



Computation of Sobol' indices using Embedded Variance Deconvolution

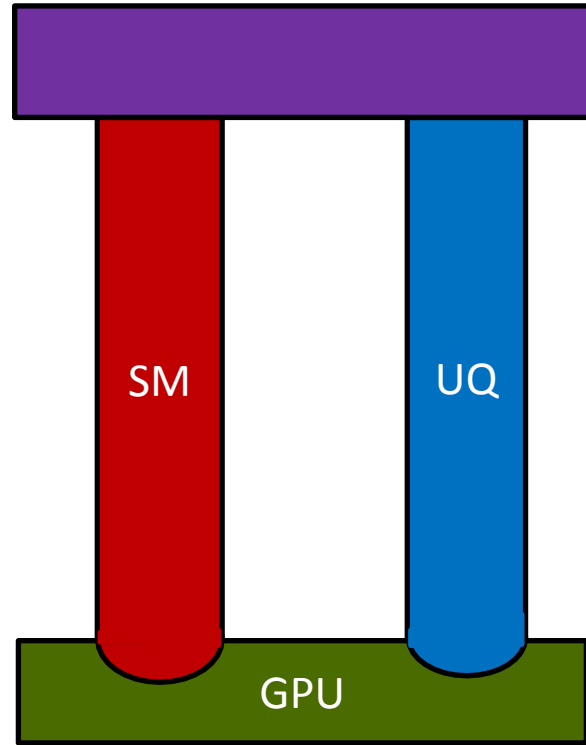
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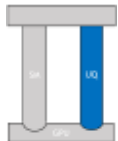
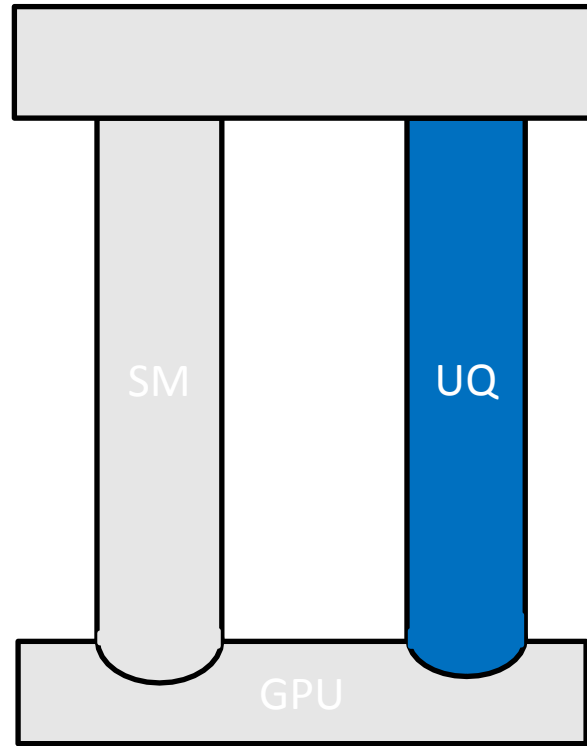
Supported by the Laboratory Directed Research and Development program at Sandia National Laboratories, a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's 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.

