



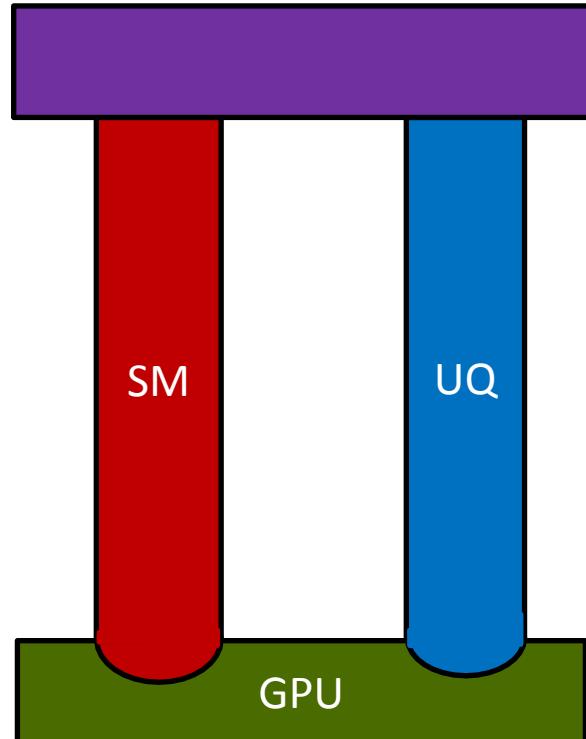
# Computation of Sobol' indices using Embedded Variance Deconvolution

James Petticrew, Atomic Weapons Establishment

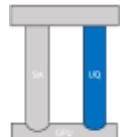
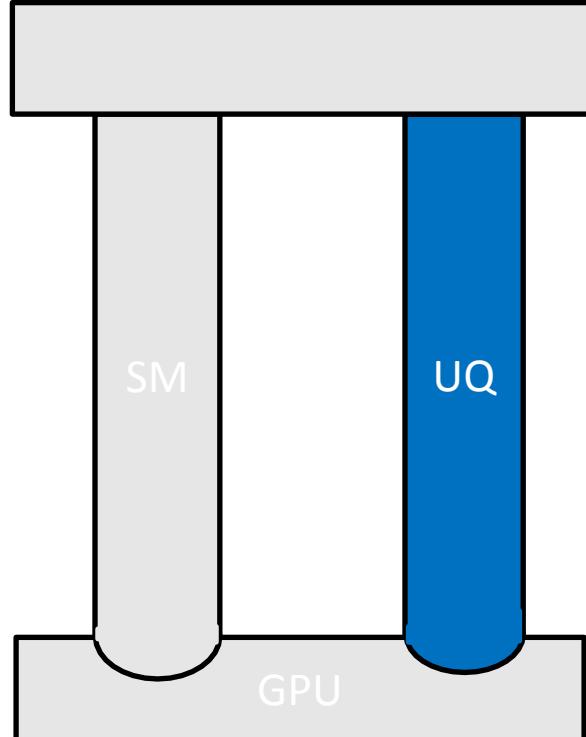
Aaron J. Olson, Sandia National Laboratories

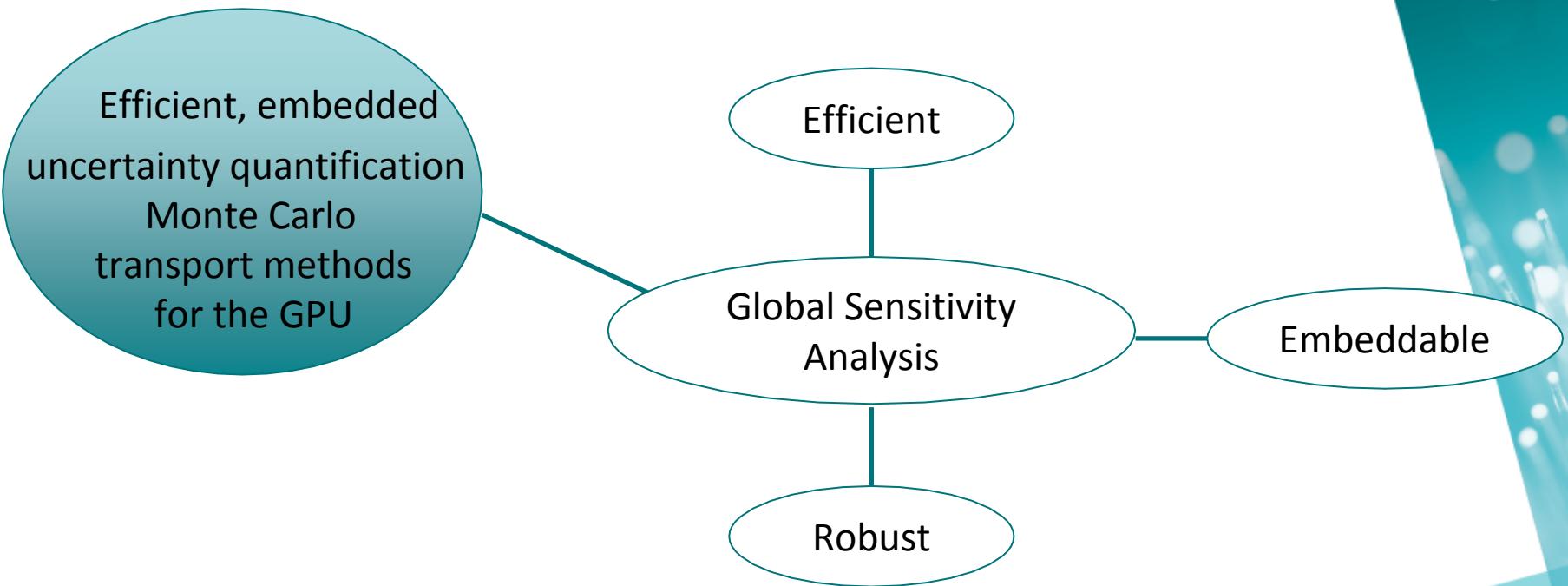
Supported by the Laboratory Directed Research and Development program at Sandia National Laboratories, a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DENA0003525. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

