Monte Carlo Solution for Uncertainty Propagation in Particle Transport with a Stochastic Galerkin Method

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Overview

- Given a deterministic system of equations for uncertainty quantification
  - Stochastic Collocation Method (SCM)
  - Stochastic Galerkin Method (SGM, aka SFEM)
- How do we efficiently solve these with Monte Carlo?

- We compare various approaches and implementations:
  - Brute-force (Monte Carlo approach)
  - SCM (quadrature-based approach)
    - Separate (Independent or Correlated) Calculations
    - Intrusive Correlated Sampling
  - SGM (solution of coupled equations)

Transport Equation with Random Parameters

- The mono-energetic transport equation with isotropic scattering:

$$\vec{\Omega} \cdot \nabla \psi(\vec{r}, \vec{\Omega}, \omega) + \Sigma_t(\omega)\psi(\vec{r}, \vec{\Omega}, \omega) = \frac{\Sigma_s(\omega)}{4\pi} \phi(\vec{r}, \omega)$$

- We consider the total and scattering cross sections to be independently uncertain (and the distribution of uncertainty is uniform):

$$\Sigma_t(\omega) = \langle \Sigma_t \rangle + \widehat{\Sigma}_t \, \xi_t(\omega) \qquad \Sigma_s(\omega) = \langle \Sigma_s \rangle + \widehat{\Sigma}_s \, \xi_s(\omega)$$

- Using the polynomial chaos spectral approach, we represent the angular flux as an expansion of random Legendre polynomials:

$$\begin{aligned} \psi(\vec{r}, \vec{\Omega}, \omega) &\equiv \psi(\vec{r}, \vec{\Omega}, \xi_t(\omega), \xi_s(\omega)) \\ &= \sum_{l=0}^{\infty} \sum_{m=0}^{\infty} \psi_{l,m}(\vec{r}, \vec{\Omega}) \, P_l(\xi_t(\omega)) P_m(\xi_s(\omega)) \end{aligned}$$

- The flux expansion coefficients are found from orthogonality:

$$\psi_{l,m}(\vec{r}, \vec{\Omega}) = a_{lm} \int_{-1}^{1} \int_{-1}^{1} \psi(\vec{r}, \vec{\Omega}, \xi_t(\omega), \xi_s(\omega)) \, P_l(\xi_t(\omega)) P_m(\xi_s(\omega)) d\xi_t d\xi_s \qquad a_{lm} = (2l+1)(2m+1)$$

Uncertainty Propagation by Monte Carlo

- The brute-force approach, which we use for benchmarking purposes, is to randomly sample from the uncertain cross section distribution:

$$\Sigma_t(\xi_t) = \langle \Sigma_t \rangle + \widehat{\Sigma}_t \, \xi_t \qquad \Sigma_s(\xi_s) = \langle \Sigma_s \rangle + \widehat{\Sigma}_s \, \xi_s$$

- Solve the transport problem for that realization:

$$\vec{\Omega} \cdot \nabla \psi(\vec{r}, \vec{\Omega}, \xi_t, \xi_s) + \Sigma_t(\xi_t) \psi(\vec{r}, \vec{\Omega}, \xi_t, \xi_s) = \frac{\Sigma_s(\xi_s)}{4\pi} \, \phi(\vec{r}, \xi_t, \xi_s)$$

- Tally each flux result, either as a histogram distribution or as distribution moments:

$$\psi_{l,m}(\vec{r}, \vec{\Omega}) = a_{lm} \int_{-1}^{1} \int_{-1}^{1} \psi(\vec{r}, \vec{\Omega}, \xi_t, \xi_s) \, P_l(\xi_t) P_m(\xi_s) d\xi_t d\xi_s$$

Uncertainty Propagation
by the Stochastic Collocation Method

- In SCM, the integration of the flux expansion moments

$$\psi_{l,m}(\vec{r},\vec{\Omega}) = a_{lm} \int_{-1}^{1}\int_{-1}^{1} \psi(\vec{r},\vec{\Omega},\xi_t,\xi_s)\, P_l(\xi_t) P_m(\xi_s) d\xi_t d\xi_s$$

  is replaced by a quadrature rule:

$$\psi_{l,m}(\vec{r},\vec{\Omega}) \approx a_{lm} \sum_{k=1}^{K}\sum_{n=1}^{K} w_k\, w_n \psi_{k,n}(\vec{r},\vec{\Omega})\, P_l(\xi_t^k) P_m(\xi_s^n)$$

- The flux at each quadrature point is determined by solving the transport equation with cross sections evaluated at the corresponding point. In general, this does not require a modification of the transport code.

$$\vec{\Omega}\cdot\nabla\psi_{k,n}(\vec{r},\vec{\Omega}) + \Sigma_t^k \psi_{k,n}(\vec{r},\vec{\Omega}) = \frac{\Sigma_s^n}{4\pi}\, \phi_{k,n}(\vec{r})$$

Uncertainty Propagation by SCM with Correlated Random Number Sequences

- For each quadrature cross section pair, we solve the transport equation using the same *random number sequence* for each corresponding history.