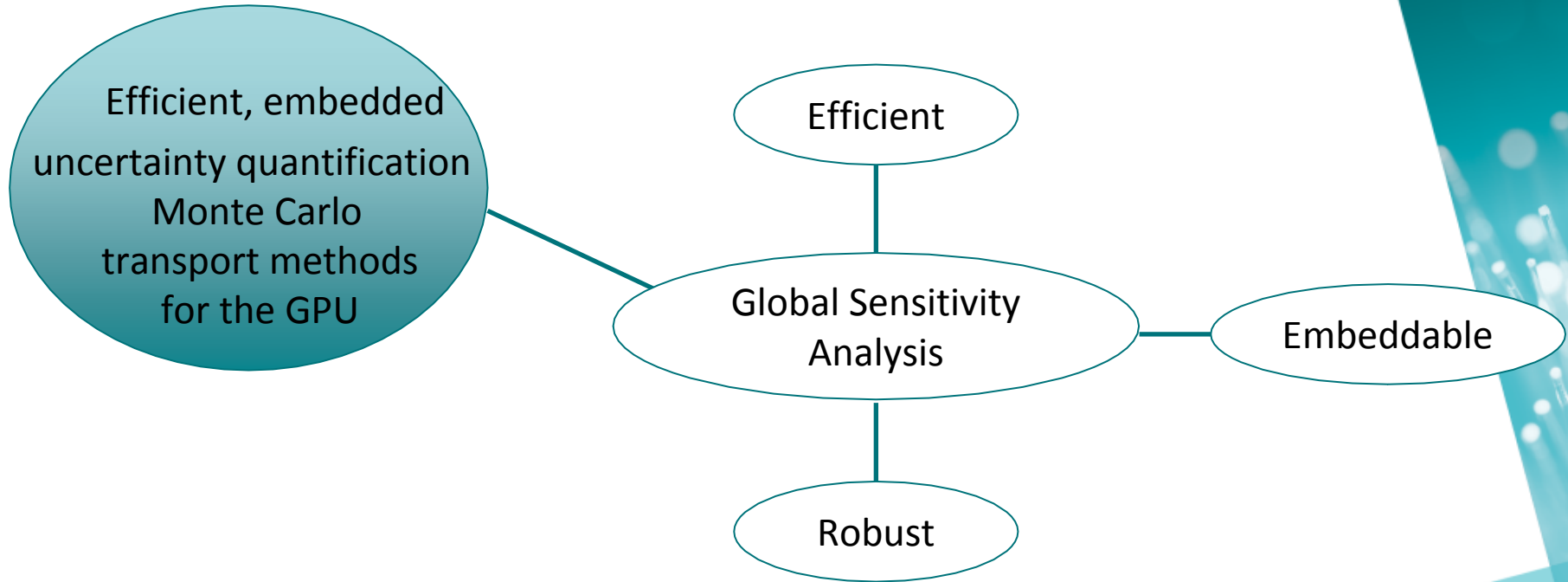


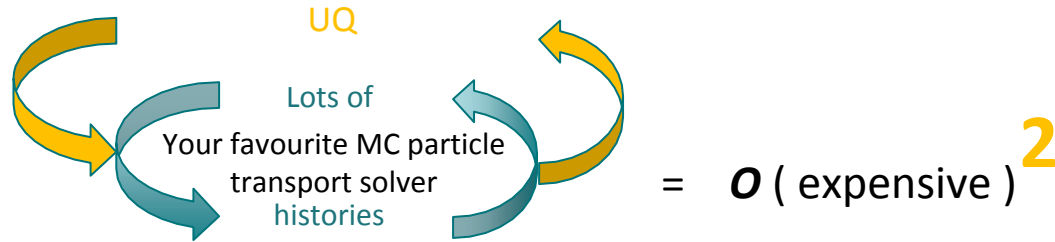
Develop efficient, embedded **stochastic media (SM)** and **uncertainty quantification (UQ)** Monte Carlo transport methods **for the GPU**.