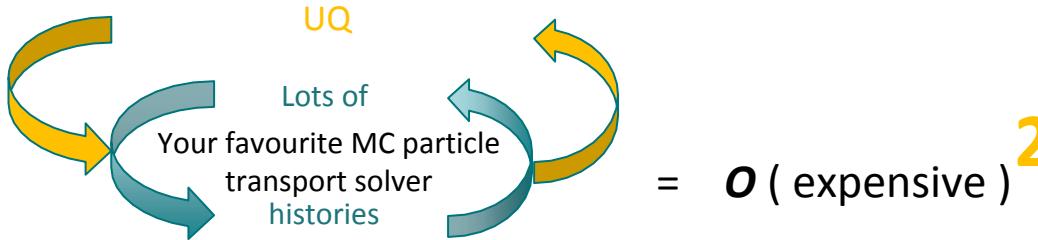
Develop efficient, embedded stochastic media (SM) and  
uncertainty quantification (UQ) Monte Carlo transport methods for the GPU.



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







Screening, emulators,  
reliability methods

Efficient



Embeddable



Robust

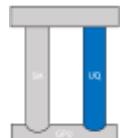


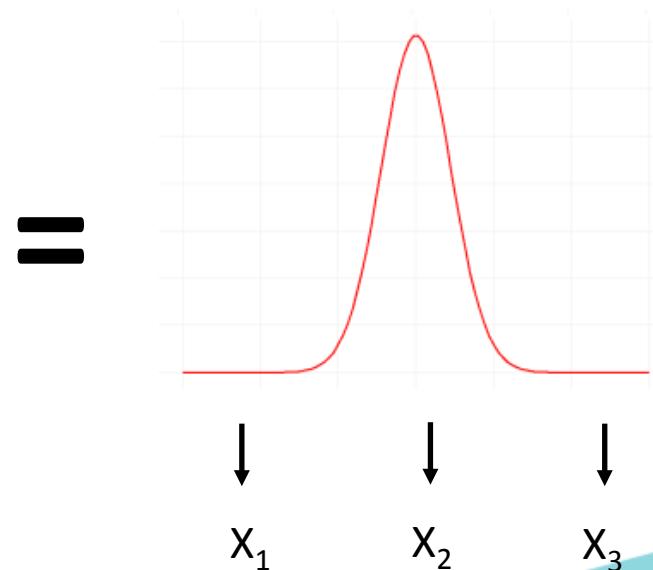
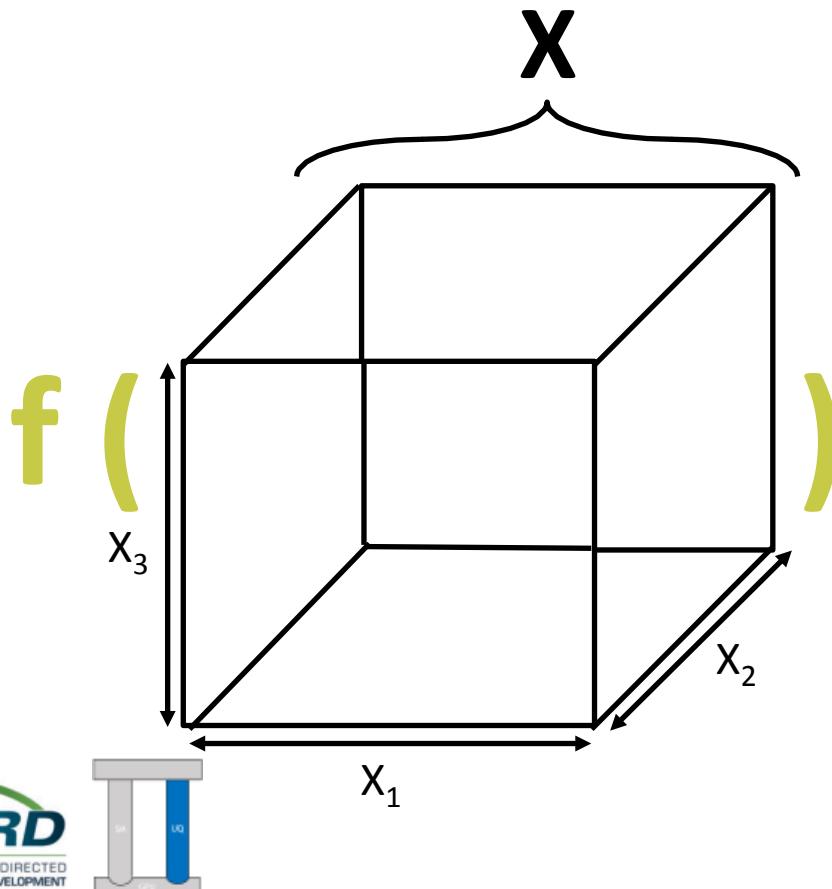
Embedded variance-based  
sensitivity analysis

