Automated Monte Carlo Biasing for Photon-Generated Electrons Near Surfaces

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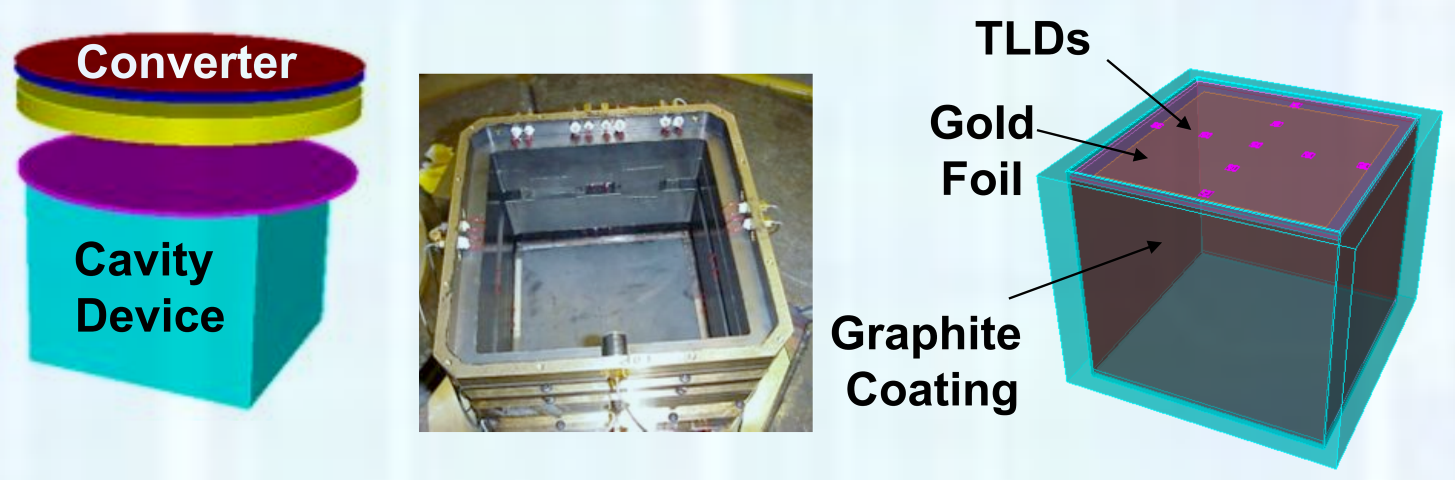
Problem

Our goal is to produce an automated technique for the biasing of electron-photon radiation transport Monte Carlo calculations, even for problems with rapidly varying importance. The most automated biasing methods rely on accurate representations of particle importance as a function of phase space. The primary challenge is obtaining sufficiently accurate importance maps, where importance varies rapidly within complex geometry. This requires adaptive, efficient data structures.

Test problem: Photoelectrons emitted into a cavity device:



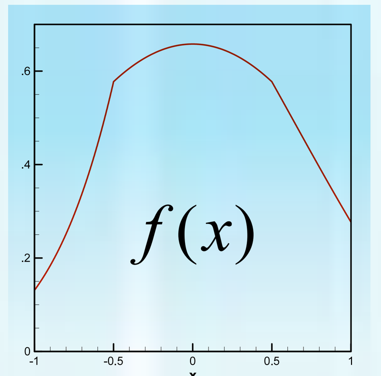
Approach

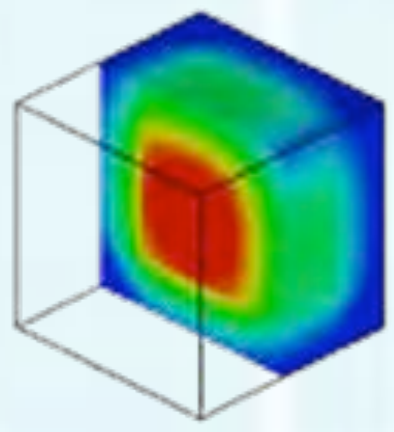
We determine particle importance maps using adaptive adjoint-flux tally structures, which are independent of the material geometry. We explored algorithms based on h-adaptivity (spatial partitioning), p-adaptivity (functional representation), and hp-adaptivity (both). We used tree data structures for spatial partitioning and orthogonal functional expansions for continuous representation.

The refinement criterion in the adaptivity algorithm needs to be based on the desired result. For weight-window settings, the desired outcome is importance within a specified relative point-wise error. For weight-windows settings, h-adaptivity was the best choice. More-advanced biasing methods, such as importance sampling, may benefit from hp-adaptivity algorithms.

