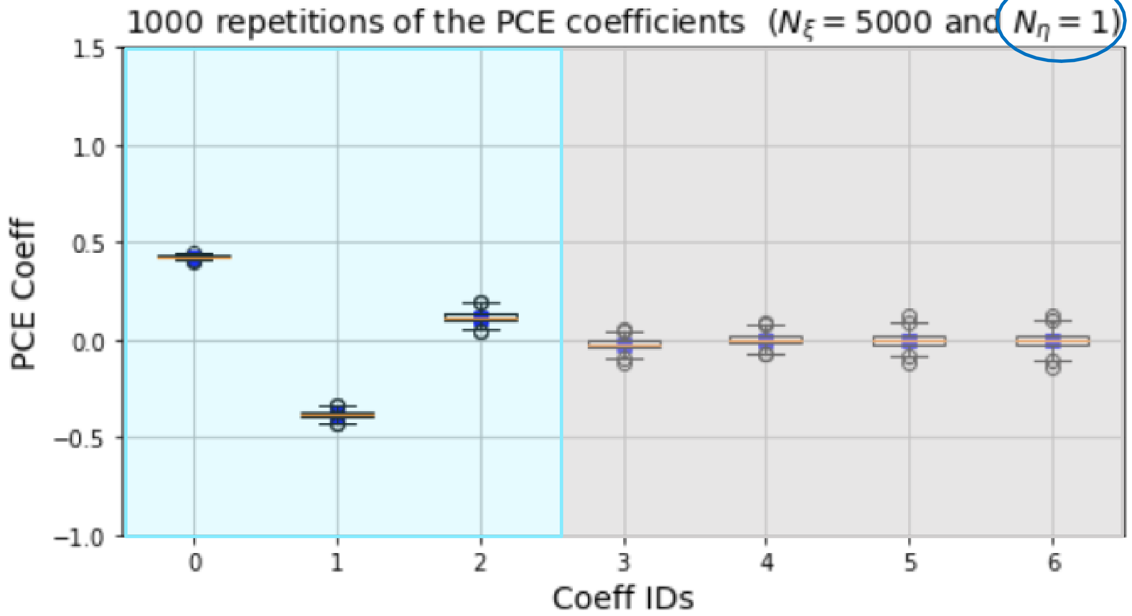
$$\mathbb{V}ar\left[\hat{\beta}_k^s\right] = \frac{1}{b_k^2}\frac{N_\eta \mathbb{V}ar\left[\Psi_k Q\right] + \mathbb{E}\left[\Psi_k^2 \sigma^2\right]}{N}$$

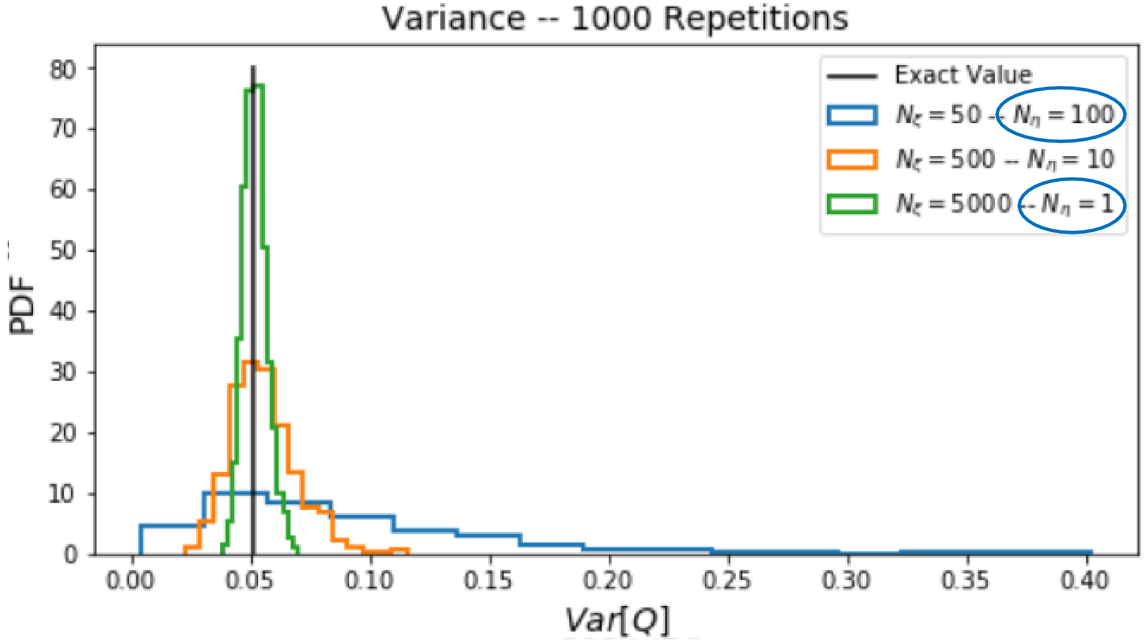
Accomplishments (ANS/M&C papers):

- Initial PCE tools (Geraci, 2021)