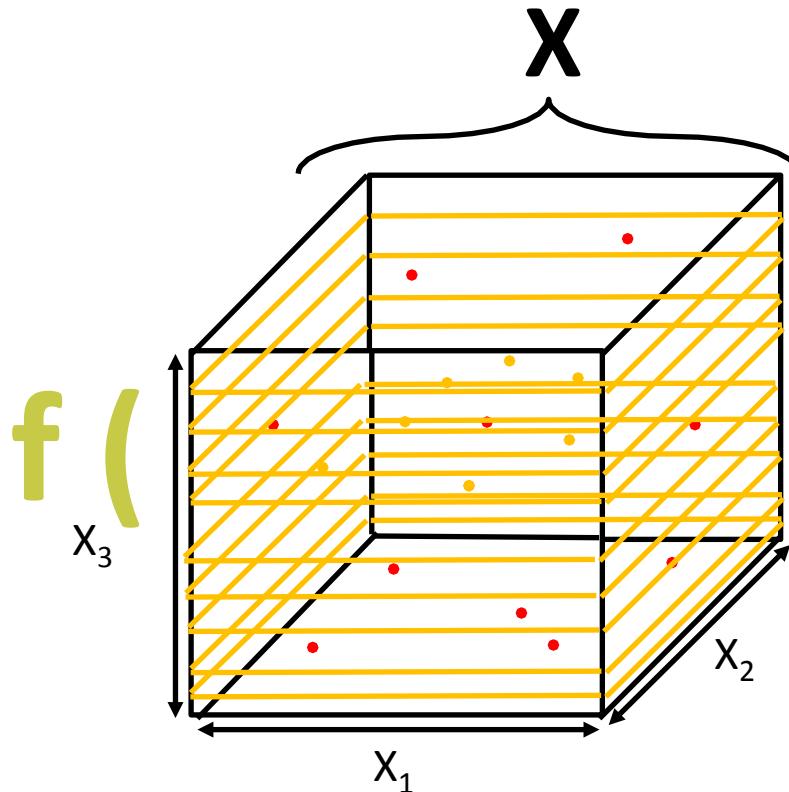


## 1. Sobol' indices

## 2. EVADE







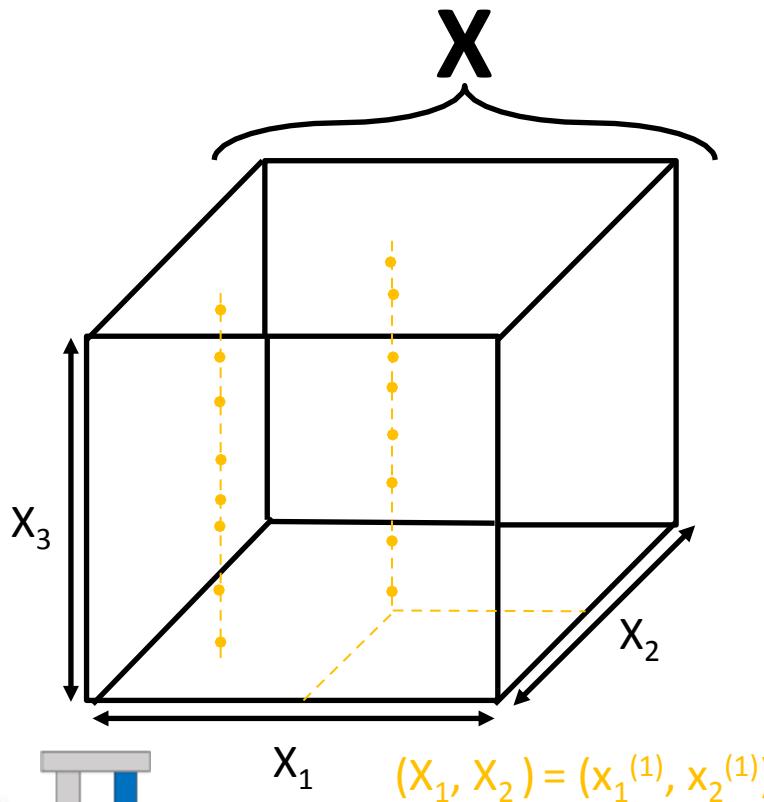
$$X_3 = x_3^{(1)}$$

1 -

$$\frac{E[\text{Var}[Y|X_3=x_3^{(1)}]]}{\text{Var}(Y)}$$

$$\frac{\text{Var}(Y)}{\text{Var}(Y)}$$

:= Main effect Sobol' index for  $X_3$