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







Screening, emulators,
reliability methods

Embedded variance-based
sensitivity analysis

Efficient



Embeddable

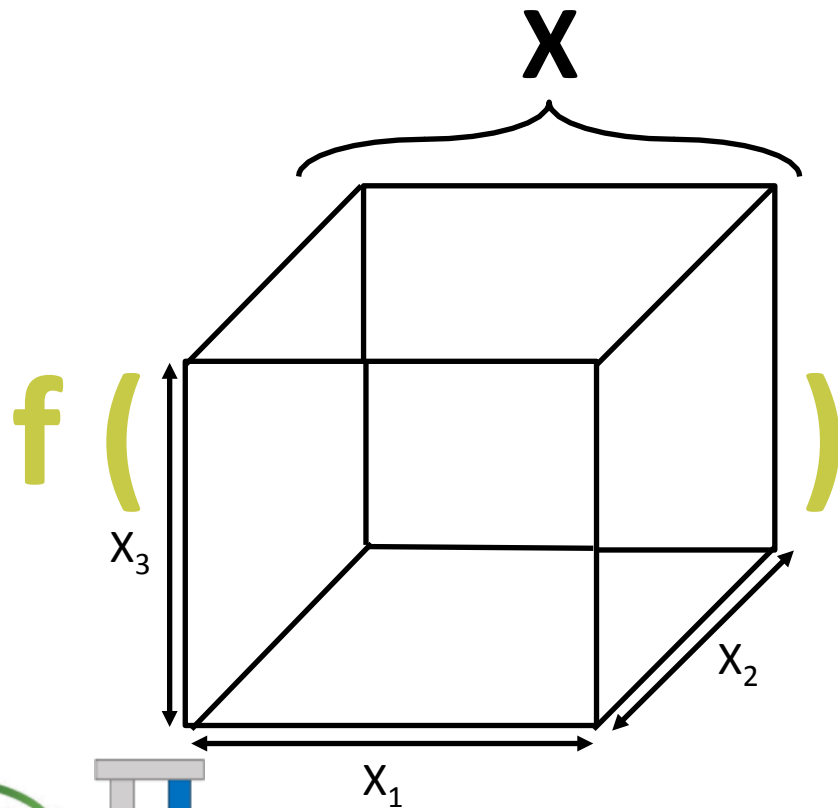


Robust

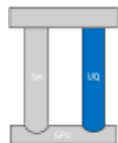
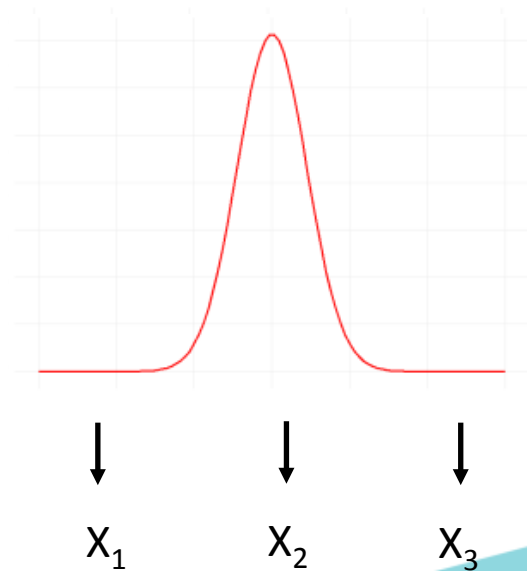