P

$$Q(\xi) = \sum_k$$





LDRD
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Progress: MMCS Sobol' Indices Tools

Develop efficient uncertainty quantification (UQ) and stochastic media (SM) Mixed Monte Carlo Sampling (MMCS) transport methods for the GPU

Four MMCS goals:

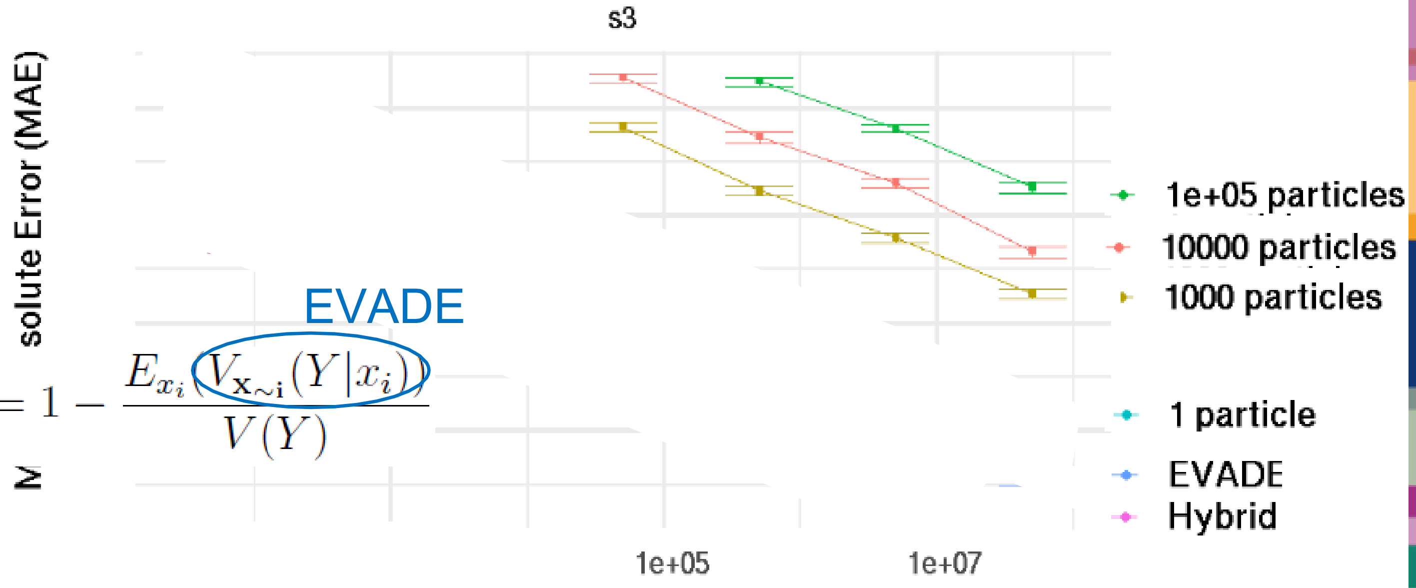
- Develop UQ methods
- Develop data-driven SM capabilities
- Adapt UQ tools to incorporate SM uncertainty
- Efficiently embed methods on the GPU

Accomplishments (ANS/M&C papers):

- Initial PCE tools (Geraci, 2021)
- Initial sampling-based Sobol indices (Petticrew, 2021)

COMPUTATION OF SOBOL' INDICES USING EMBEDDED VARIANCE DECONVOLUTION

James M. Petticrew[1], Aaron J. Olson[2]



EVADE

$$S_i = 1 - \frac{E_{x_i}\left(V_{\mathbf{x}_{\sim i}}(Y|x_i)\right)}{V(Y)}$$

EVADE

$$S_{T_i} = \frac{E_{\mathbf{x}_{\sim i}}\left(V_{x_i}(Y|\mathbf{x}_{\sim i})\right)}{V(Y)}$$

EVADE

$$V(Y) = E\left(V(Y|x)\right) + V\left(E(Y|x)\right)$$

EVADE-based: MC convergence, efficient

"Traditional" in MMCS limit: Surprisingly well-performing

New "hybrid": Traditional sampling w/ EVADE

LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Progress: Deep Learning SM Tool

Develop efficient uncertainty quantification (UQ) and stochastic media (SM) Mixed Monte Carlo Sampling (MMCS) transport methods for the GPU

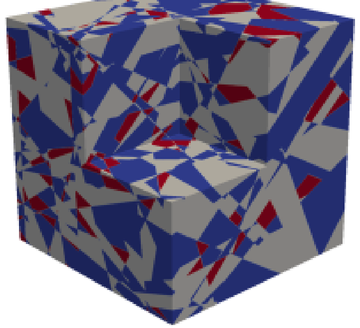
Four MMCS goals:

- Develop UQ methods
- Develop data-driven SM capabilities
- Adapt UQ tools to incorporate SM uncertainty
- Efficiently embed methods on the GPU

Accomplishments (ANS/M&C papers):