$$\frac{E(\text{Var}[Y|X_1, X_2])}{\text{Var}(Y)}$$

:= Total effect Sobol' index for  $X_3$

$$1 - \frac{E(\text{Var}[Y|X_3])}{\text{Var}(Y)}$$

:= Main effect Sobol' index for  $X_3$

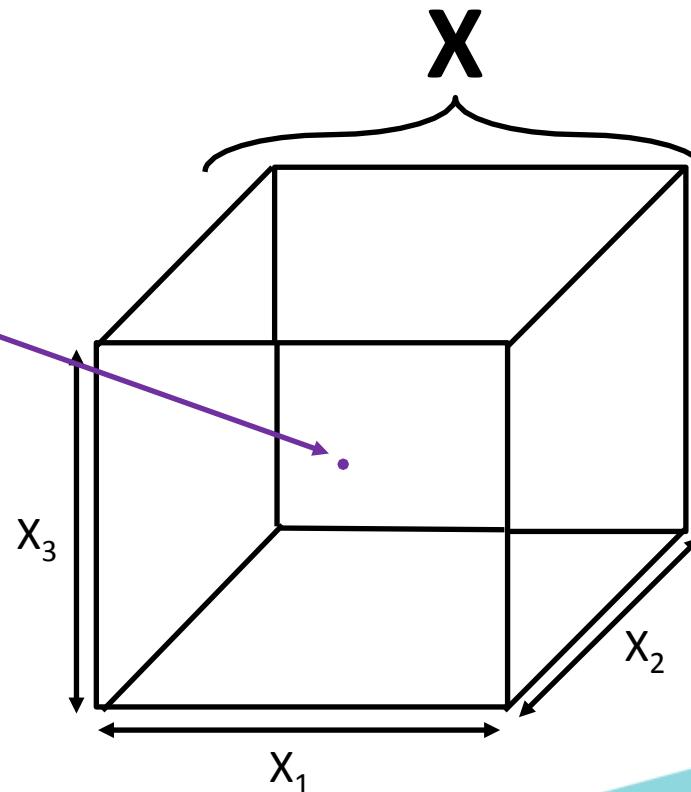
$$x^{(1)} := (x_1^{(1)}, x_2^{(1)}, x_3^{(1)})$$

