

# Development of Continuous-Energy Eigenvalue Sensitivity Coefficient Calculation Methods in the Shift Monte Carlo Code

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# Introduction

- The need to model more complex problems with increased accuracy has motivated the extension of TSUNAMI-3D's eigenvalue sensitivity coefficient methodology to continuous-energy applications.
- Fundamental limitations in the TSUNAMI methodology prevent its use for continuous-energy sensitivity coefficient calculations, and there has been a push to develop new methods for sensitivity coefficient calculations.
- This study examines two existing methods for performing eigenvalue sensitivity coefficient calculations, and introduces two new methods that show potential for continuous-energy applications.
- These methods were implemented in the Shift Monte Carlo code within the Denovo framework of the SCALE code package.
- Each method was used to obtain sensitivity coefficients for several test problems, and was compared in terms of accuracy, speed, and efficiency.

# Contributon Method

- The Contributon Method calculates the importance of a neutron during a collision by simulating secondary neutrons at the site of the collision and tracking how many fissions are created by each secondary particle.
- The importance of an event is given by:

$$\phi^*(\tau_s) = \int_V G(\tau_s \rightarrow r) F^*(r) dr ,$$

where...

$G(\tau_s \rightarrow r)$  = The number of fission neutrons created at  $r$  by a neutron originating in phase space  $\tau_s$ .

$F^*(r)$  = The average importance of a fission neutron born at  $r$ .

# CLUTCH Method



- A new method for calculating sensitivity coefficients has been developed based on Contribution Theory. This method, known as the CLUTCH (Contribution-Linked eigenvalue sensitivity/Uncertainty estimation via Tracklength importance Characterization) method, requires the simulation of **no** secondary particles, and instead calculates the importance of a neutron by examining its random walk postmortem.

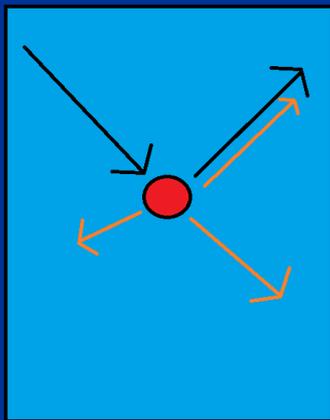


Illustration of the  
Contribution Process

- The implementation, performance, and memory requirements of the CLUTCH method are similar to that of the Differential Operator method for calculating sensitivity coefficients.
- The CLUTCH method requires the calculation of  $F^*(r)$  before tallying sensitivity coefficients.

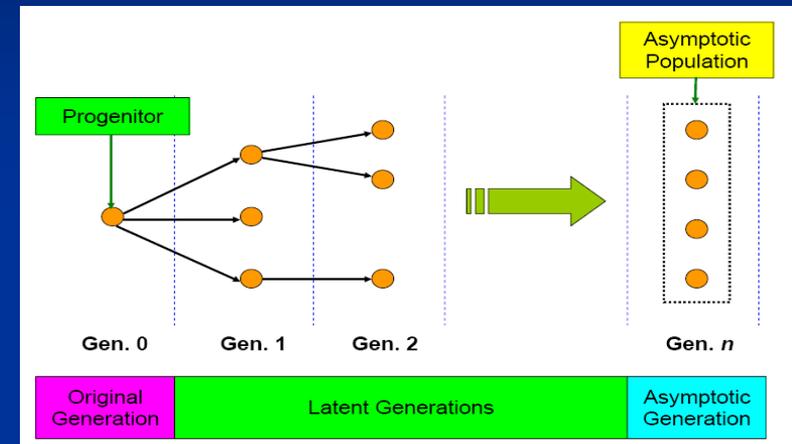
# Iterated Fission Probability Method

- The Iterated Fission Probability (IFP) method calculates adjoint-weighted tallies by assuming that the importance of a neutron at a collision is proportional to the “asymptotic population” of neutrons in some future generation that are progeny of the original neutron.
- When calculating sensitivity coefficients, the IFP method stores data (reaction rates, flux tallies, etc.) for every neutron for some number of “latent generations” until tallying the asymptotic population associated with the original event.
- The IFP method allows for accurate sensitivity coefficient calculations with a small increase in problem runtime, but can have large memory requirements for complex systems.
- The number of latent generations used by the IFP method was varied in this study so that the IFP sensitivity coefficient calculations used a minimum number of latent generations.
- An IFP calculation using 20 latent generations was used to generate reference sensitivity coefficients for this study.

# Contributon-IFP Hybrid Method

New Method!