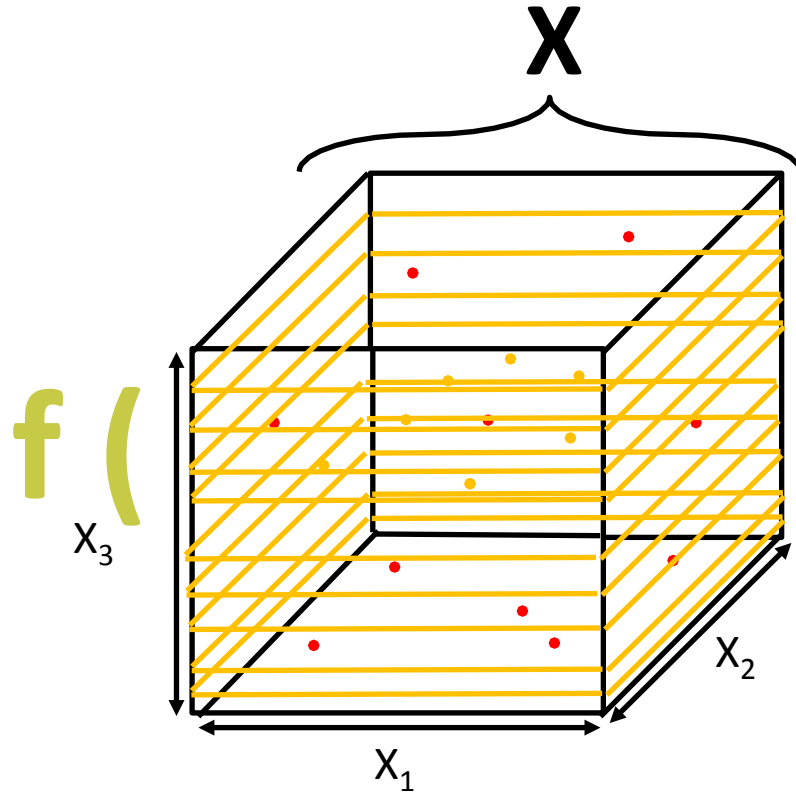
1. Sobol' indices

2. EVADE



=

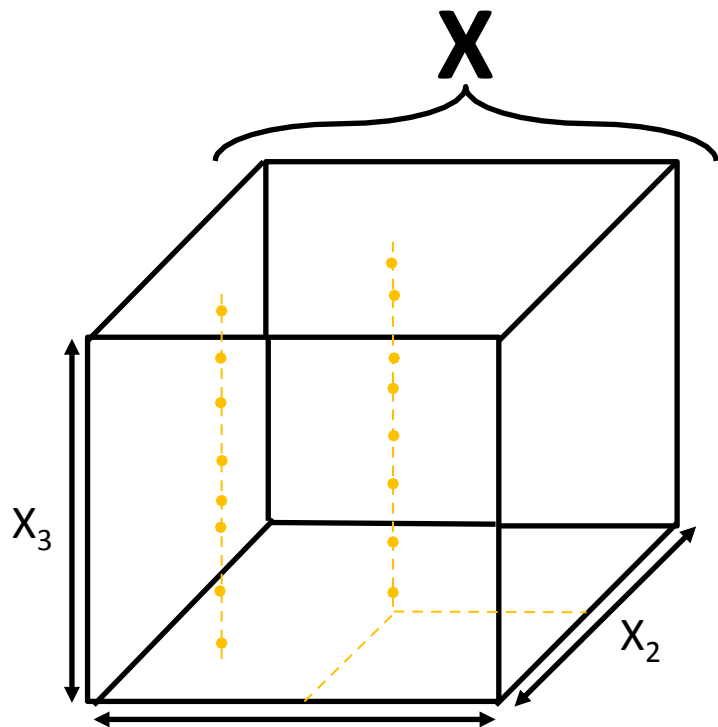




$$X_3 = x_3^{(1)}$$

$$1 - \frac{E[\text{Var}[Y|X_1, X_2, x_3^{(1)}]]}{\text{Var}(Y)}$$

:= Main effect Sobol' index for X_3


 X_1

$$(X_1, X_2) = (x_1^{(1)}, x_2^{(1)})$$

$$E(\text{Var}[Y | (X_1, X_2)]) = (x_1^{(1)}, x_2^{(1)})]$$

 $\text{Var}(Y)$

:= 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

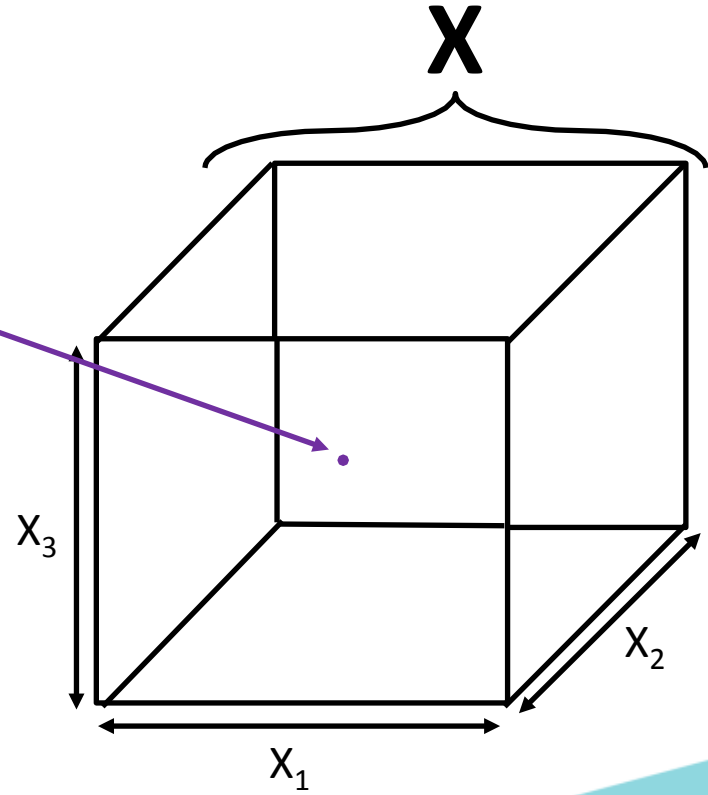
$$\mathbf{x}^{(1)} := (x_1^{(1)}, x_2^{(1)}, x_3^{(1)})$$

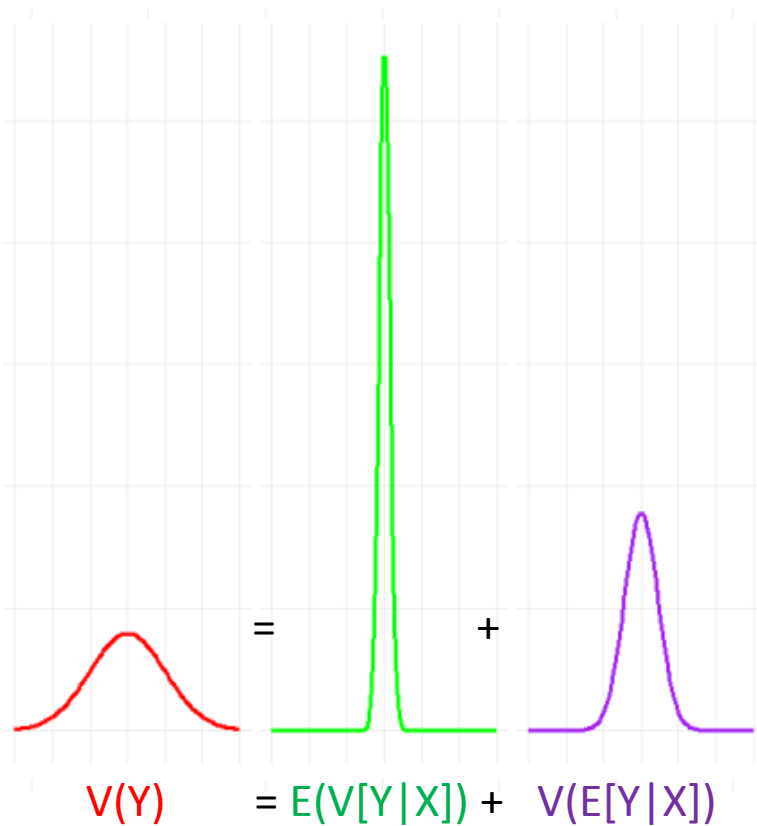
$$y^{(1)} := f(\mathbf{x}^{(1)})^{(1)}$$