Uncertainty Propagation by SCM with Correlated Sampling Monte Carlo

- For each quadrature cross section pair, we solve the transport equation using the same *random numbers* to achieve the same sample outcomes along the same particle path for each corresponding history.

- The latter imposes greater correlation to achieve better efficiency but does require modifications to the Monte Carlo transport code.

Correlated Sampling in Monte Carlo

- We sample event outcomes using a nominal cross section case. We adjust the particle weight based on the probability of the sampled outcome in each SCM case. As in biasing schemes, the weight adjustment is the ratio of the true probability of an outcome to the probability as simulated.

$$w_{out,k,n} = \frac{p_{k,n}}{p_{sim}} w_{in,k,n}$$

- We are biasing the sampled distance to interaction and the absorption probability. (Our nominal case uses survival biasing.) The following weight adjustments are made when a particle moves and interacts:

$$w_{out,k,n} = \frac{\langle \Sigma_t \rangle + \widehat{\Sigma}_t \xi_t^k}{\langle \Sigma_t \rangle} \exp\left[-\widehat{\Sigma}_t \xi_t^k s \right] w_{in,k,n}$$ Particle moves to an interaction

$$w_{out,k,n} = \exp\left[-\widehat{\Sigma}_t \xi_t^k s \right] w_{in,k,n}$$ Particle moves to a non-interaction

$$w_{out,k,n} = \frac{\langle \Sigma_s \rangle + \widehat{\Sigma}_s \xi_s^k}{\langle \Sigma_t \rangle + \widehat{\Sigma}_t \xi_t^k} w_{in,k,n}$$ Particle interaction event

- Since the nominal case is the same for all quadrature points, an array of weights can be used to track and tally all cases in a single simulation.

Uncertainty Propagation by the Stochastic Galerkin Method

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- In SGM, we exploit the orthogonality of the uncertainty basis functions

$$\xi P_m(\xi) = \frac{m+1}{2m+1} P_{m+1}(\xi) + \frac{m}{2m+1} P_{m-1}(\xi)$$

to derive an infinite set of coupled moment equations:

$$\vec{\Omega} \cdot \nabla \psi_{l,m}(\vec{r}, \vec{\Omega}) + \langle \Sigma_t \rangle \psi_{l,m}(\vec{r}, \vec{\Omega}) + \hat{\Sigma}_t \left[\left(\frac{l+1}{2l+3} \right) \psi_{l+1,m} + \left(\frac{l}{2l-1} \right) \psi_{l-1,m} \right]$$
$$= \frac{\langle \Sigma_s \rangle}{4\pi} \phi_{l,m}(\vec{r}) + \frac{\hat{\Sigma}_s}{4\pi} \left[\left(\frac{m+1}{2m+3} \right) \phi_{l,m+1} + \left(\frac{m}{2m-1} \right) \phi_{l,m-1} \right]$$

These equations can be truncated in various ways. We consider truncations at $l + m = K - 1$, resulting in $K(K+1)/2$ moments (designated SG-1) and at $l = K - 1$ and $m = K - 1$ resulting in K^2 moments (designated SG-2)

Uncertainty Propagation by SGM using Interaction-Based Weight Adjustments

- We regroup the equation and write it in matrix notation as

$$\vec{\Omega} \cdot \nabla \mathbf{\Psi} + \mathbf{A_t} \mathbf{\Psi} = \hat{\mathbf{A}}_\mathbf{t} \mathbf{\Psi} + \mathbf{A_s} \int_{4\pi} \mathbf{\Psi} d\Omega$$

- We sample distance to interaction

$$\vec{\Omega} \cdot \nabla \mathbf{\Psi} + \langle \Sigma_t \rangle \mathbf{\Psi} = 0$$