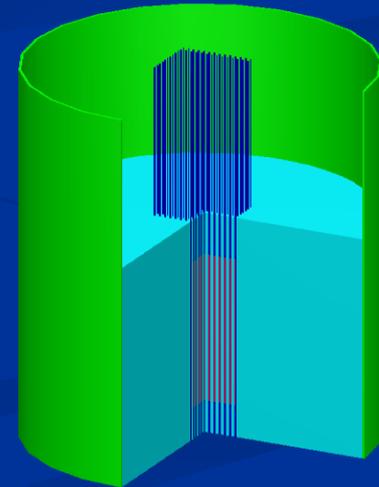
Illustration of the IFP Process [7]



- A new sensitivity coefficient method has been developed that combines the IFP approach for calculating the importance of an event using its asymptotic population with the Contributon notion of simulating secondary particles.
- Instead of storing reaction rate tallies for a number of latent generations when a progenitor causes a fission event, this new approach uses that same number of latent generations of secondary particles to simulate the fission chain created by the fission event.
- This creates an estimate for the asymptotic population for an event before allowing the initiating particle to continue its random walk, and greatly reduces the memory requirements of the method.

# Method Proof of Principle

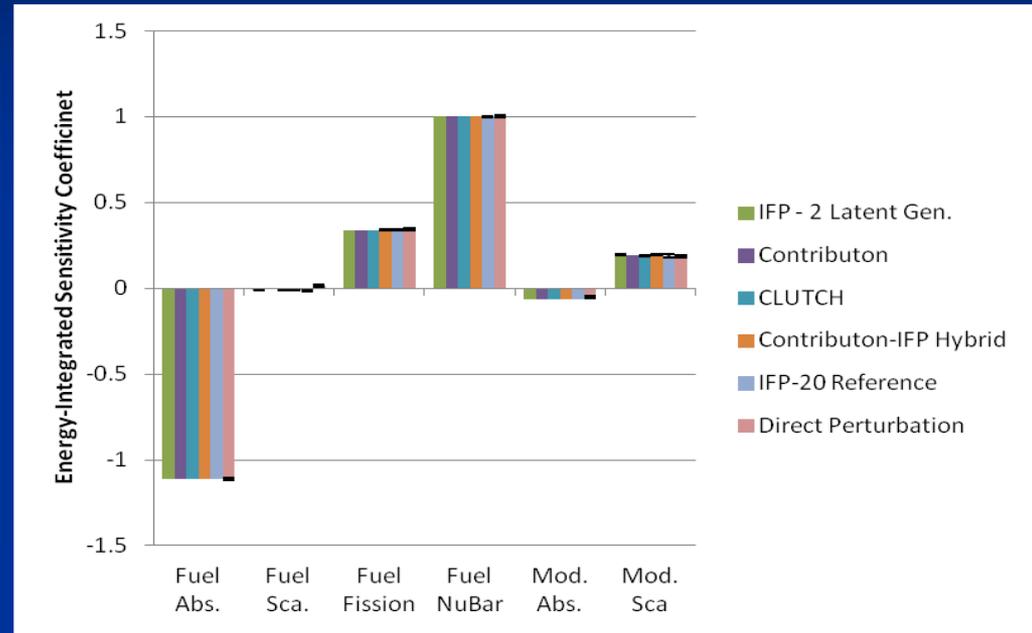
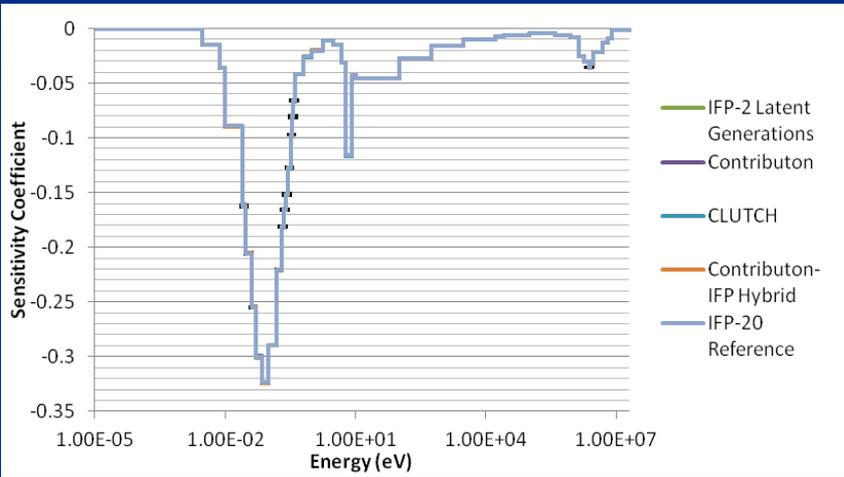
- The energy-, material-, and reaction-dependent sensitivity coefficients calculated using each method were compared with those from a reference IFP simulation in Shift using 20 latent generations, and also to Direct Perturbation calculations.
- The difference between the reference and calculated sensitivity coefficients was expressed in terms of the effective number of standard deviations, and a chi-squared test was performed on these quantities to determine if the calculations differed significantly.
- All calculations used a 44-group cross-section library that was generated by CENTRM.
- The test problems examined in this study include:
  - An infinitely-reflected, 2.7%-enriched, PWR fuel pin
  - Godiva
  - MIX-COMP-THERM-004-001, a benchmark model of a criticality safety accident where a cask containing an assembly of reprocessed fast reactor fuel is partially flooded with water. Referred to in this study as MCT.