- Initial PCE tools (Geraci, 2021)
- Initial sampling-based Sobol indices (Petticrew, 2021)
- Initial machine learning SM capability (Davis, 2021)

Markovian mixing (N-ary)



USING DEEP NEURAL NETWORKS TO PREDICT MATERIAL TYPES IN CONDITIONAL POINT SAMPLING APPLIED TO MARKOVIAN MIXTURE MODELS

Warren L. Davis IV[1], Aaron Olson[1], Gabriel Popoola[1], Dan Bolintineanu[1], Theron Rodgers[1], and Emily Vu[1,2]

Method	Sample0	Sample1	Sample2	Sample3	Sample4	Average
CoPS2	.147	.146	.154	.151	.147	.149
DNN	.169	.153	.112	.129	.166	.146

Figure: Jensen-Shannon divergence for 1-D predictions

Method	Sample0	Sample1	Sample2	Sample3	Sample4	Average
CoPS2	84.8	83.6	90.2	86.1	83.2	85.6
DNN	87.8	87.3	91.1	87.4	86.0	87.9

Figure: Accuracy percentages for 3-D predictions

LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Progress: SM Benchmarking Capabilities

Develop efficient uncertainty quantification (UQ) and stochastic media (SM) Mixed Monte Carlo Sampling (MMCS) transport methods for the GPU

Four MMCS goals:

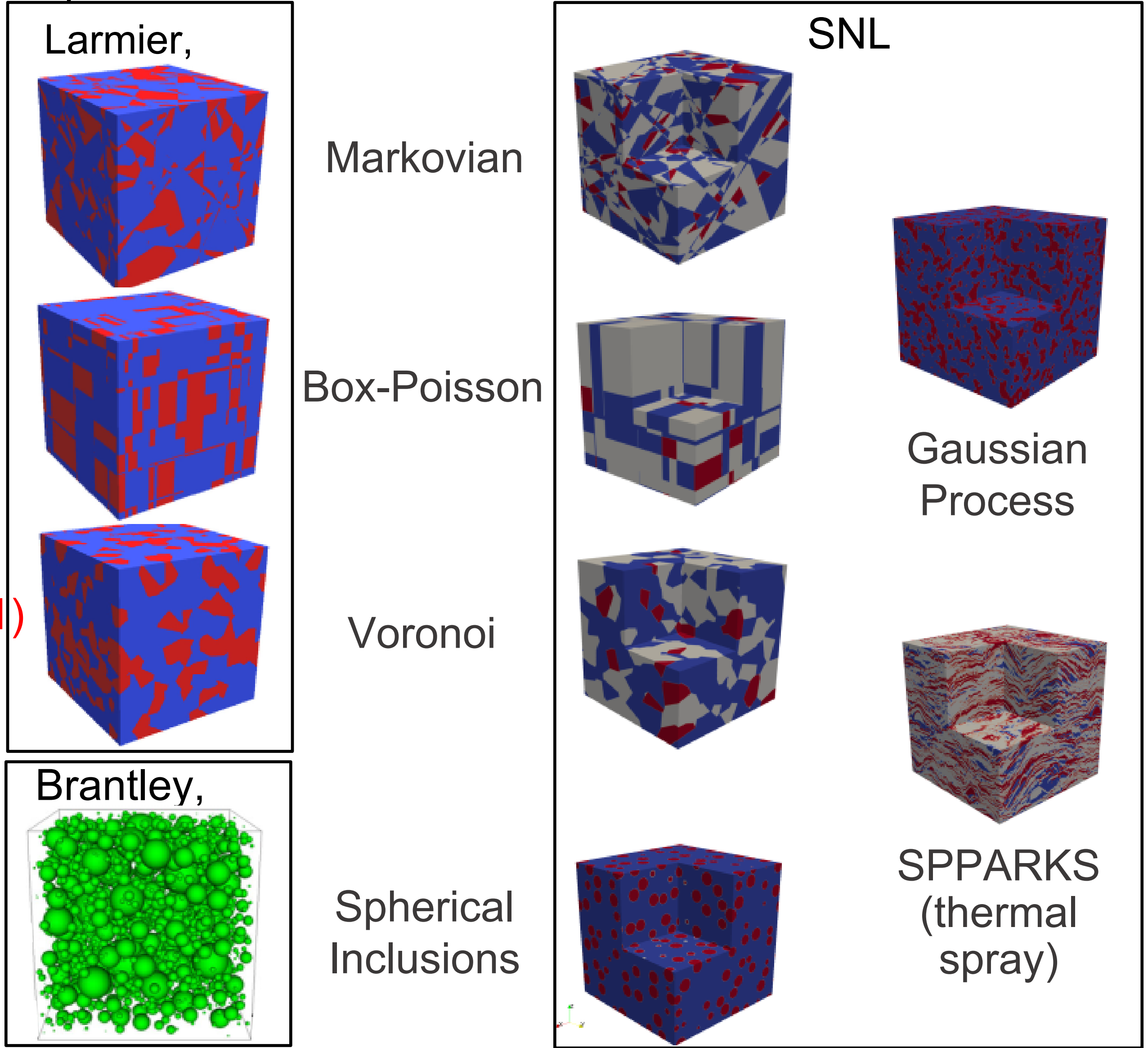
- Develop UQ methods
- Develop data-driven SM capabilities
- Adapt UQ tools to incorporate SM uncertainty
- Efficiently embed methods on the GPU