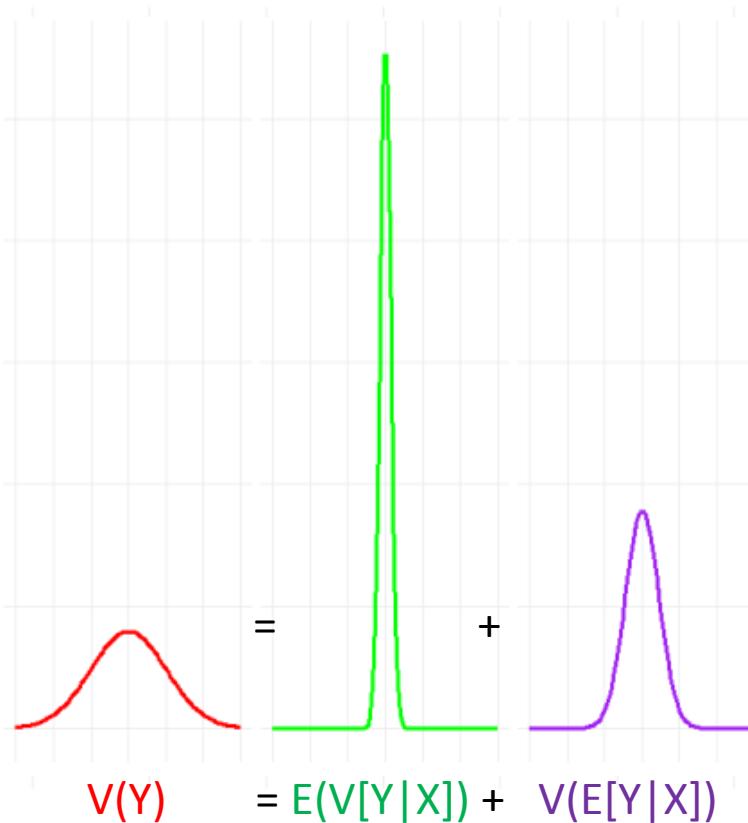
$$y^{(1)} := f(x^{(1)})^{(1)}$$

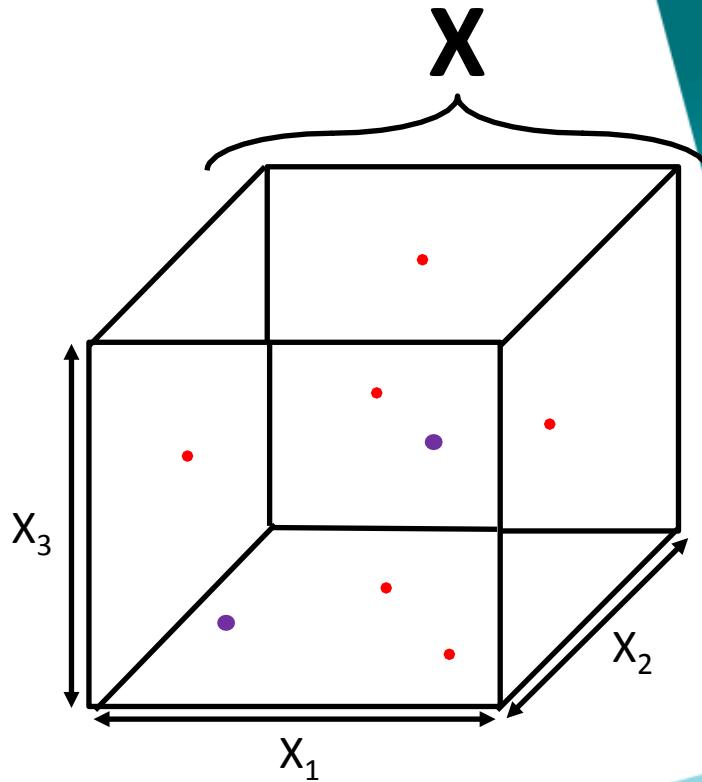
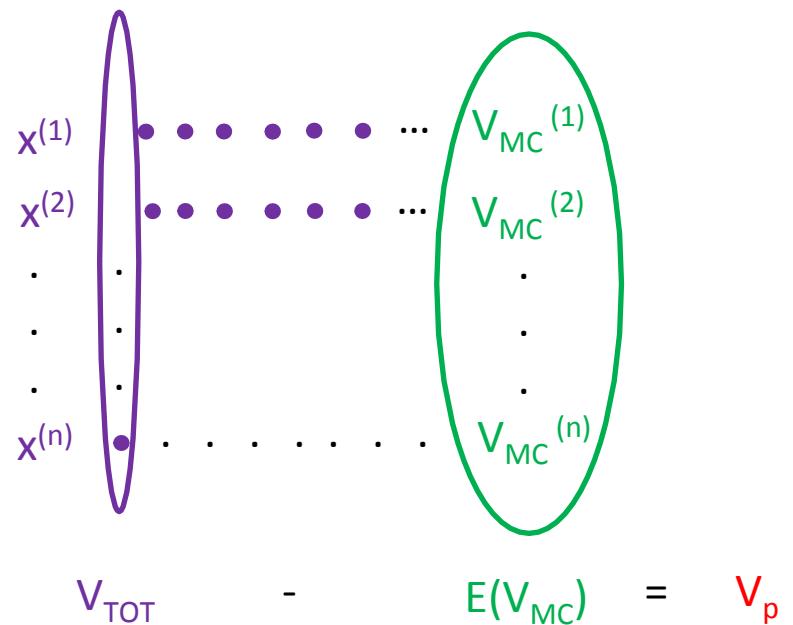
$$y^{(2)} := f(x^{(1)})^{(2)}$$