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

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

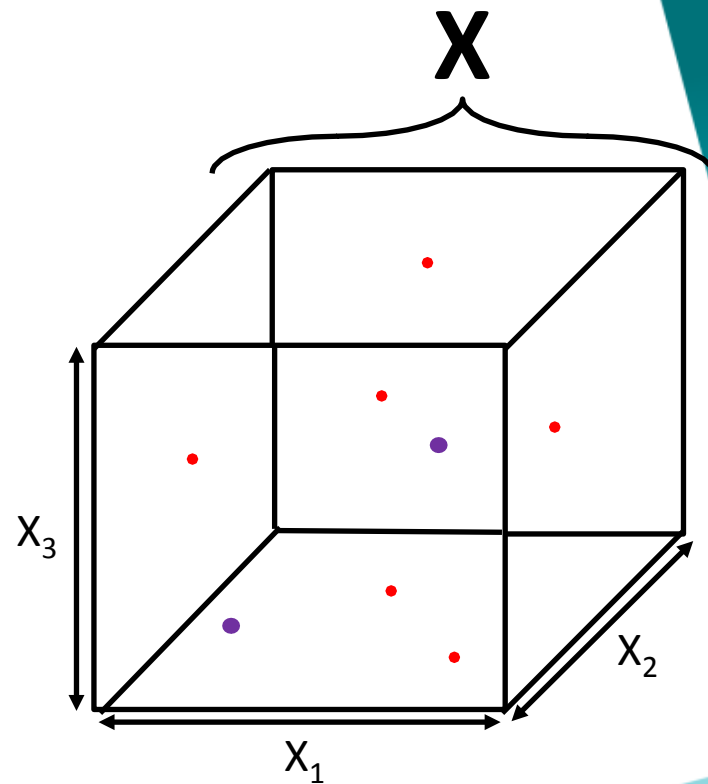
$$V_{MC}(Y | X = \mathbf{x}^{(1)}) = \text{Var}(f(\mathbf{x}^{(1)}))$$





$$\begin{array}{c}
 x^{(1)} \\
 x^{(2)} \\
 \vdots \\
 x^{(n)}
 \end{array}
 \begin{array}{c}
 \cdots \\
 \cdots \\
 \cdots \\
 \cdots
 \end{array}
 \begin{array}{c}
 V_{MC}^{(1)} \\
 V_{MC}^{(2)} \\
 \vdots \\
 V_{MC}^{(n)}
 \end{array}$$