Accomplishments (ANS/M&C papers):

- Initial PCE tools (Geraci, 2021)
- Initial sampling-based Sobol indices (Petticrew, 2021)
- Initial machine learning SM capability (Davis, 2021)
- SM benchmarking capabilities (Olson, 2021)

THEORY AND GENERATION METHODS FOR N-ARY STOCHASTIC MIXTURES WITH MARKOVIAN MIXING STATISTICS

Aaron Olson[1], Shawn Pautz[1], Dan Bolintineanu[1], and Emily Vu[1,2]



Progress: Proposed Test Problem

Develop efficient uncertainty quantification (UQ) and stochastic media (SM) Mixed Monte Carlo Sampling (MMCS) transport methods for the GPU

Four MMCS goals:

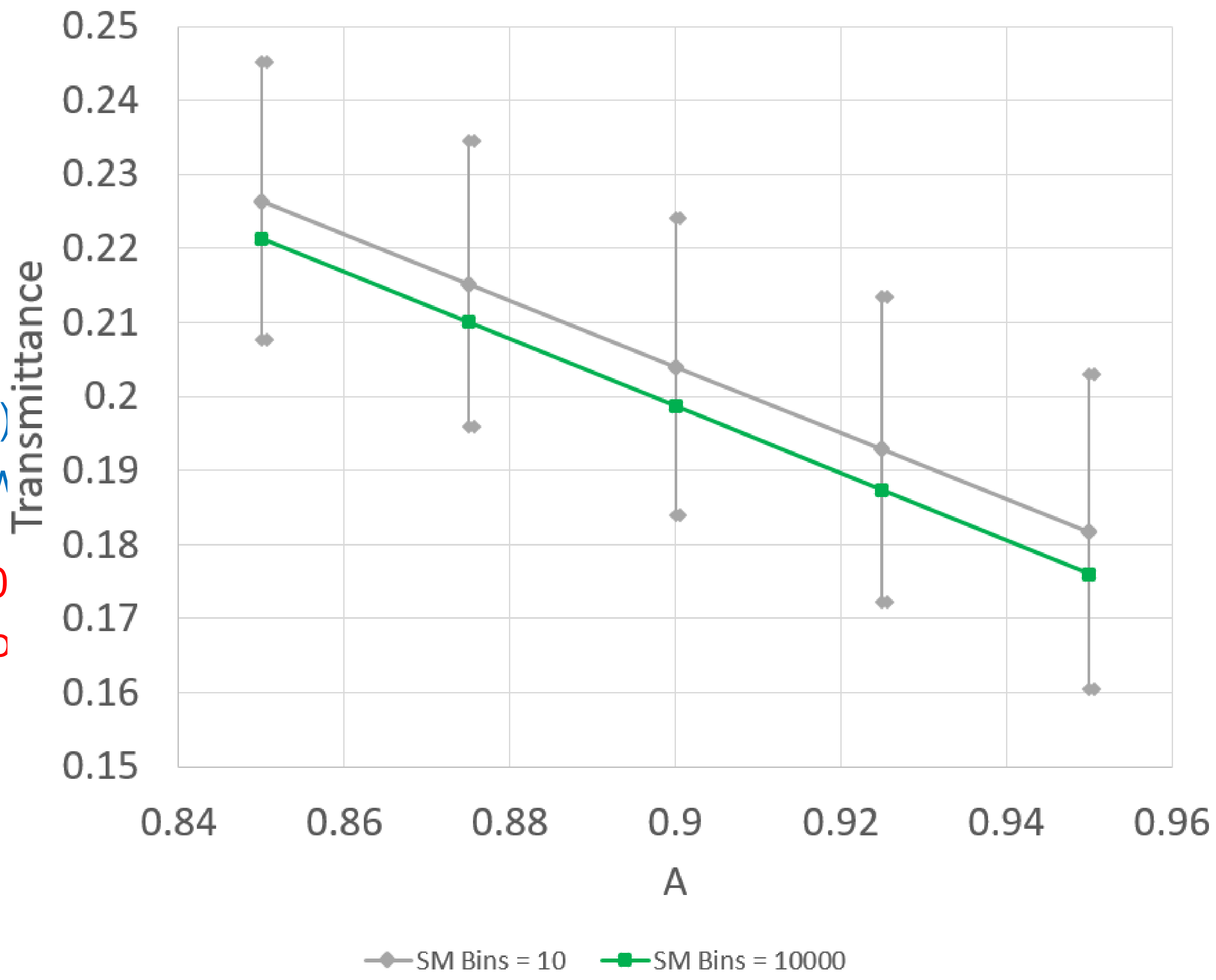
- Develop UQ methods
- Develop data-driven SM capabilities
- Adapt UQ tools to incorporate SM uncertainty
- Efficiently embed methods on the GPU