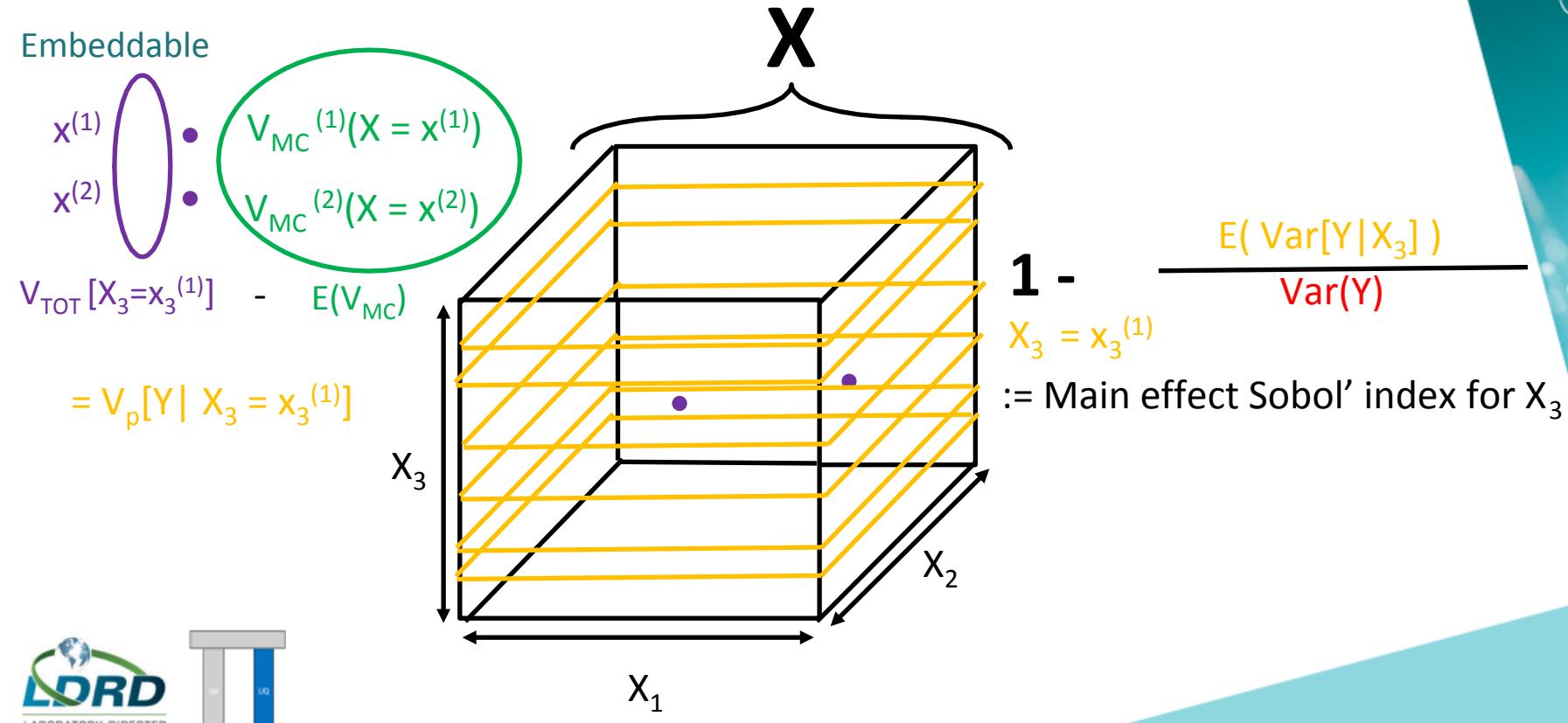
$$y^{(1)} \neq y^{(2)}$$

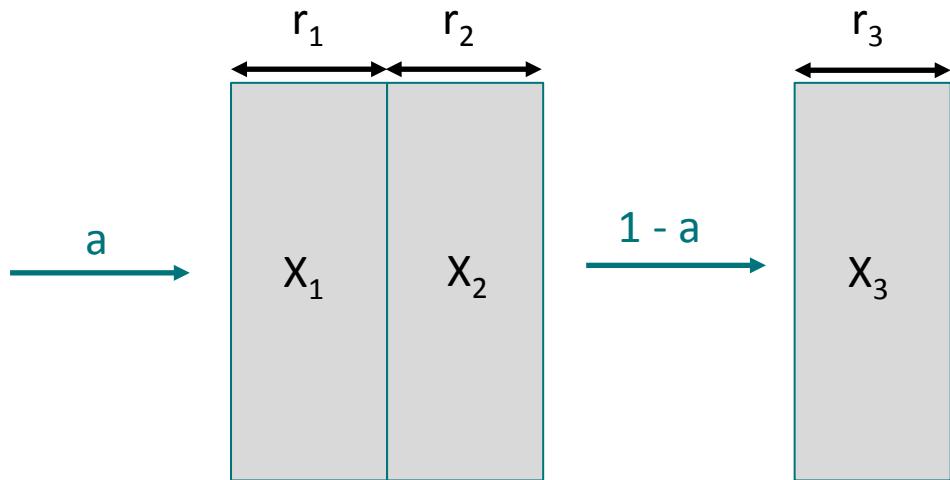
$$V_{MC}(Y | X = x^{(1)}) = \text{Var}(f(x^{(1)}))$$