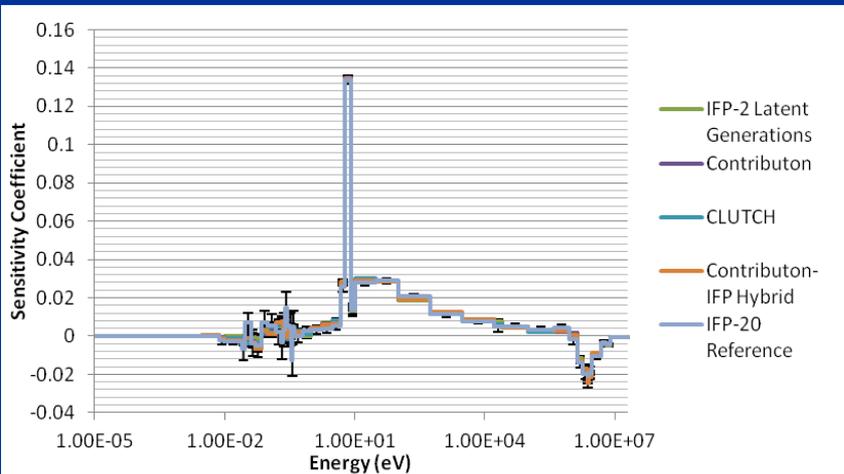
KENO-3D image of the MCT problem.

# Fuel Pin Sensitivity Coefficients

## Fuel Absorption Sensitivity Coefficient



## Moderator Scatter Sensitivity Coefficient

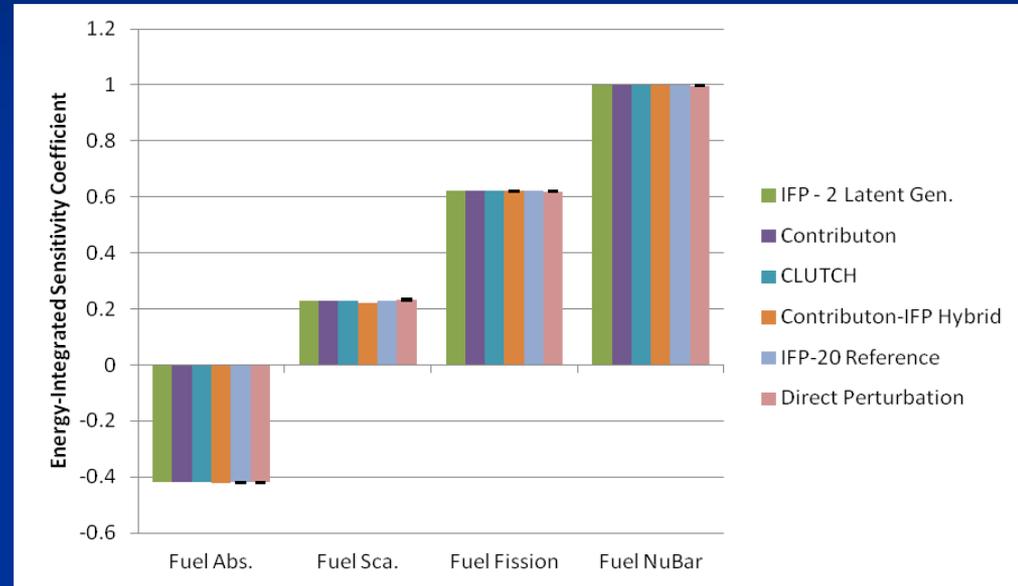
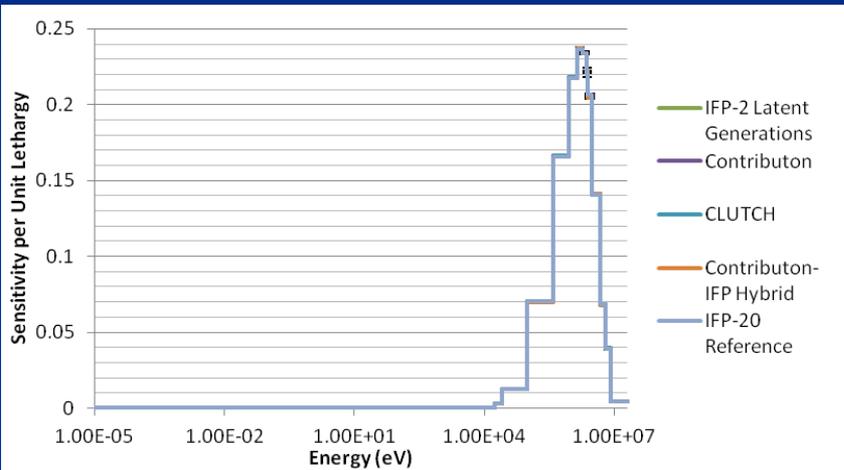