Accomplishments (ANS/M&C papers):

- Initial PCE tools (Geraci, 2021)
- Initial sampling-based Sobol indices (Petticrew 2021)
- Initial machine learning SM capability (Davis, 20
- SM benchmarking capabilities (Olso 2021)
- Proposed test problem

Estimation of Sobol indices:

Surrogate over fractional source distribution "A":



LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Progress: GPU Prototyping

Develop efficient uncertainty quantification (UQ) and stochastic media (SM) Mixed Monte Carlo Sampling (MMCS) transport methods for the GPU

Four MMCS goals:

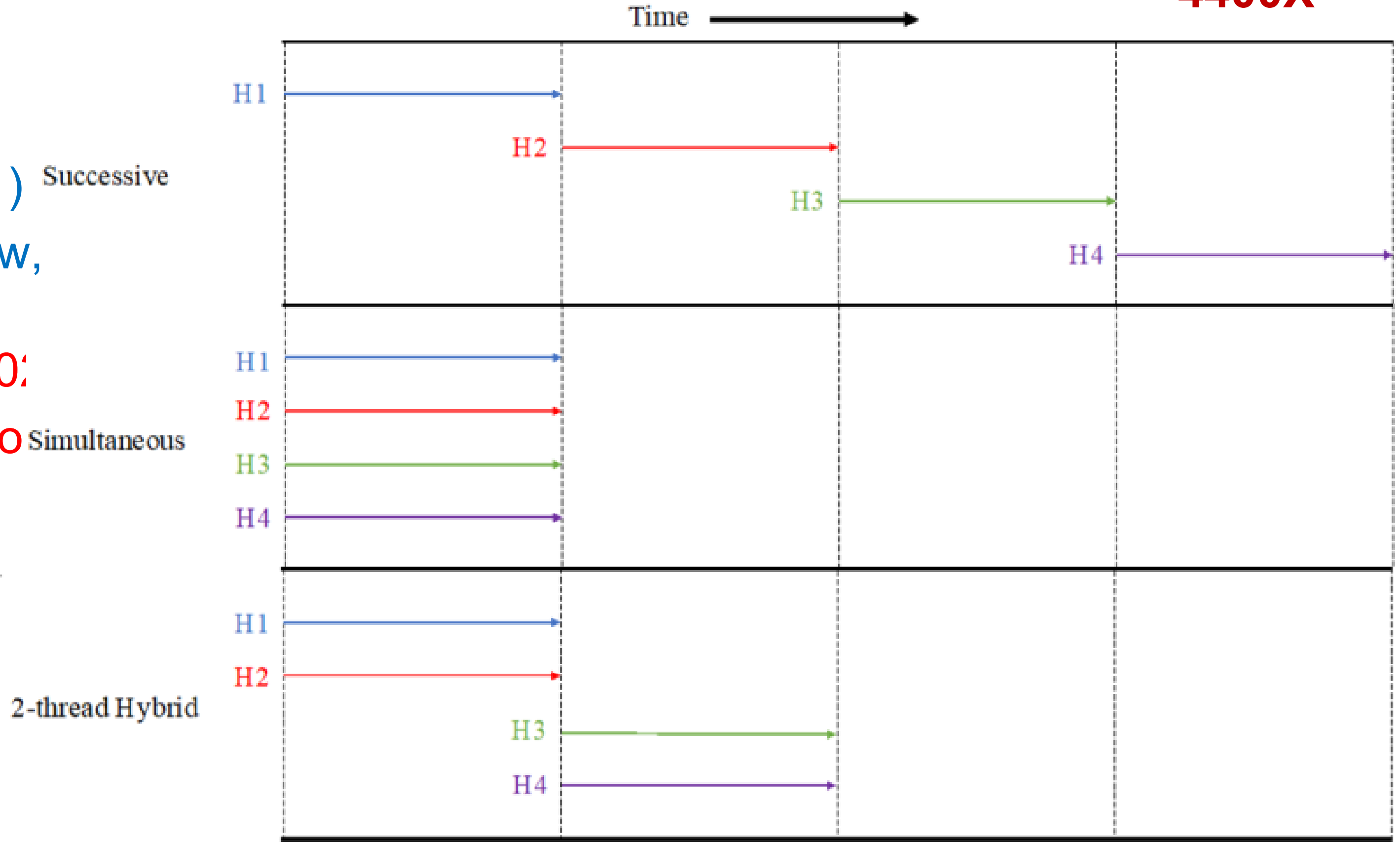
- Develop UQ methods
- Develop data-driven SM capabilities
- Adapt UQ tools to incorporate SM uncertainty
- Efficiently embed methods on the GPU

Accomplishments (ANS/M&C papers):

- Initial PCE tools (Geraci, 2021)
- Initial sampling-based Sobol indices (Petticrew, 2021)
- Initial machine learning SM capability (Davis, 20
- SM benchmarking capabilities (Olso 2021)
- Proposed test problem
- Prototyped SM algorithm on GPU (Kersting, 2021)