- We randomly select between scattering and streaming events, with the fraction of scattering events given by

$$f_s = \frac{\langle \Sigma_s \rangle + \hat{\Sigma}_s}{\hat{\Sigma}_t + \langle \Sigma_s \rangle + \hat{\Sigma}_s}$$

and particle weight adjustments given by either

$$\mathbf{w_o} = -\mathbf{w_i} \frac{1}{1 - f_s} \frac{\hat{\mathbf{A}}_\mathbf{t}}{\langle \Sigma_t \rangle} \quad \text{or} \quad \mathbf{w_o} = \mathbf{w_i} \frac{1}{f_s} \frac{\mathbf{A_s}}{\langle \Sigma_t \rangle}$$

Uncertainty Propagation by SGM using Streaming- and Scattering-Based Weight Adjustments

- Using the same matrix notation, we again sample distance to interaction as

$$\vec{\Omega} \cdot \nabla \mathbf{\Psi} + \langle \Sigma_t \rangle \mathbf{\Psi} = 0$$

- Weights are adjusted for streaming based on the eigenvalue problem

$$\vec{\Omega} \cdot \nabla \mathbf{\Psi} = \hat{\mathbf{A}}_{\mathbf{t}} \mathbf{\Psi}$$

with the general solution

$$\vec{\psi}(\vec{r}_0 + s\vec{\Omega}) = \sum_{j=1}^{J} c_j \vec{V}_j \exp\left(\lambda_j s\right) \quad \text{, where} \quad \sum_{j=1}^{J} c_j \vec{V}_j = \vec{\psi}(\vec{r}_0)$$

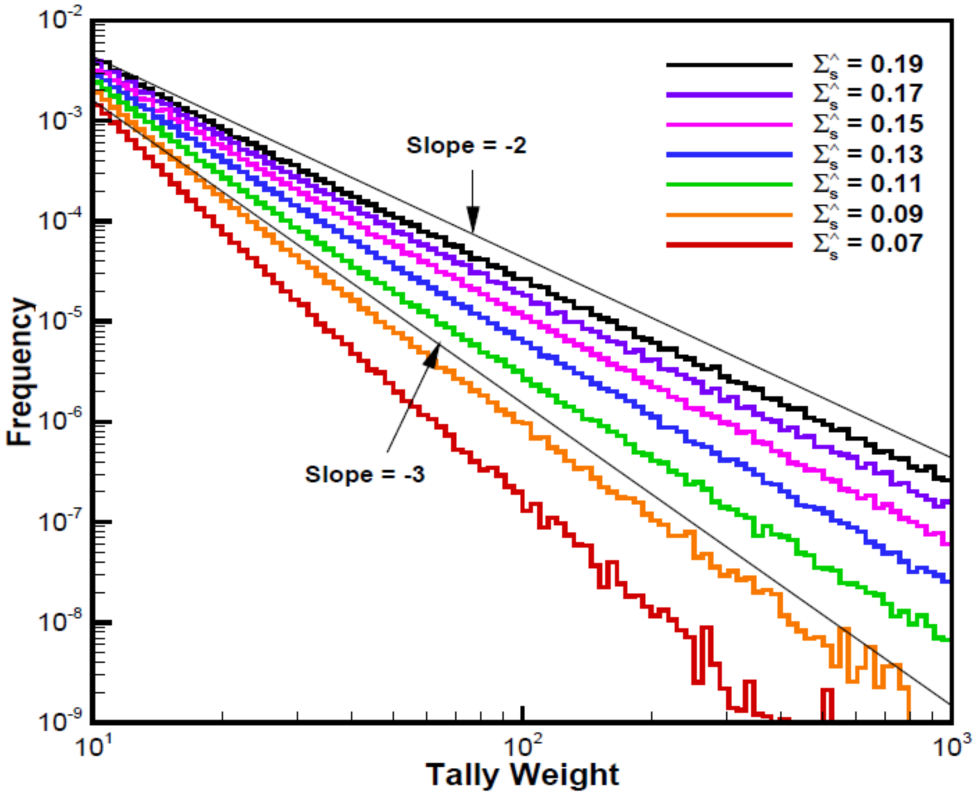
- Scattering interactions are based on

$$\vec{\Omega} \cdot \nabla \mathbf{\Psi} = \frac{\langle \Sigma_s \rangle}{\langle \Sigma_t \rangle} \frac{\mathbf{A_s}}{\langle \Sigma_s \rangle} \int_{4\pi} \mathbf{\Psi} d\Omega$$

where the ratio of the mean cross sections can be treated by sampling for particle absorption or treated as a survival biasing weight adjustment.