$V_{TOT} - E(V_{MC}) = V_p$



Embeddable

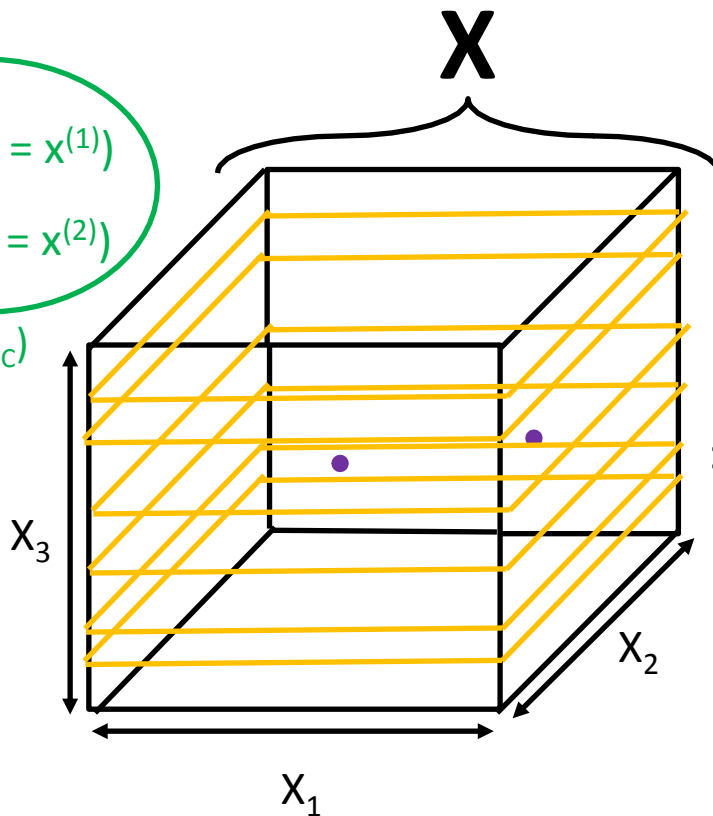
$x^{(1)}$
 $x^{(2)}$

$$V_{MC}^{(1)}(X = x^{(1)})$$

$$V_{MC}^{(2)}(X = x^{(2)})$$

$$V_{TOT}[X_3=x_3^{(1)}] - E(V_{MC})$$

$$= V_p[Y | X_3 = x_3^{(1)}]$$



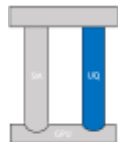
1 -

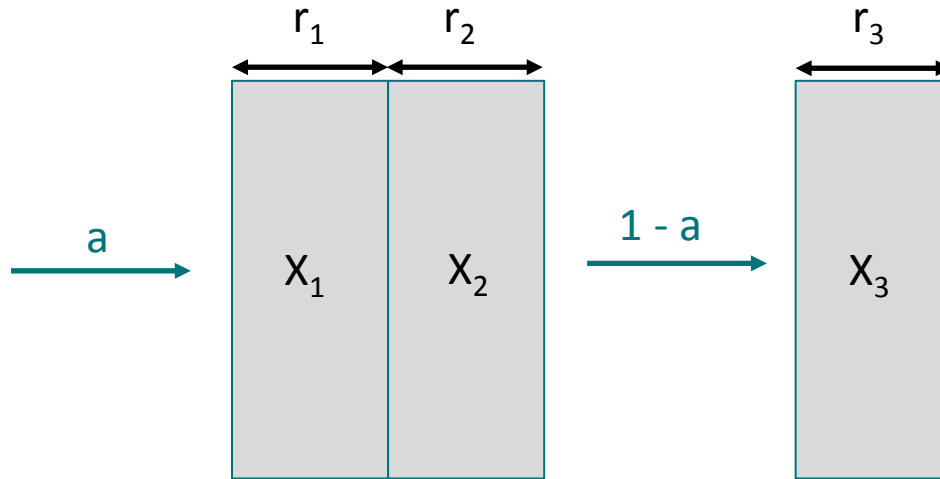
$$X_3 = x_3^{(1)}$$

:= Main effect Sobol' index for X_3

