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Comparison of CADIS Implementations in Attila4MC and ADVANTG

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Introduction

Consistent Adjoint Driven Importance Sampling (CADIS) is a widely accepted deterministic variance reduction (VR) method that is used to accelerate Monte Carlo codes for deep penetration shielding problems [1].

- AutomateD VAriaNce reduction Generator (ADVANTG) [2] commonly used to generate CADIS parameters to accelerate Monte Carlo N-Particle (MCNP) [3] fixed-source calculations
	- Reads MCNP5 runtape files as input and defines geometry based on Constructive Solid Geometry (CSG)
- Attila4MC deterministically generates CADIS parameters to accelerate MCNP calculations
	- Uses a first-order tetrahedral unstructured mesh (UM) geometry [5]

Literature on the use of UM deterministic solvers for VR is, at present, limited [6]. This presentation aims to expand on it with a well known benchmark, the Ueki Shielding Experiments [2, §7.1].

Introduction

Starting with MCNP6.1, the MCNP code has gained the ability to track particles on UM [4].

- Main purpose is to permit computational geometries that are difficult or impossible to describe using CSG
- Added benefit is the ability to use a UM deterministic solver to perform the "deterministic phase" of CADIS calculations

Attila4MC CADIS Implementation

Attila4MC 10.2 performs the deterministic phase of CADIS calculations on a **UM composed of first-order tetrahedral elements**.

- Requires a multigroup cross section library and a multigroup or a discrete energy source spectrum
	- The group structure of the source spectrum does not have to align with that of the library
- Angular domain is discretized using discrete ordinates (S_N) with the Triangular Chebyshev-Legendre (TCL) angular quadrature by default
	- User-specified S_N order
	- Custom quadrature sets are also accepted
- The external and scattering sources and the angular flux are expanded and stored in spherical harmonics
	- User-specified P_N order

Attila4MC CADIS Implementation

- Attila4MC uses the **Linear Discontinuous (LD) finite element spatial discretization method**
- Once a multigroup adjoint flux field is evaluated, it is mapped to a specified Cartesian axis-aligned weight window (WW) grid
- An exact adjoint solution is not required for an accurate MCNP calculation: the goal is only to generate an importance function to accelerate the Monte Carlo calculation

The resulting WW field and the consistently biased source definition are then provided to the MCNP phase of the calculation.

ADVANTG CADIS Implementation

ADVANTG 3.0.3 performs the deterministic phase of CADIS calculations on a **user-specified Cartesian axis-aligned grid.**

- Materials within grid elements are mixed automatically based on the CSG from an MCNP5-compatible input
- Like Attila4MC, ADVANTG requires a multigroup cross section library
	- ADVANTG accepts any source energy spectrum but will only bias it if able to do so

ADVANTG CADIS Implementation

- Discrete ordinates with a Quadruple Range (QR) quadrature set and spherical harmonics expansions were used, consistent with [2, §7.1]
	- Multiple angular and spatial discretization methods are available in ADVANTG
- The S_N solver in ADVANTG 3.0.3 uses step characteristic spatial differencing with one unknown per grid element
- Similar to Attila4MC, once an adjoint multigroup flux field is computed, WW lower bounds are generated and the source is biased (if possible). The WW field and the source definition are then provided to the MCNP phase of the calculation

CADIS Motivating Tally

For either software, a "CADIS motivating tally" is the tally that the deterministic phase of a CADIS calculation is aimed at accelerating.

- Acts as the adjoint source in the deterministic phase of the calculation
- Only adjoint volume sources are supported in Attila4MC 10.2
- Can only be used to directly accelerate an F4 tally

ADVANTG 3.0.3 is also capable of ray tracing from the F5 tally to evaluate the last-collided component of the adjoint flux, followed by a normal second-to-last collided adjoint volume source calculation.

• ADVANTG 3.0.3 CADIS calculations can be motivated with F4 or F5 tallies

Note that any number and type of tallies can still be requested in the MCNP phase of the calculation.

Ueki Shielding Experiment MCNP CSG Model

Modeled to replicate [2, §7.1].

- Paraffin block is centered at $(0, 0, 0)$
- 252Cf neutron point source at (0.001 cm, 0, 0)
- Watt fission source spectrum, source rate 4.05×10^7 n/s
- Graphite shield thicknesses of 0, 2, 5, 10, 15, 20, 25, 30, and 35 cm
- Detector is modeled as air
- ENDF/B-VII cross sections are used for all MCNP phases

Unstructured Mesh Model

UM generated using Attila4MC's mesh generation tool

- Used software basic guidelines: no special refinement for shield thickness
- The **UM is identical to the CSG** (within the discretization error), except:
	- Conical air volume opening in the paraffin block is segmented \rightarrow smaller conical air volume (length 0.5 cm) exists at the apex of the 45° conical opening
	- Created to emulate a small forward volume source for Attila4MC used for source spectrum biasing
	- However, the **MCNP phases are all run with the true forward point source**

Unstructured Mesh Model

Calculation Specs

In all calculations:

- Detector is represented with both an F4 and F5 tally
	- F5 tally located identical to [2], 20 cm from the shield (110 cm from source)
	- F4 tally calculated over $5 \times 5 \times 5$ cube, centered at this point (F5)
- Uses same flux-to-dose response function, ANSI/ANS-6.1.1-1991 [10]

Attila4MC 10.2 and ADVANTG 3.0.3 were used to run the deterministic phases of calculations, using the BUGLE-96 multigroup cross section library [9].