Stability Limitations in the Stochastic Galerkin Method

- The uncertainty in the cross sections imposes stability limitations on the SGM equations. With no uncertainty in the total cross section, we can show that ratio of the absorption cross section to the (uniform) uncertainty in the scattering cross section must be greater than the largest point in a Gauss-Legendre quadrature of order K.



	$\hat{\Sigma}_t$				
$\hat{\Sigma}_s$	0.00	0.01	0.02	0.04	0.08
0.03	-8.35	-7.47	-5.51	-4.09	-2.76
0.05	-4.59	-4.52	-4.04	-3.16	-2.45
0.07	-3.61	-3.42	-3.19	-2.72	-2.24
0.09	-3.01	-2.91	-2.76	-2.46	-2.08
0.11	-2.65	-2.59	-2.48	-2.26	-1.97
0.13	-2.39	-2.36	-2.28	-2.11	-1.87
0.15	-2.21	-2.19	-2.13	-2.00	-1.80
0.17	-2.08	-2.05	-2.01	-1.90	-1.74
0.19	-1.97	-1.95	-1.92	-1.82	-1.69

Test Problems

- Two test problems use slab thickness of 1.0 and the following parameters:

Problem Number	$\langle\Sigma_t\rangle$ (cm^{-1})	$\langle\Sigma_s\rangle$ (cm^{-1})	$\widehat{\Sigma}_t$ (cm^{-1})	$\widehat{\Sigma}_s$ (cm^{-1})
1	1.0	0.5	0.1	0.05
2	5.0	2.5	0.5	0.25

- In both cases, c=0.5 and uncertainties are ±10%.
- Benchmark calculations used 10^5 histories in 10^6 realizations.
- SGM and SCM calculations used 10^7 histories with K=4.
- We have examined other test problems and concluded that the method is stable and effective as long as:

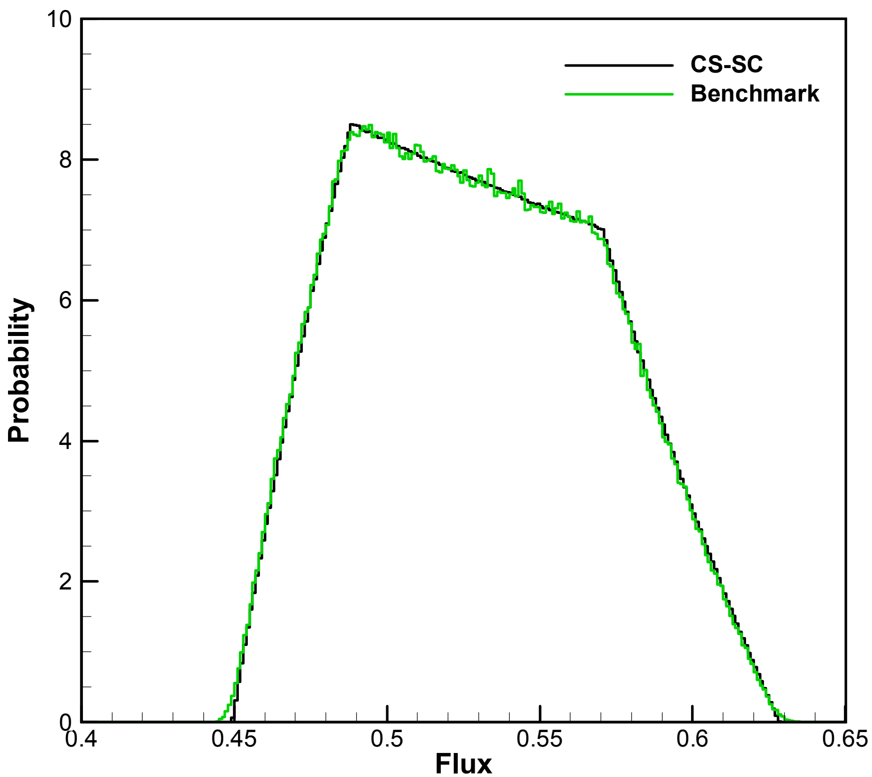
$$\Sigma_t^k > 0,\ \Sigma_s^n > 0, \text{ and } \Sigma_a^{k,n} > 0$$

- Making Σ_a uncertain, rather than Σ_t, may be a more natural approach.