Results

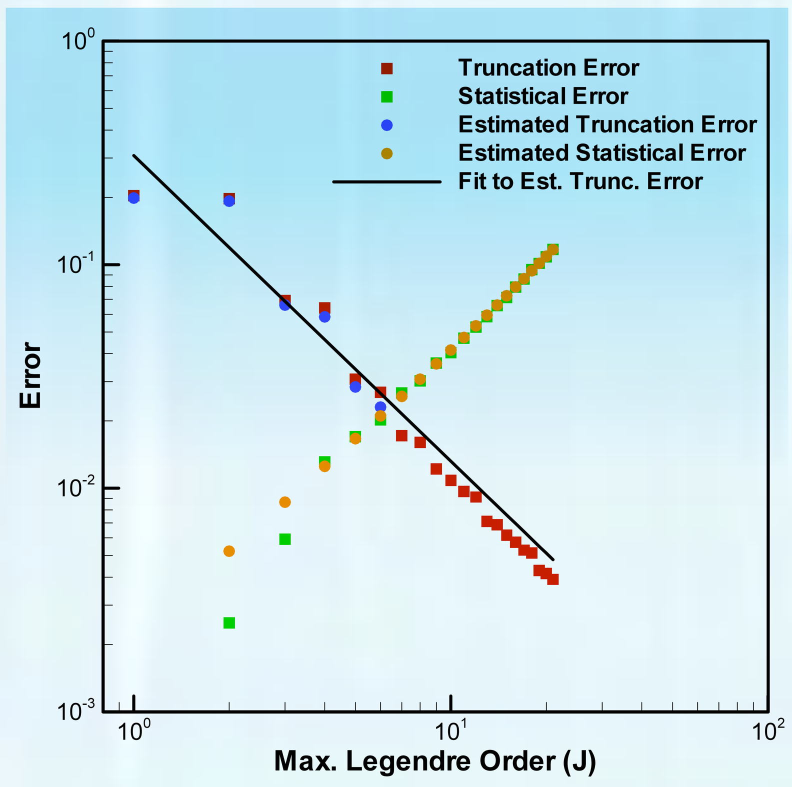
p-Adaptivity and hp-Adaptivity

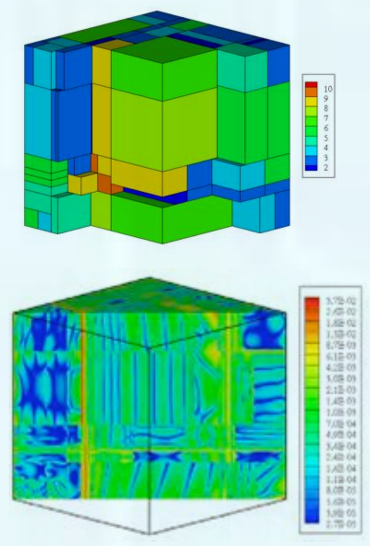




We examined functional expansions as an alternative or addition to tree data structures. Well-characterized 2-norm errors lead to a predictive adaptivity capability, though the point-wise error can be above that requested.

$$g(x,y,z) = f(x)f(y)f(z)$$





Functional Expansion Order

Absolute Point-Wise Relative Error

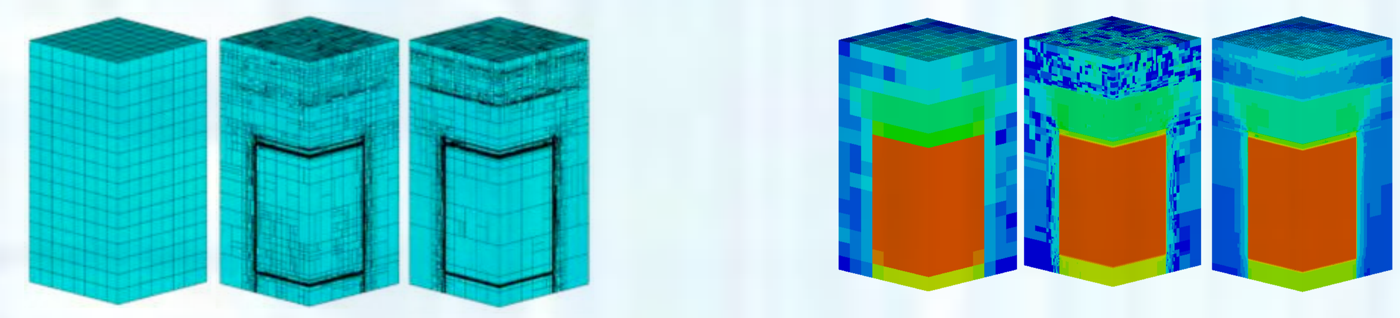
Results (cont.)

h-Adaptivity

Our h-adaptivity algorithms use a binary spatial-partitioning tree with axis-aligned splitting planes from the Mesh-Oriented datABase (MOAB).

In our simplest h-adaptivity algorithm, the tree is refined by splitting leaves that differ from neighboring leaves by more than a specified factor (e.g., 3) to a statistically significant degree (> 1 sigma).