## Energy-Integrated Sensitivity Coefficients

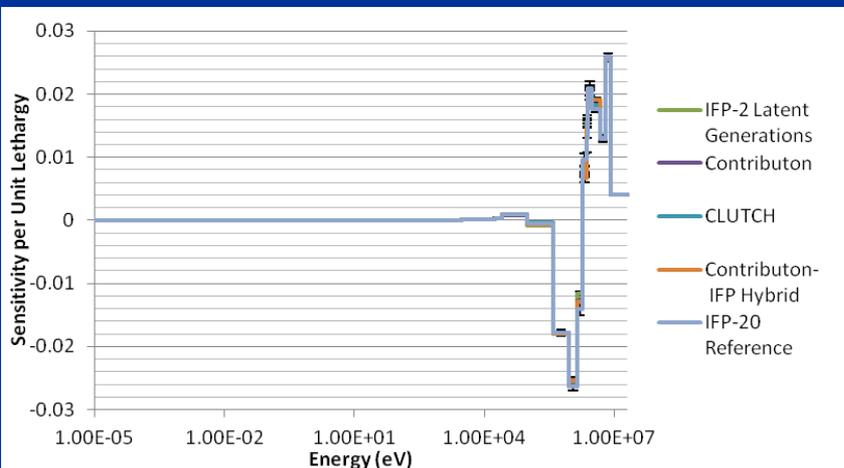
|                | <b>IFP-2</b> | <b>Contrib.</b> | <b>CLUTCH</b> | <b>Contrib.-IFP Hybrid</b> |
|----------------|--------------|-----------------|---------------|----------------------------|
| Norm. $\chi^2$ | 0.7062       | 0.8358          | 0.7831        | 0.7929                     |
| p-value        | 0.9999       | 0.9790          | 0.9964        | 0.9948                     |

# Godiva Sensitivity Coefficients

## Fuel Fission Sensitivity Coefficient



## Fuel Fission Spectrum Sensitivity Coefficient

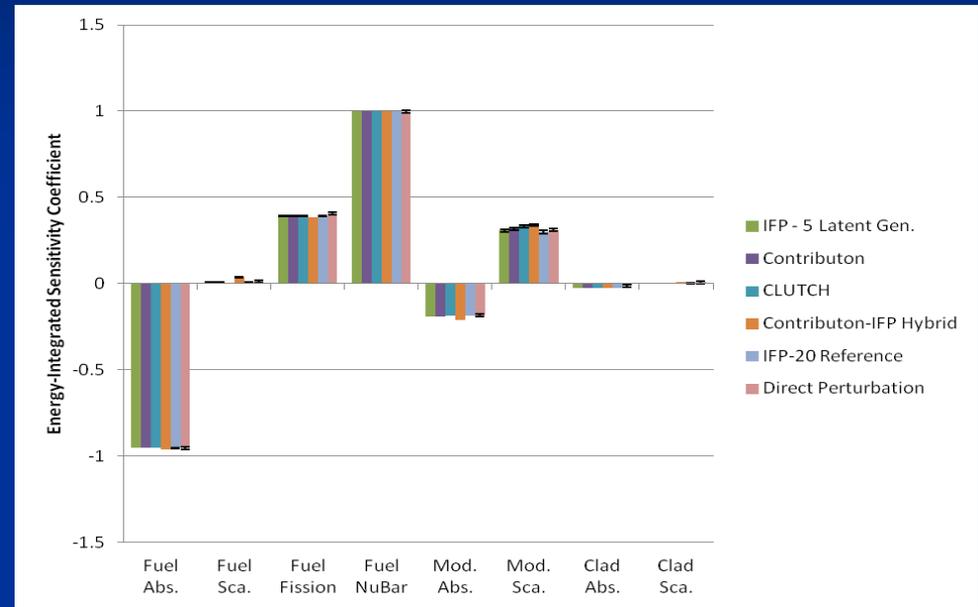
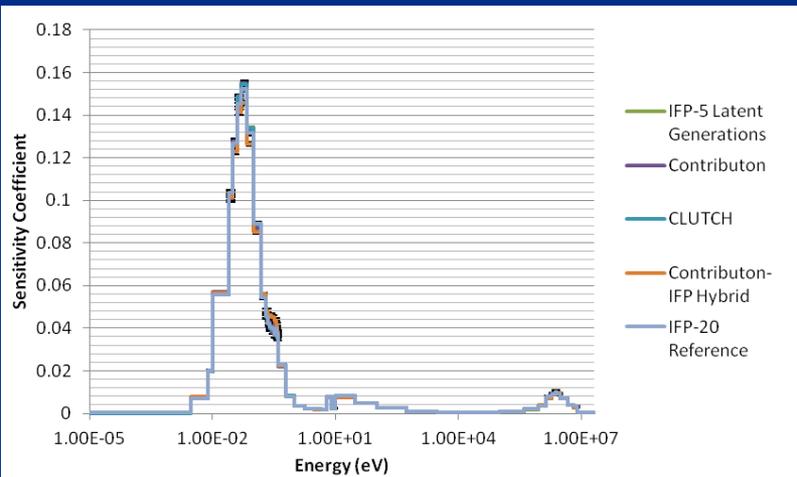