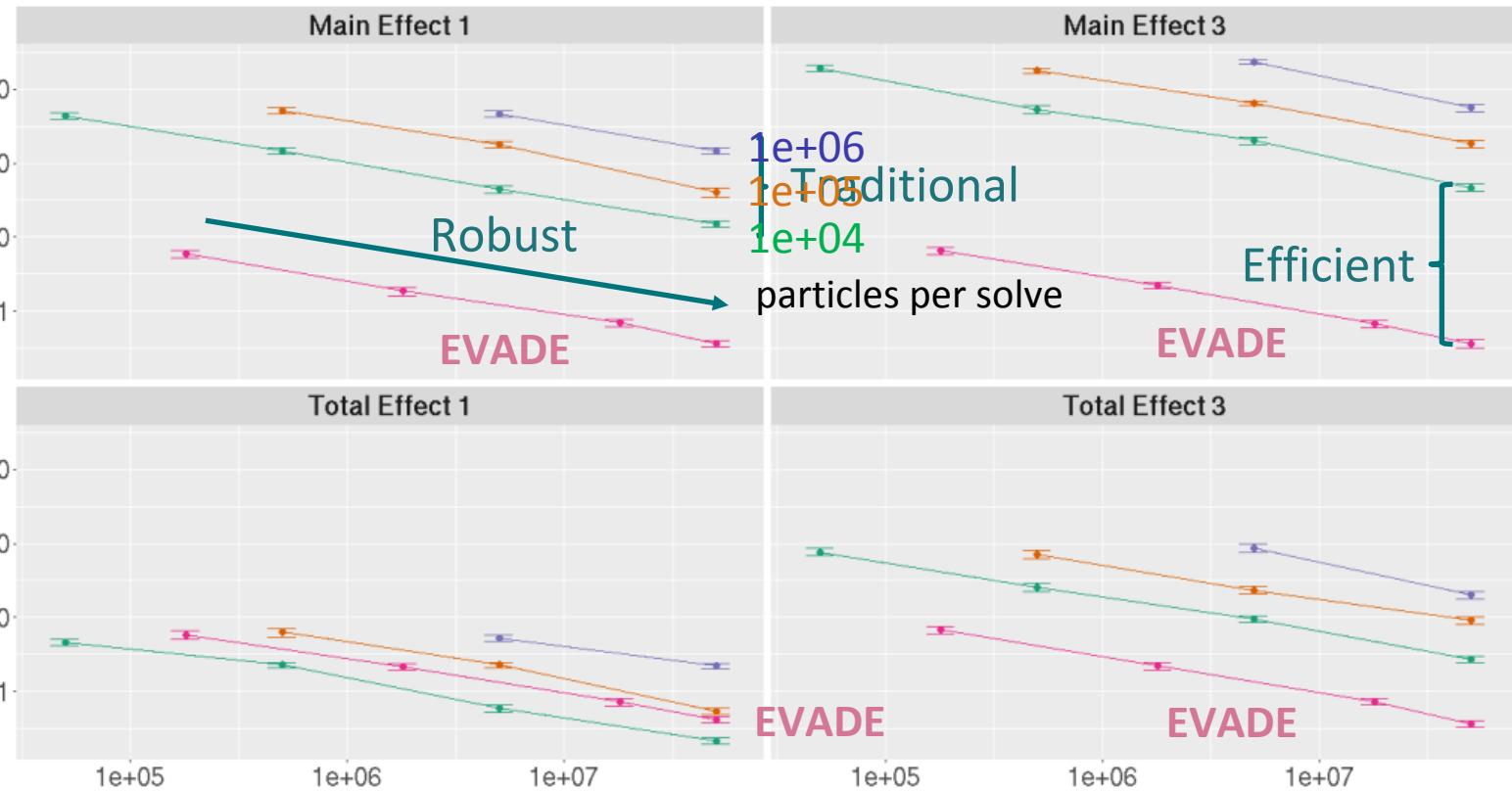


$$f(X_1, X_2, X_3) = a \exp(-r_1 X_1 - r_2 X_2 - X_3) + (1 - a) \exp(-r_3 X_3)$$

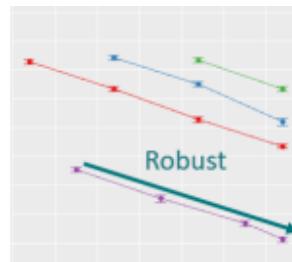
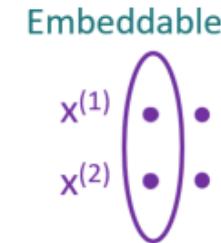
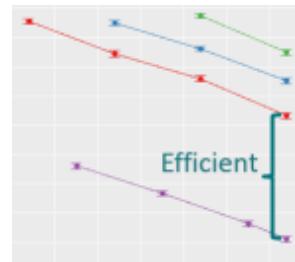
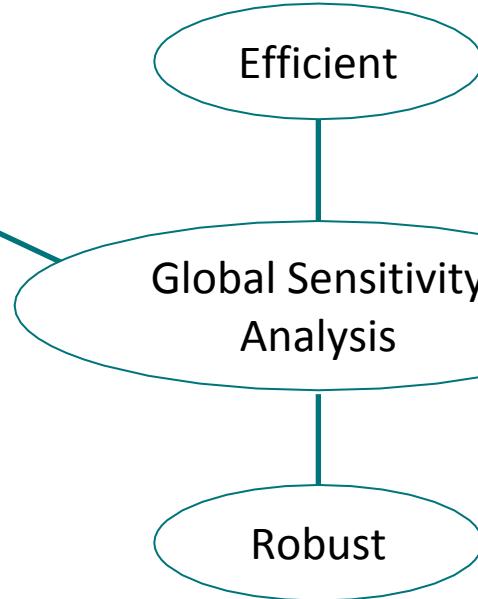


Error

Cost



Efficient, embedded  
uncertainty quantification  
Monte Carlo  
transport methods  
for the GPU



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*

for generalized mixing

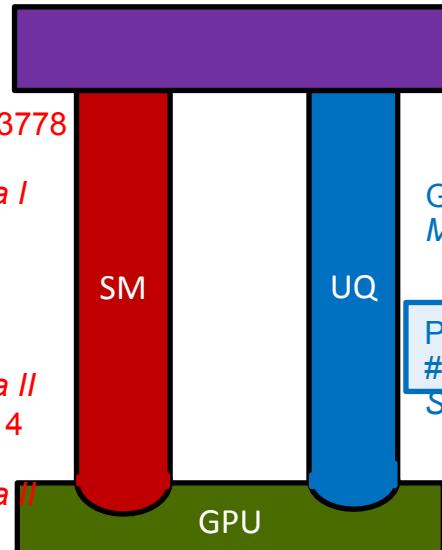
Davis, Paper #33784  
*Transport in Stochastic Media II*

memory/runtime efficiency

Vu, Paper #33614  
*Transport in Stochastic Media II*



on the GPU

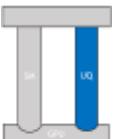


Kersting, Paper #33673  
*Monte Carlo Algorithms*

PCE surrogate models

Global sensitivity analysis

# Backup



**Main Effect 1**
**Main Effect 3**
**Total Effect 1**
**Total Effect 3**

- 1e+00 particles per solve
- 1e+01 particles per solve
- 1e+02 particles per solve