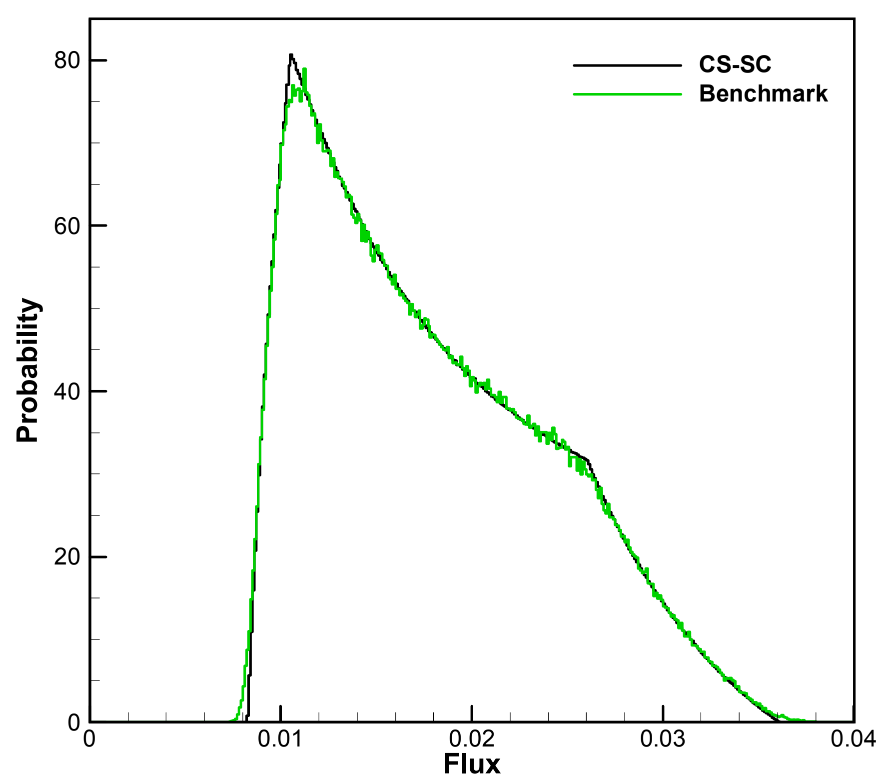
Results: Uncertainty Distributions

- $\psi(\vec{r}, \vec{\Omega}, \omega)$ distributions are obtained by randomly sampling $\xi_t(\omega)$ and $\xi_s(\omega)$ and using the flux-moment results to evaluate:

$$\psi(\vec{r}, \vec{\Omega}, \omega) = \sum_{l=0}^{K-1} \sum_{m=0}^{K-1} \psi_{l,m}(\vec{r}, \vec{\Omega}) \, P_l(\xi_t(\omega)) P_m(\xi_s(\omega))$$



Problem #1



Problem #2

Results: Figures-of-Merit

$$FOM = \frac{1}{\sigma^2 T}$$

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Problem #1:

Flux Moment		Figure of Merit						
			SCM			SGM		
l,m	$\psi_{l,m}$	MC	I-SC	CR-SC	CS-SC	SG-1S	SG-2S	SG-2I
0,0	5.30E-1	3.9E+3	5.1E+5	5.2E+4	3.0E+5	4.0E+4	3.9E+4	2.2E+5
0,1	2.38E-2	5.8E-3	4.5E+2	1.2E+4	5.0E+4	7.6E+3	7.4E+3	2.7E+4
0,2	7.51E-4	a	2.7E-1	6.2E+3	3.5E+4	5.8E+3	5.6E+3	1.7E+4
0,3	2.09E-5	a	a	3.1E+3	1.6E+4	3.1E+3	3.0E+3	9.1E+3
1,1	-4.74E-3	a	8.0E+0	3.1E+2	3.2E+4	4.7E+3	4.6E+3	8.5E+3
2,2	2.43E-5	a	a	4.6E+0	8.1E+3	b	1.5E+3	1.6E+3
3,3	-1.15E-7	a	a	4.9E-2	2.4E+3	b	4.9E+2	3.5E+2
Time (s):		44190	6589	7424	739	5306	5448	575

a Results are omitted for values with standard deviation greater than 10%.

b Flux moments omitted from the SG-1S calculation.

- Without converged benchmark results, the accuracy of the higher SCM moments might be questioned, but all results reported are within reasonable statistical agreement.