## Energy-Integrated Sensitivity Coefficients

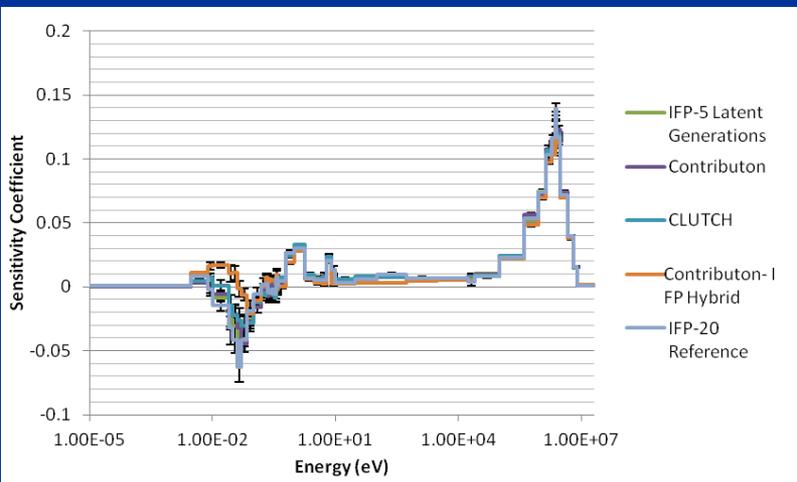
|                | <b>IFP-2</b> | <b>Contrib.</b> | <b>CLUTCH</b> | <b>Contrib.-<br/>IFP Hybrid</b> |
|----------------|--------------|-----------------|---------------|---------------------------------|
| Norm. $\chi^2$ | 0.9815       | 0.9247          | 0.8967        | 1.5607                          |
| p-value        | 0.5242       | 0.6622          | 0.7258        | 0.0013                          |

# MCT Sensitivity Coefficients

## Fuel Fission Sensitivity Coefficient



## Moderator Scatter Sensitivity Coefficient



## Energy-Integrated Sensitivity Coefficients

|                | <b>IFP-5</b> | <b>Contrib.</b> | <b>CLUTCH</b> | <b>Contrib.-<br/>IFP Hybrid</b> |
|----------------|--------------|-----------------|---------------|---------------------------------|
| Norm. $\chi^2$ | 0.6534       | 1.0803          | 1.0716        | 57.8276                         |
| p-value        | 0.9999       | 0.1437          | 0.1701        | 0.0000                          |