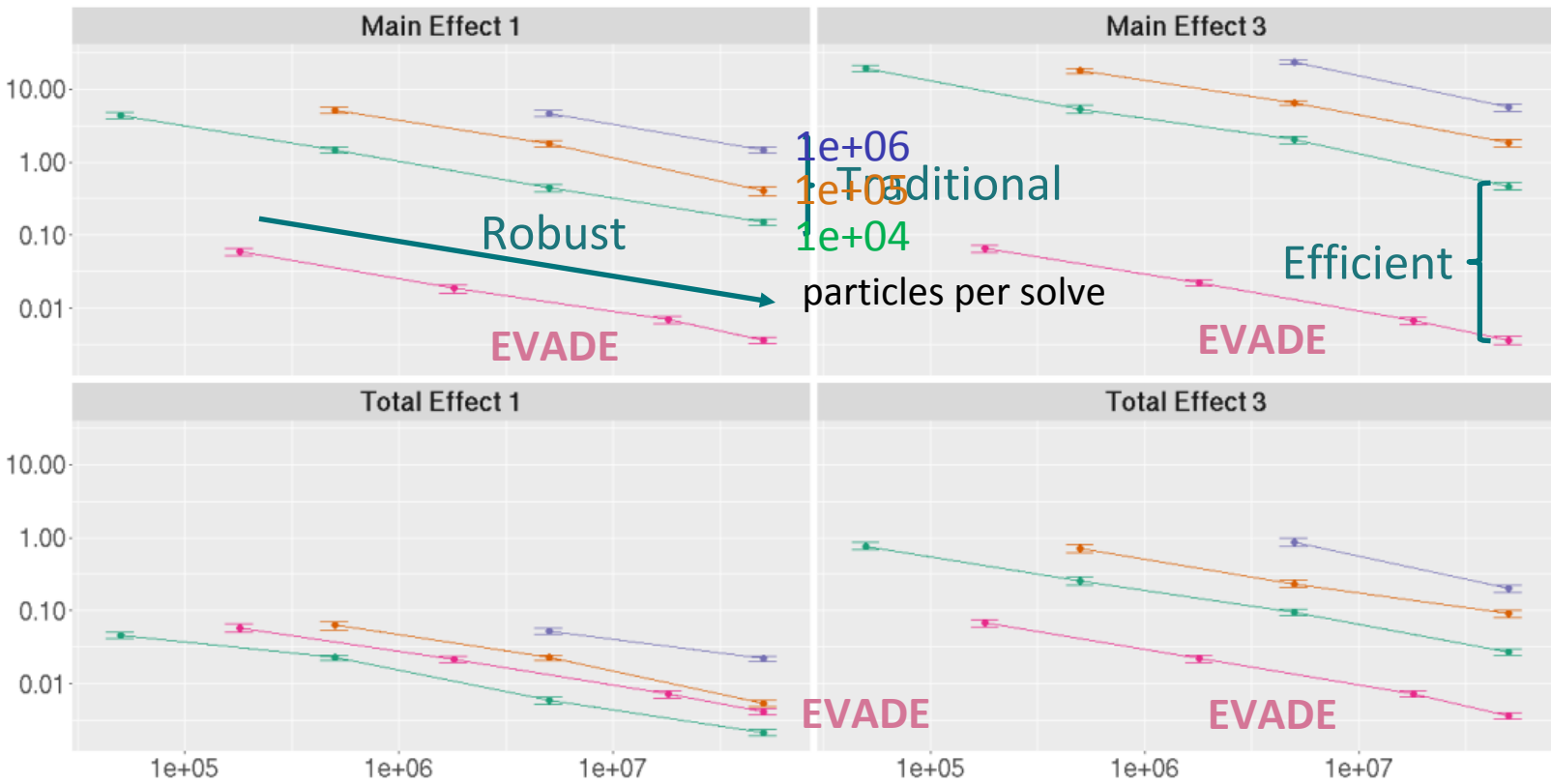
$$E(\text{Var}[Y|X_3])$$

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

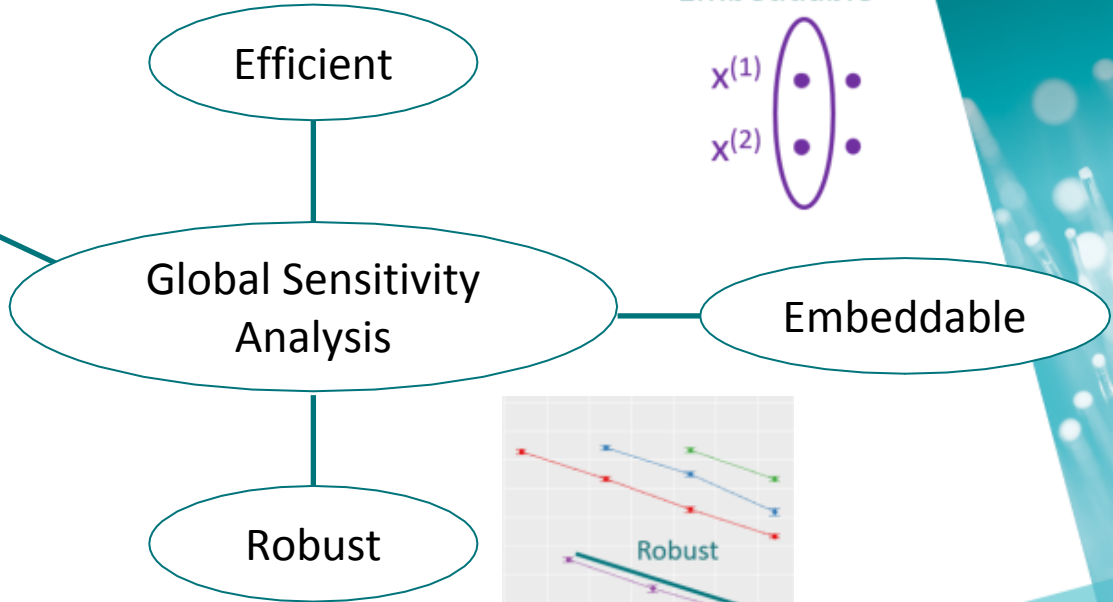




$$f(X_1, X_2, X_3) = a \exp(-r_1 X_1 - r_2 X_2 - X_3) + (1 - a) \exp(-r_3 X_3)$$



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

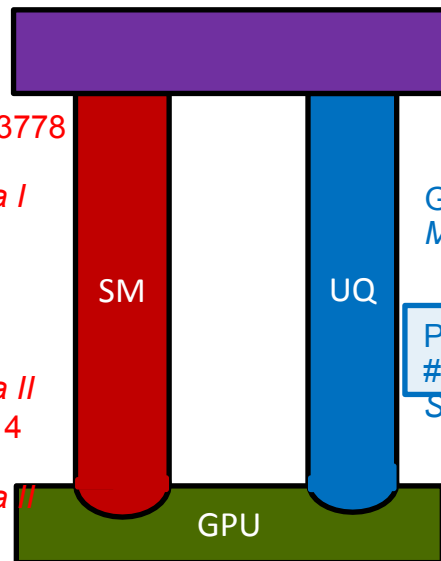
Olson, Paper #33778
*Transport in
Stochastic Media I*