	Reflectance			Runtime (s)	
	Bench. [4]	CPU	GPU	CPU	GPU
2 c	0.3438(6)	0.3135(5)	0.3133(5)	14539.8	3.3

4400X



CONDITIONAL POINT SAMPLING IMPLEMENTATION FOR THE GPU

Luke J. Kersting[1], Aaron Olson[1], and Kerry Bossler[1]

LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Progress: GPU Prototyping

Develop efficient uncertainty quantification (UQ) and stochastic media (SM) Mixed Monte Carlo Sampling (MMCS) transport methods for the GPU

Four MMCS goals:

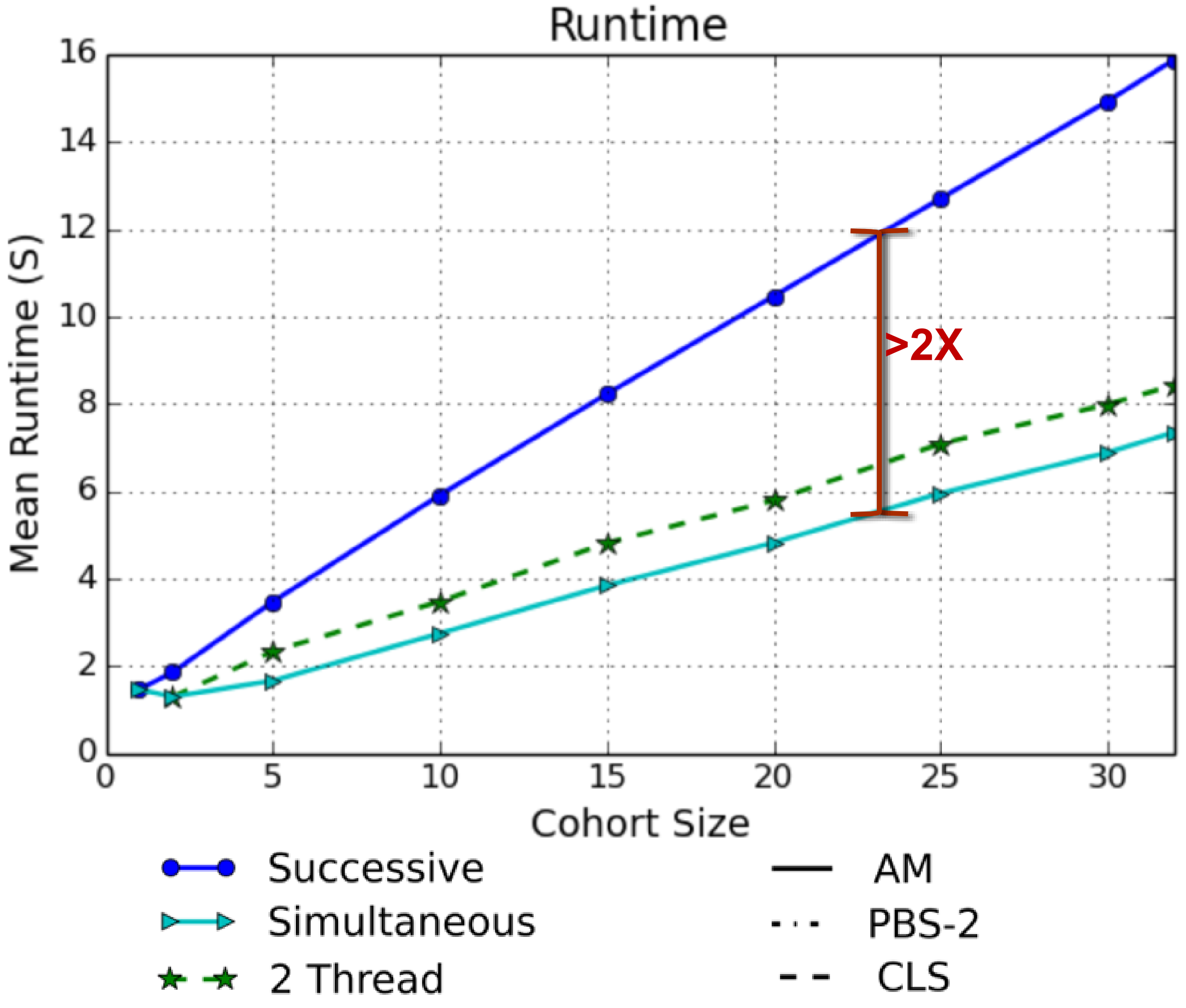
- Develop UQ methods
- Develop data-driven SM capabilities
- Adapt UQ tools to incorporate SM uncertainty
- Efficiently embed methods on the GPU

Accomplishments (ANS/M&C papers):

- Initial PCE tools (Geraci, 2021)
- Initial sampling-based Sobol indices (Petticrew, 2021)
- Initial machine learning SM capability (Davis, 2021)
- SM benchmarking capabilities (Olson, 2021)
- Proposed test problem
- Prototyped SM algorithm on GPU (Kersting, 2021)