- 1e+03 particles per solve
- 1e+04 particles per solve
- 1e+05 particles per solve
- 1e+06 particles per solve
- EVADE-based

**Table 1: Benchmark function numerical results after 3e+07 particle histories**

Method	$s_1$	$s_2$	$s_3$	$s_{T_1}$	$s_{T_2}$	$s_{T_3}$
Analytic	0.0635	0.0635	0.8725	0.0638	0.0638	0.8730
1e4 hist. solve	$0.0462 \pm 0.0250$	$0.0870 \pm 0.0268$	$0.749 \pm 0.0844$	$0.0644 \pm 0.0004$	$0.0644 \pm 0.0003$	$0.876 \pm 0.0045$
1e5 hist. solve	$0.0920 \pm 0.0810$	$0.0366 \pm 0.0812$	$0.761 \pm 0.339$	$0.0641 \pm 0.0009$	$0.0646 \pm 0.0008$	$0.892 \pm 0.0156$
1e6 hist. solve	$-0.1024 \pm 0.2578$	$0.5619 \pm 0.2742$	$0.9059 \pm 1.0310$	$0.0653 \pm 0.0037$	$0.0623 \pm 0.0035$	$0.9215 \pm 0.0371$
EVADE 4 hist. plane	$0.0627 \pm 0.0006$	$0.0623 \pm 0.0009$	$0.8730 \pm 0.0007$	$0.0638 \pm 0.0007$	$0.0627 \pm 0.0009$	$0.8737 \pm 0.0006$
EVADE 30 hist. plane	$0.0634 \pm 0.0007$	$0.0645 \pm 0.0007$	$0.8729 \pm 0.0004$	$0.0642 \pm 0.0005$	$0.0638 \pm 0.0005$	$0.8722 \pm 0.0007$