MCNP6.2 was used for all MCNP calculations, using 107 histories and performed on the Los Alamos National Laboratory "Snow" supercomputer using a single node with 36 threads.

• Each calculation was given its own allocation on a backend processing node to avoid conflicts with other processes. Each processor is an Intel Xeon E5- 2695 v4 at 2.10 GHz.

Summary of Run Configurations

9 unique calculations are performed for each shield thickness varying by:

- Deterministic solver used (ADVG for ADVANTG, A4MC for Attila4MC)
- CADIS-motivating tally used (F4 or F5)
- Geometry used for tracking (CSG or UM)

Two sets of discretization settings are used, also denoted ADVG and A4MC, with ADVG indicating the settings used in Ref. [2, §7.1] and A4MC indicating the settings recommended for Attila4MC calculations:

Deterministic Phase Discretization Settings

Summary of Run Configurations

Nomenclature example \rightarrow ADVG-A4MC/F5 + UM indicates a run with:

- **Deterministic phase** run by ADVANTG
- With **discretization settings** adapted from Attila4MC
- **Motivated by** an F5 tally
- **Tracked on** UM

Reminder: **Attila4MC can only be motivated using an F4 tally**. ADVANTG can run using either type of tally. Other than this restriction, the configurations used are selected to provide a broad and impartial comparison.

Computed and Experimental Results Comparison

To evaluate the accuracy of the calculations performed in this study, the ratios of the computed-to-experimental (C/E) attenuation factors were plotted.

The computed and experimentally measured attenuation factors differ by less than 5 % in most cases, and in all cases, by less than 10 %, **consistent with the C/E ratios reported in the original experiment** and for a different shielding material for both F4 and F5 tallies.

Figure of Merit Comparison – F4

Comparison of the efficiencies of CADIS implementations of ADVANTG and Attila4MC for the purpose of accelerating an **F4 tally**:

On average, **the most efficient configuration for the F4 detector tally appears to be A4MC-A4MC/F4, tracked either on the UM or on CSG**. This is particularly evident with shield thicknesses of 10–35 cm.

Figure of Merit Comparison – F4 Observations

A possible explanation for worse performance at low shield thicknesses is that in streaming-dominated problems, WWs provide indirect biasing only.

- It may be that the deterministic S_N solver of Attila4MC produces ray effects with the relatively coarse angular quadrature used
- The ADVANTG S_N solver does not benefit from LD spatial discretization in these calculations
	- Its ray tracing capability with an F5 motivating tally reduces the ray effects that Attila4MC presumably suffers from in the low-*T* configurations.
	- This conclusion is further supported by the fact that the F4-motivated (i.e., solved without ray tracing) ADVANTG configurations performed noticeably worse than either ADVG-A4MC/F5 or ADVG-ADVG/F5

The drop in Attila4MC's FOM at *T* = 35 cm may be explained by the fact that for this deep penetration problem the 10 cm mesh element edge length through the shield is likely too coarse (no refinement of mesh for varying shield thicknesses).

Figure of Merit Comparison – F4 Observations

ADVANTG, when motivated by the F5 tally, does not appear to suffer from using Attila4MC's discretization settings despite the spatial coarseness.

• This suggests that the grid from Ref. [2, §7.1] may be somewhat overrefined, hurting the deterministic calculation time but not the FOM.

ADVANTG's F4-motivated cases are substantially more sensitive to discretization.

- Substituting in Attila4MC's coarser spatial discretization but finer angular quadrature increases the FOMs to be roughly consistent with the F5 motivated cases
- This makes sense: refining the angular quadrature in a pure adjoint volume source problem will eventually approach the accuracy of the last-collided ray trace and earlier-collided volume source adjoint solution

Figure of Merit Comparison – F5

Comparison of the efficiencies of CADIS implementations of ADVANTG and Attila4MC for the purpose of accelerating an **F5 tally**:

The most efficient runs are the ADVANTG F5-motivated configurations.

Note that for this simple geometry, FOMs from runs on CSG were generally higher than on the UM, however, the magnitude of the difference is not consistent with other geometries [11].

Figure of Merit Comparison – F5 Observations

There appears to be no discernible difference between ADVG-ADVG/F5 and ADVG-A4MC/F5.

A4MC-A4MC/F4 performs comparably for most of the shielded runs, but its FOM drops for the thickest shields and for the unshielded case.

- Consistent with the interpretations for the F4 tally results
- In a streaming-dominated case, the last-collided component that ADVANTG resolves through ray tracing will dominate the adjoint solution
	- Challenging for an S_N solver without this capability to match it

For the thickest shields, the reduced FOM is likely due to the excessively coarse mesh element element edge length in the shield (similar to F4 tally results).

Summary and Future Work

Attila4MC 10.2 and ADVANTG 3.0.3 perform comparably in a straightforward CADIS calculation, with both packages requiring minimum to no fine-tuning to achieve acceleration.

- When optimizing for a point tally, ADVANTG has an advantage, but Attila4MC can also substantially accelerate such a tally.
- Attila4MC appears to have a slight edge at accelerating a small volume tally, but its main benefit comes from the fact that it is able to work with CAD geometries directly.

Future work includes studying the performance of the two software packages in more complex geometries, their discretization sensitivities, and their implementations of FW-CADIS.

Questions?

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