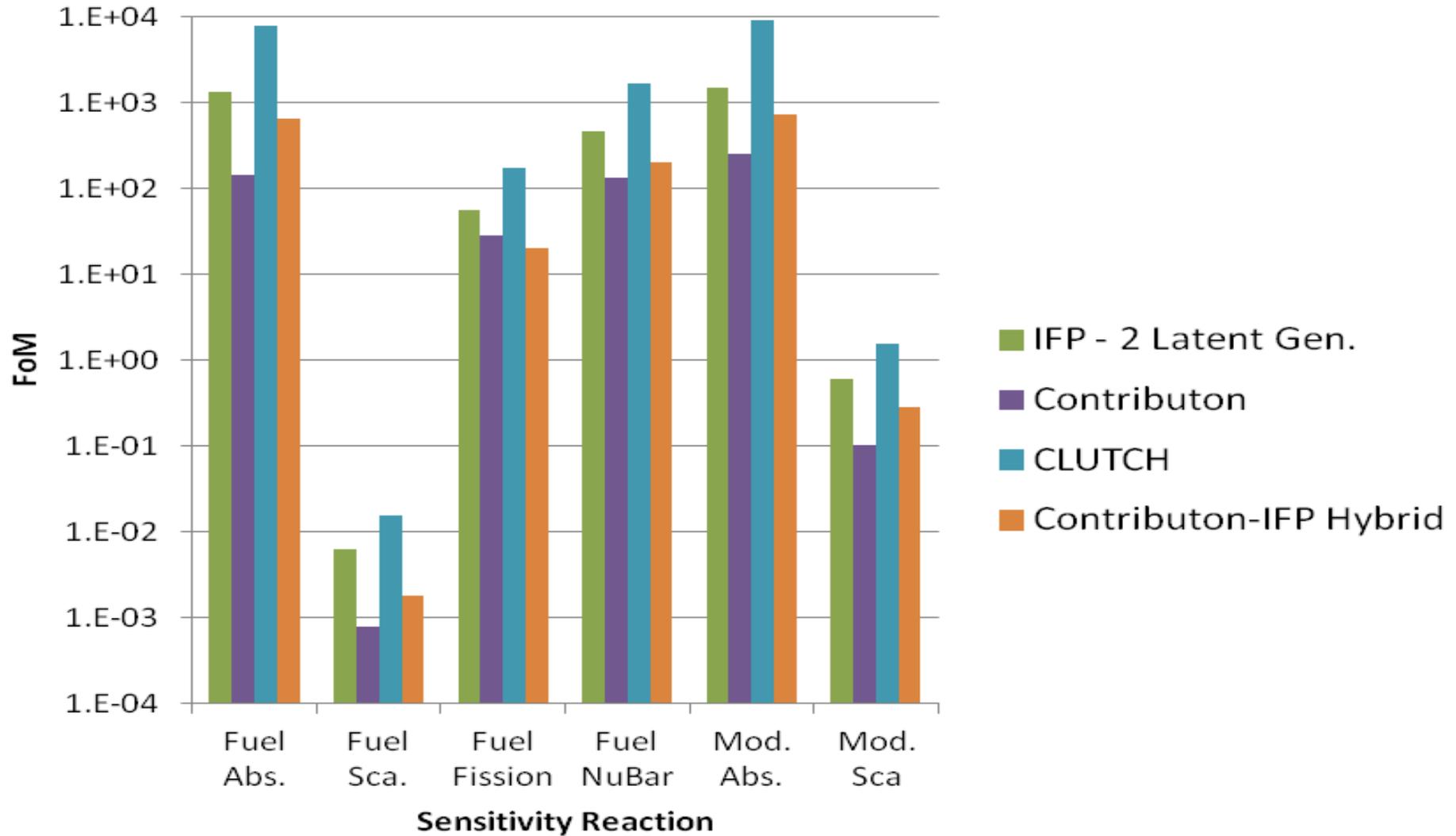
# Sensitivity Method Efficiency Comparison

- The efficiency of each sensitivity coefficient method was quantified by calculating the Figures of Merit (FoM) for each material-averaged, energy-integrated sensitivity coefficient.
- A commonly-used metric for evaluating the efficiency of Monte Carlo simulations, the Figure of Merit is defined as:

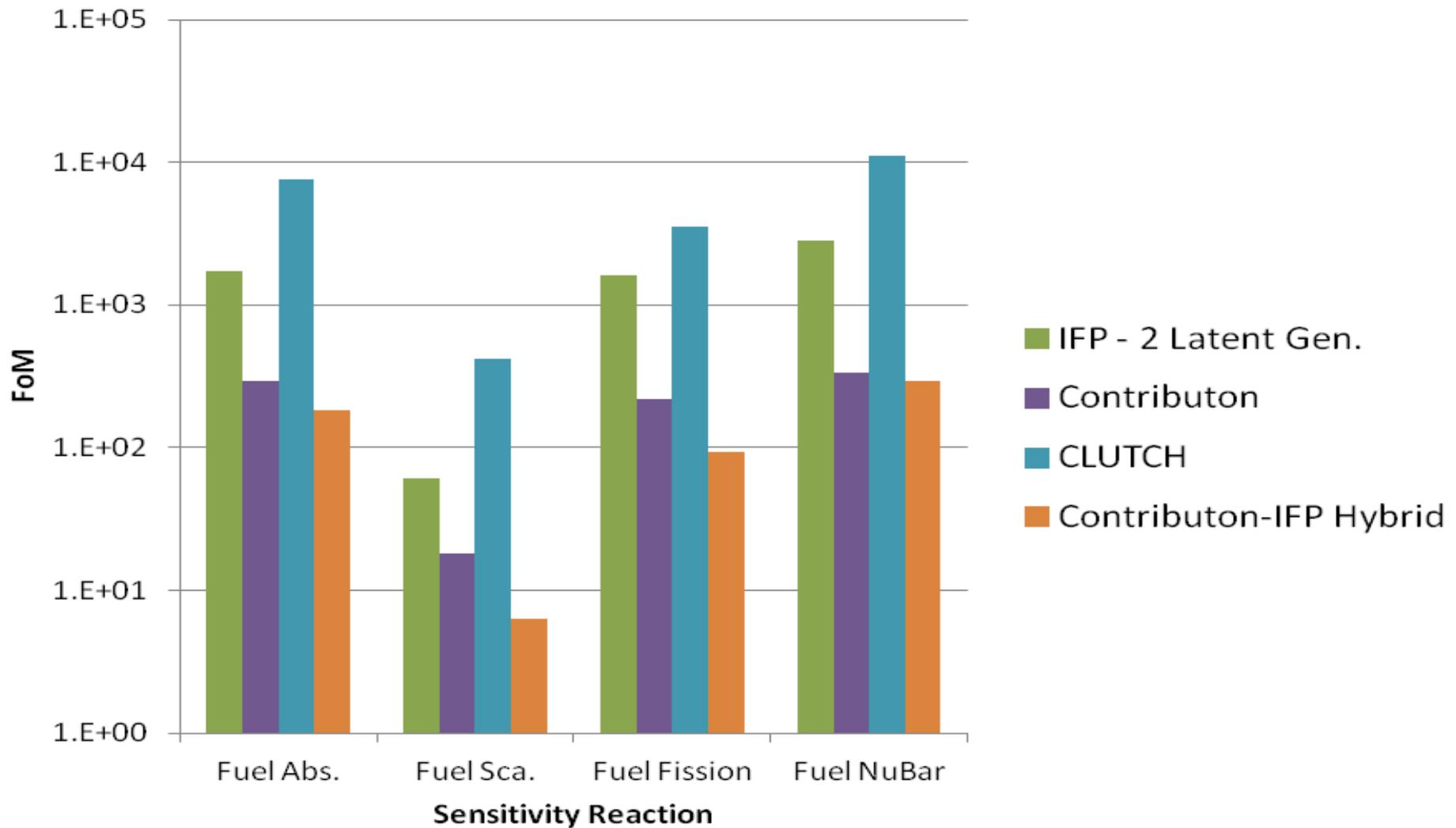
$$FoM = \frac{1}{R^2 T},$$

where  $R$  is the relative error for the parameter of interest and  $T$  is the simulation runtime.