Results: Figures-of-Merit

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Problem #1:

Flux Moment		Figure of Merit						
			SCM			SGM		
l,m	$\psi_{l,m}$	MC	I-SC	CR-SC	CS-SC	SG-1S	SG-2S	SG-2I
0,0	1.78E-2	1.4E+2	5.3E+3	4.9E+2	2.3E+3	3.2E+2	3.1E+2	3.0E+3
0,1	2.58E-3	2.6E-2	3.4E+1	6.9E+2	2.8E+3	4.2E+2	4.0E+2	2.5E+3
0,2	2.23E-4	a	1.4E-1	1.0E+3	4.3E+3	6.4E+2	6.2E+2	1.9E+3
0,3	1.57E-5	a	a	1.3E+3	5.5E+3	8.2E+2	8.0E+2	1.8E+3
1,1	-1.84E-3	1.6E-2	7.1E+0	2.8E+2	3.0E+3	4.4E+2	4.2E+2	2.6E+3
2,2	5.72E-5	a	a	4.2E+1	3.9E+3	b	5.8E+2	2.3E+3
3,3	-1.19E-6	a	a	3.3E+0	3.6E+3	b	5.2E+2	1.3E+3
Time (s):		57210	6380	5576	683	5876	6053	591

a Results are omitted for values with standard deviation greater than 10%.

b Flux moments omitted from the SG-1S calculation.

- Without converged benchmark results, the accuracy of the higher SCM moments might be questioned, but all results reported are within reasonable statistical agreement.

Conclusions

- The SCM correlated random number sequence approach is effective for calculating low-order moments of uncertainty distributions.
- While the SCM correlated-sampling approach is most efficient, it has drawbacks:
  - It requires an intrusive implementation: modifying the particle weight array, adding the biasing-based weight-adjustment logic, and implementing the array-based tally logic.
  - It may introduce memory issues when scaled to large numbers of uncertain parameters, high quadrature orders, and/or highly differential tallies.
- The stochastic Galerkin method (SGM) has better scaling than SCM (with tensor product quadrature) for large numbers of uncertain parameters.
- The most appealing approach for us appears to be a post-processing tool that uses correlated-sampling weight manipulation to enable SCM with any quadrature scheme, including adaptive sparse-grid quadrature.

Backup Slides

Results: Uncertainty Distributions

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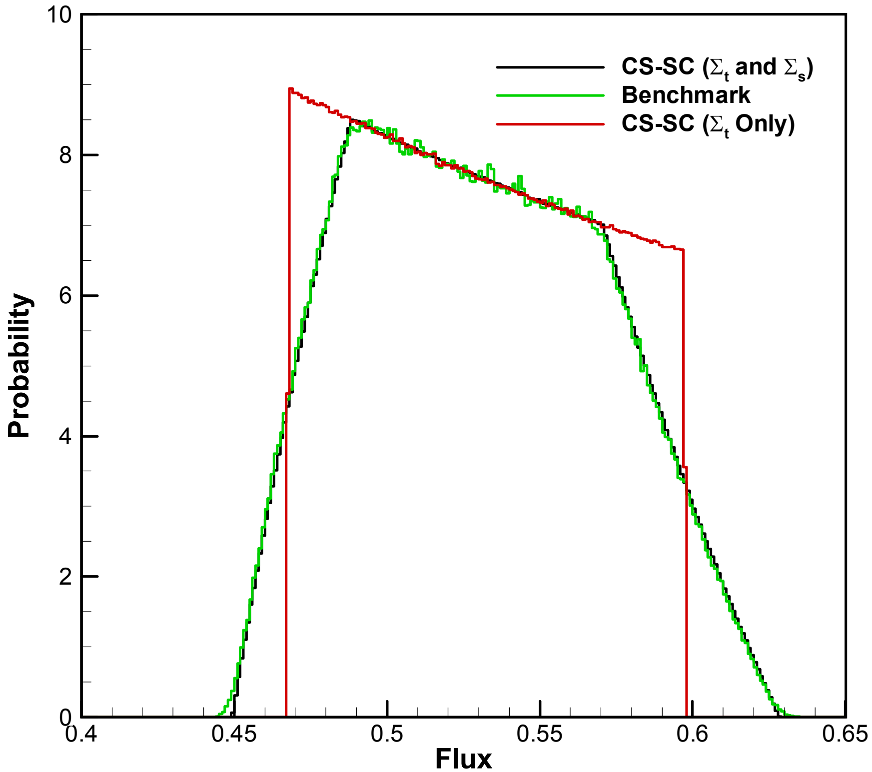

Problem #1

Results: Convergence Behavior

- Representative behavior is shown here for the moment $\psi_{2,2}$