**for generalized
mixing**

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

**memory/runtime
efficiency**

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



Geraci, Paper #33671
Monte Carlo Methods

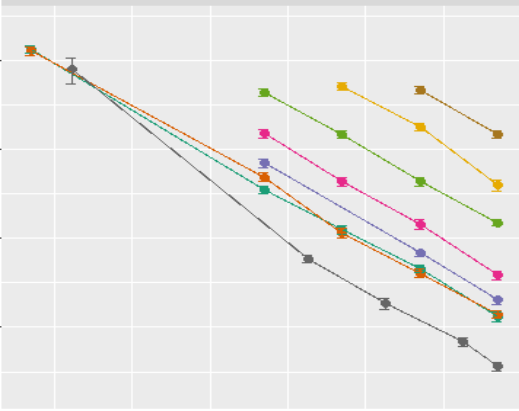
PCE surrogate models

Petticrew, Paper
#33657
Sensitivity Analysis

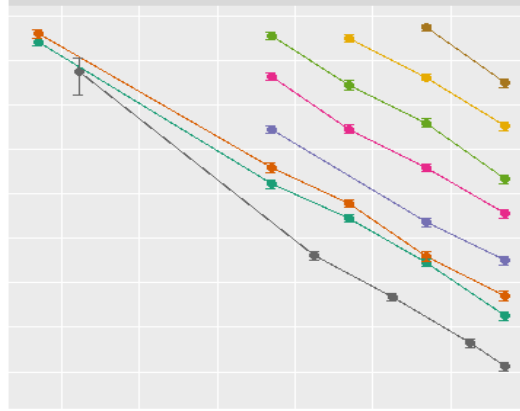
**Global sensitivity
analysis**

Backup

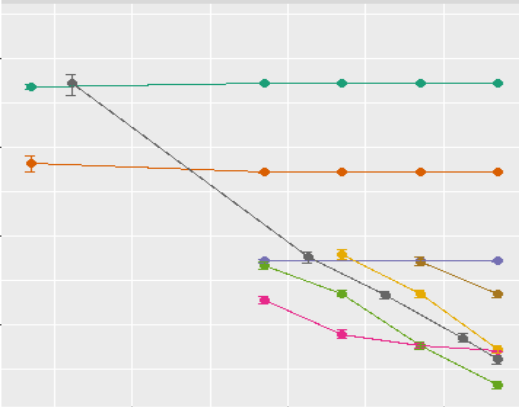
Main Effect 1



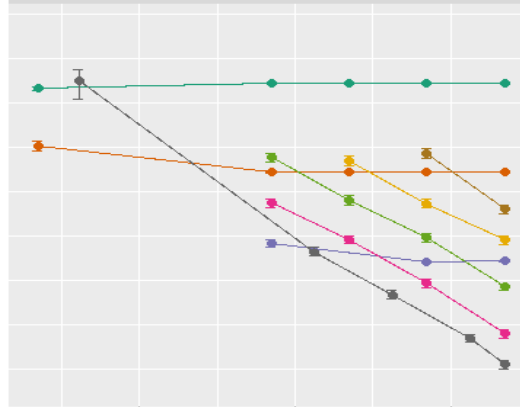
Main Effect 3



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 ± 0.0250	0.0870 ± 0.0268	0.749 ± 0.0844	0.0644 ± 0.0004	0.0644 ± 0.0003	0.876 ± 0.0045
1e5 hist. solve	0.0920 ± 0.0810	0.0366 ± 0.0812	0.761 ± 0.339	0.0641 ± 0.0009	0.0646 ± 0.0008	0.892 ± 0.0156
1e6 hist. solve	-0.1024 ± 0.2578	0.5619 ± 0.2742	0.9059 ± 1.0310	0.0653 ± 0.0037	0.0623 ± 0.0035	0.9215 ± 0.0371
EVADE 4 hist. plane	0.0627 ± 0.0006	0.0623 ± 0.0009	0.8730 ± 0.0007	0.0638 ± 0.0007	0.0627 ± 0.0009	0.8737 ± 0.0006
EVADE 30 hist. plane	0.0634 ± 0.0007	0.0645 ± 0.0007	0.8729 ± 0.0004	0.0642 ± 0.0005	0.0638 ± 0.0005	0.8722 ± 0.0007