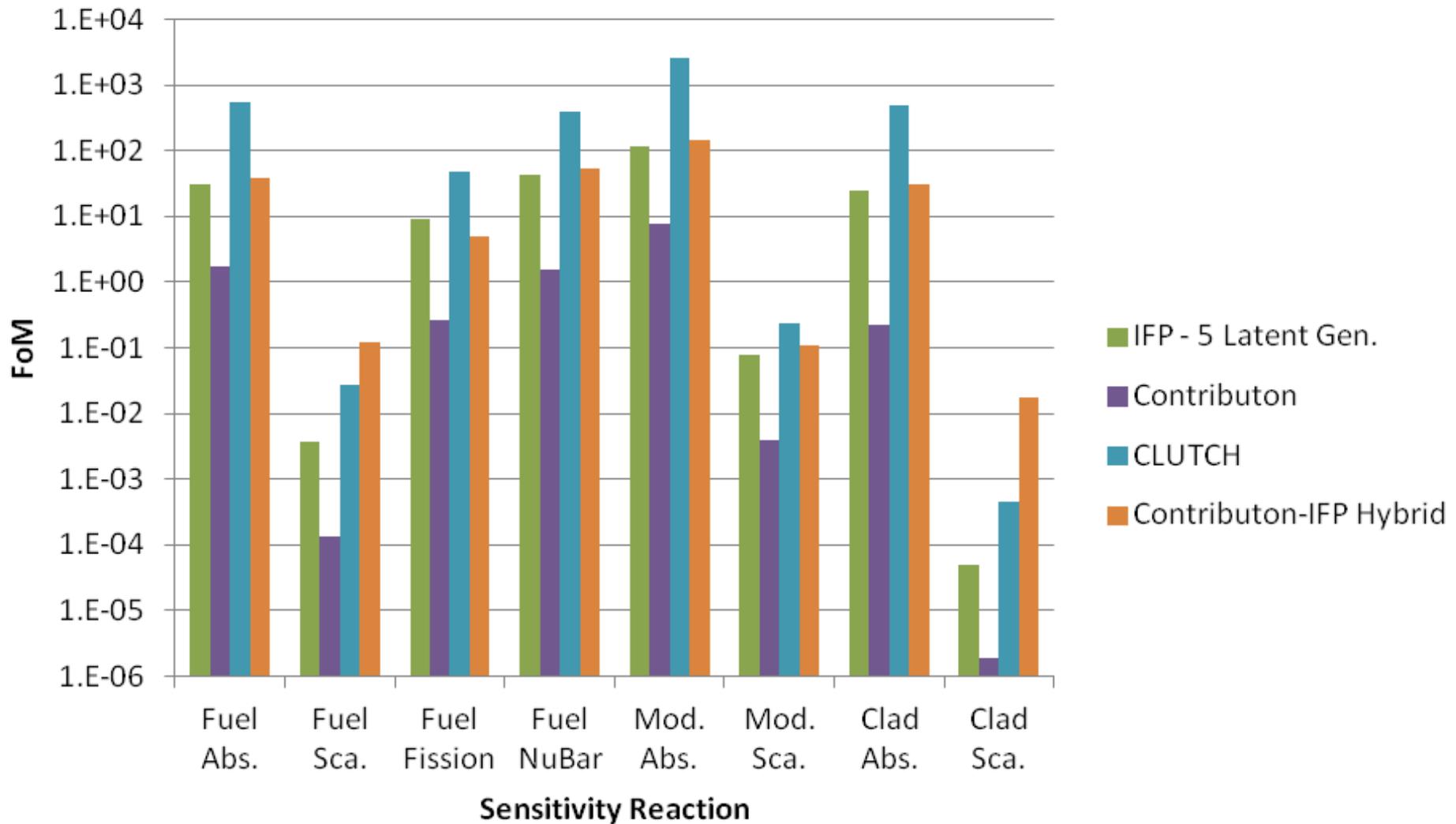
# Fuel Pin FoM



# Godiva FoM



# MCT FoM



# Conclusions

- Several methods for calculating eigenvalue sensitivity coefficients have been implemented in the Shift Monte Carlo code and have been compared in terms of accuracy, speed, and efficiency.
- A new method for performing sensitivity coefficient calculations, known as the CLUTCH method, has been developed, and has shown the potential to calculate accurate sensitivity coefficients with a high degree of efficiency.
- Future studies will apply the CLUTCH methodology to continuous-energy sensitivity coefficient calculations and will calculate isotope-dependent sensitivity coefficients.

# References

- *SCALE: A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design*, ORNL/TM-2005/39, Version 6.1, Oak Ridge National Laboratory, Oak Ridge, Tennessee (June 2011). Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-785.
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- E. E. Lewis, W. F. Miller, Jr., *Computational Methods of Neutron Transport*, American Nuclear Society, La Grange Park, Illinois, USA (1993).

# Iterated Fission Probability Memory Requirements

- The Iterated Fission Probability method allows for accurate sensitivity coefficient calculations with a small increase in problem runtime, but can have large memory requirements for complex systems.
- Consider the PWR problem mentioned earlier...

*38,000 unique isotope – regions*

*× 12 reactions per isotope*

*× 44 energy groups*

*× 11 generations of storage*

*× 10,000 particles per generation*

*× 8 bytes per double*

*= 17,656 gigabytes of memory*

# Contributon Method Evaluation

- The Contributon Method has low memory requirements because sensitivity coefficients are tallied at the site of every collision.

*38,000 unique isotope – regions*  
*× 12 reactions per isotope*  
*× 44 energy groups*  
*× 8 bytes per double*  
*= 0.16 gigabytes of memory*

- Unfortunately, the Contributon Method causes HUGE increases in a problem's runtime, and also requires the calculation of  $F^*(r)$  before tallying sensitivity coefficients.

# CLUTCH Memory Requirements

- Like the Differential Operator method, the CLUTCH method requires one to store reaction rate tallies for every collision a particle sees from birth until death.
- Unlike the IFP method, this information is freed after a particle dies and is not carried for multiple generations.

*38,000 unique isotope – regions*

*× 12 reactions per isotope*

*× 44 energy groups*

*× 400 collisions per particle*

*× 8 bytes per double*

*= 64.2 gigabytes of memory*