CONDITIONAL POINT SAMPLING IMPLEMENTATION FOR THE GPU

Luke J. Kersting[1], Aaron Olson[1], and Kerry Bossler[1]



LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Progress: Limited-memory Algorithm

Develop efficient uncertainty quantification (UQ) and stochastic media (SM) Mixed Monte Carlo Sampling (MMCS) transport methods for the GPU

Four MMCS goals:

- Develop UQ methods
- Develop data-driven SM capabilities
- Adapt UQ tools to incorporate SM uncertainty
- Efficiently embed methods on the GPU

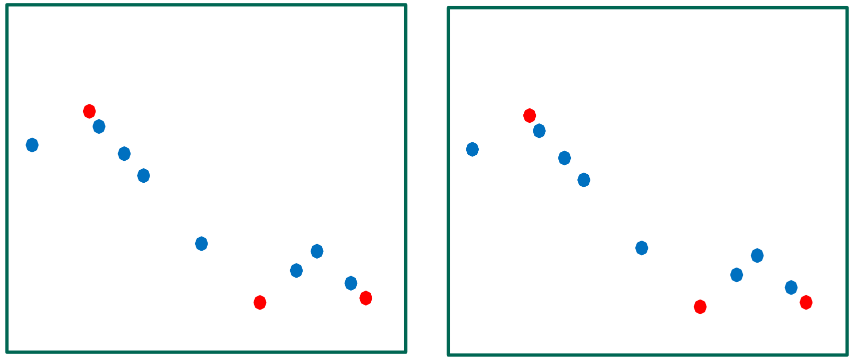
Accomplishments (ANS/M&C papers):

- Initial PCE tools (Geraci, 2021)
- Initial sampling-based Sobol indices (Petticrew, 2021)
- Initial machine learning SM capability (Davis, 2021)
- SM benchmarking capabilities (Olson, 2021)
- Proposed test problem
- Prototyped SM algorithm on GPU (Kersting, 2021)
- "Limited-memory" SM algorithm (Vu, 2020; Vu, 2021)

Recent Memory Versions of Conditional Point Sampling for Transport in 1D Stochastic Media

Emily H. Vu*† and Aaron J. Olson†

Full memory: Recent memory:



	CoPS2-1	CoPS2-2	CoPS2-3	CoPS2-∞
Transmittance RMS E_R	0.362	0.288	0.257	0.042
Runtime (min.)	282	293	296	598

LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Progress: Limited-memory Algorithm

Develop efficient uncertainty quantification (UQ) and stochastic media (SM) Mixed Monte Carlo Sampling (MMCS) transport methods for the GPU

Four MMCS goals:

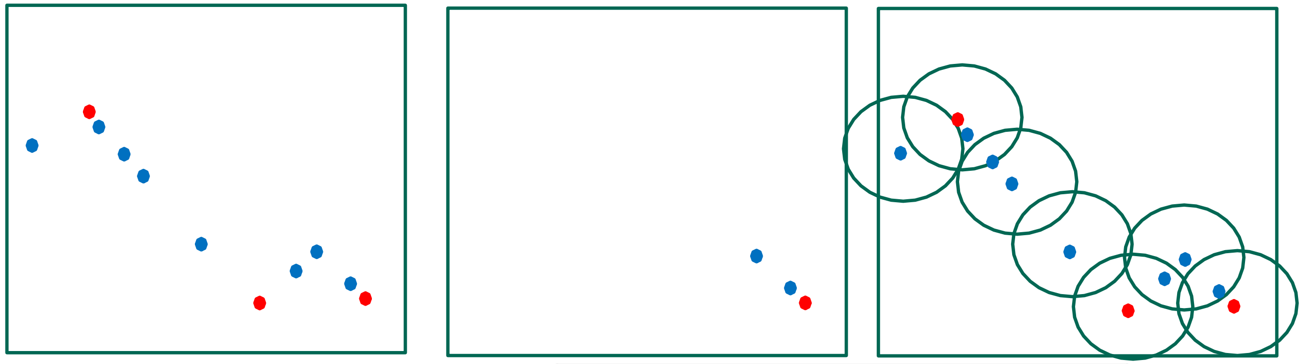
- Develop UQ methods
- Develop data-driven SM capabilities
- Adapt UQ tools to incorporate SM uncertainty
- Efficiently embed methods on the GPU

Accomplishments (ANS/M&C papers):