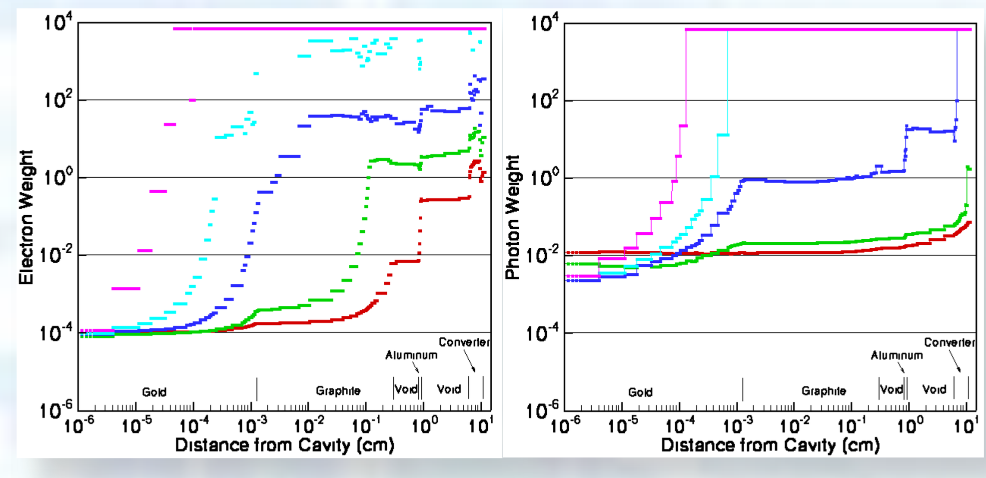
We iterate on adjoint calculations and tree refinement.



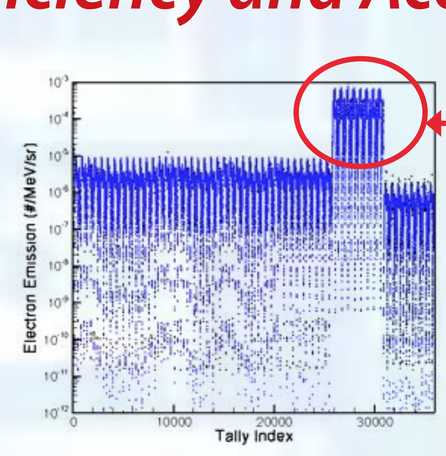
Weight-Window Biasing

Weight-windows settings are determined from the adjoint fluxes on the spatial-partitioning tree. Using particle splitting and roulette, weight windows force particle weights to be inversely proportional to particle importance (but do not control particle population).

The test problem demonstrates the challenge to capture rapidly varying importance.

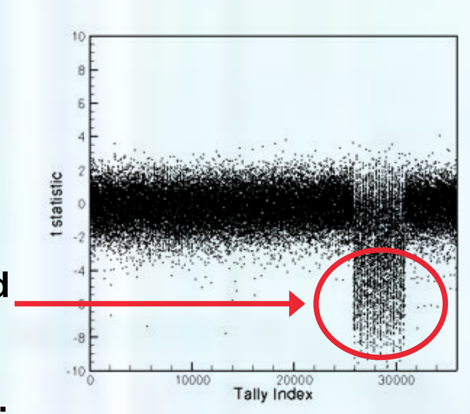


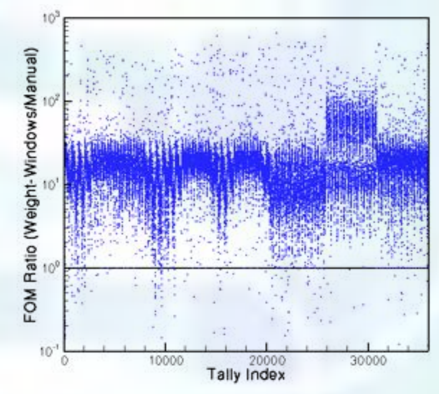
Efficiency and Accuracy Improvements



Emission is dominated by electrons off of the gold foil.

Weight-window results revealed a systematic error with our manual biasing.





The new biasing method achieved an order of magnitude improvement in the runtime Figure of Merit (FOM).

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

x = tally mean

σ^2 = tally variance

T = Monte Carlo time

Significance

- We have achieved an order-of-magnitude speed-up, while obtaining more accurate results.
  - The manually-biased test-problem run time was 100s of processor-days. Applications may require 2–4 orders-of-magnitude more.
  - This may apply to stockpile applications, such as electron-emission distributions for cavity system-generated electromagnetic pulse and dose enhancement near material interfaces. Deep-penetration satellite radiation-environment analysis may benefit from a similar biasing approach.
- We have explored adaptivity algorithms for Monte Carlo tallies, which may eventually be applied to many result distributions within the Integrated TIGER Series codes to improve automation.

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