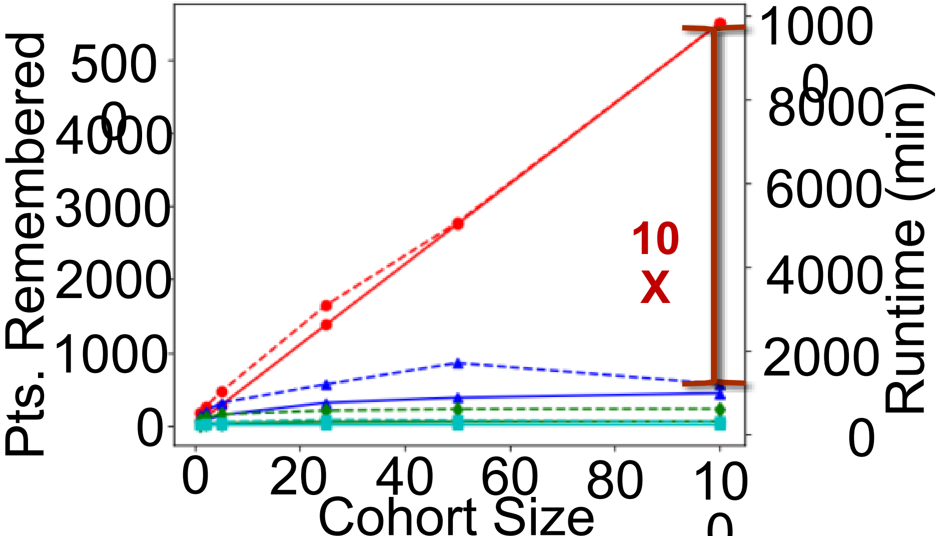
- Initial PCE tools (Geraci, 2021)
- Initial sampling-based Sobol indices (Petticrew, 2021)
- Initial machine learning SM capability (Davis, 2021)
- SM benchmarking capabilities (Olson, 2021)
- Proposed test problem
- Prototyped SM algorithm on GPU (Kerst
- “Limit
2020;

AMNESIA RADIUS VERSIONS OF CONDITIONAL POINT SAMPLING FOR RADIATION TRANSPORT IN 1D STOCHASTIC MEDIA

Emily H. Vu[1,2] and Aaron J. Olson[2]



Cohort size 1E6:
0.7d vs. 190yr
13s vs. 15.8d



LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Progress: UNM Collaboration

Develop efficient uncertainty quantification (UQ) and stochastic media (SM) Mixed Monte Carlo Sampling (MMCS) transport methods for the GPU

Four MMCS goals:

- Develop UQ methods
- Develop data-driven SM capabilities
- Adapt UQ tools to incorporate SM uncertainty
- Efficiently embed methods on the GPU

Accomplishments (ANS/M&C papers):

- Initial PCE tools (Geraci, 2021)
- Initial sampling-based Sobol indices (Petticrew, 2021)
- Initial machine learning SM capability (Davis, 2021)
- SM benchmarking capabilities (Olson, 2021)
- Proposed test problem
- Prototyped SM algorithm on GPU (Kersting, 2021)
- “Limited memory” SM algorithm (Vu, 2020; Vu, 2021)

Sensitivity Analysis in Coupled Radiation Transport Simulations

Christopher M. Perfetti[a], Brian Franke[b], Ron Kensek[b], Aaron Olson[b]

“Coupled CLUTCH”

- 1D transport
- Photon/electron
- 3 groups
- 10 cells

REVISITING THE LOCKWOOD ALBEDO MEASUREMENTS FOR VALIDATION OF THE INTEGRATED TIGER SERIES ELECTRON-PHOTON TRANSPORT CODE

R b

Rowdy Davis[1], Ronald P. Kensek[2], Christopher M. Perfetti[1] and Aaron Olson[2]

ITS Validation Suite:

- 7 experiments
- Assessment: Expand Lockwood albedo simulations

Improvements:

- Quantitative error metric
- More simulations
- Experimental errors

UNM collaboration goals/accomplishments:

- Adapt local sensitivity methods/prototype on GPUs

UNM Collaboration

- Validation/calibration simulations
- Sensitivity method implementation/prototyping
- XS calibration foundation

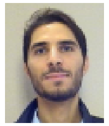
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

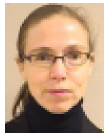
Opportunity: CEMeNT Collaboration?

Develop efficient uncertainty quantification (UQ) and stochastic media (SM) Mixed Monte Carlo Sampling (MMCS) transport methods for the GPU

Four MMCS goals:

- Develop UQ methods
- Develop data-driven SM capabilities
- Adapt UQ tools to incorporate SM uncertainty
- Efficiently embed methods on the GPU





Accomplishments (ANS/M&C papers):

- Initial PCE tools (Geraci, 2021)
- Initial sampling-based Sobol indices (Petticrew, 2021)
- Initial machine learning SM capability (Davis, 2021)
- SM benchmarking capabilities (Olson, 2021)
- Proposed test problem
- Prototyped SM algorithm on GPU (Kersting, 2021)
- “Limited memory” SM algorithm (Vu, 2020; Vu, 2021)

Wish list:

- Develop PCE term selection/regression approaches
- Quantify Sobol performance, new and traditional
- Expand MMCS PCE/Sobol prototyping
- Design MMCS UI/co-implementation strategies
- Your ideas!

Internship Job Posting:

- Sandia Careers: https://bit.ly/2XzEuGD
- Posting number: 674437
- Posting live until Feb. 22

UNM collaboration goals/accomplishments:

- Adapt local sensitivity methods/prototype on GPUs

CEMeNT collaboration?

- Student internship
- Other