Detector Response Forward Modelling Using Kernel Density Estimator Intermediate Staged Sources

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INTRODUCTION

Accurate simulations of the neutron and gamma particle transport from sources off a line of sight, into vanishingly small solid angle detectors along a line of sight (LOS), pose particular challenges that have not been shared by, for example, collimated sources. For instance, the transport is dominated heavily by scattering and absorption processes. Simplified approximations of transport to detectors, such as the use of point or ring detectors on diagnostic particles launched by physical processes that transport particles undergo, become problematic. One may require the full transport of particles from source, to detectors, through the underlying geometry in order to unambiguously forward model the instrumental response.

Unfortunately, the vanishingly small solid angle of the detector requires staged transport in order to get adequate statistics for the forward model. This report describes a relatively unexplored method, the use of kernel density estimators (KDE)[1, 2], as a single random variable intermediate stage source to transport particles with sufficient statistics up to the detectors. KDE sources require significantly less memory – on the order of the collection of particles one uses to construct them – to represent the necessary domain correlations than gridded, high dimension, high resolution sources. Several other research efforts have also successfully employed KDEs as random variable particle samplers in MC simulations of criticality and forward modeling[3, 4].

This proceeding applies the KDE staged transport into an off-LOS example problem. The **Background** section describes the physical problem that is modeled, and the tools used to perform the transport. The **Results** section summarizes the main results: the justifications for using the KDE, the application of KDEs as intermediate sources in this problem, and the robustness of the KDE approach. The **Summary and Further Work** section summarizes the main results, describes improvements in characterizing the KDE source approach, and introduces alternative representations of source functions that may share similar advantages to KDE representations of sources.

BACKGROUND

The efficacy of KDE staged transport in an off-axis source problem is demonstrated. A monochromatic, isotropic neutron point source emits off-axis in an air-filled experimental canister, into negligible solid angle proton recoil telescopes (PRT) several meters up the LOS. The source confusion problem, where a high emission source off the line of sight may overwhelm the on-axis signal at the PRTs, is explored.

The geometry is an experimental platform that consists of a few cubic meters of cylindrical air canister that contains the source, a narrow air cylindrical LOS with PRTs a few meters above, highly neutron reflecting metal walls, and a final wrapping layer of air. The reflecting walls are 0.5 cm Fe at 10^3 gm/cm^3, to act as highly neutron reflecting walls. Fe is chosen so that the atomic number is high enough to minimize elastic downscatter of neutron energies. A lead scattering ball along the same horizontal plane, underneath the LOS, represents a high-atomic-number platform that contains the un-modelled on-axis source. The source is 10^{19} 3.5 MeV neutrons emitted from a point, isotropically, over a 10 ns time scale. Its emission rate is,

$$\dot{n}(t) = 10^{17} t e^{-t/10} \text{ ns}^{-1}. \quad (1)$$

Here t is a time in units of ns. The source is aligned approximately 18 cm horizontally from the LOS axis. Fig. (1) shows the experimental platform with relative source location.

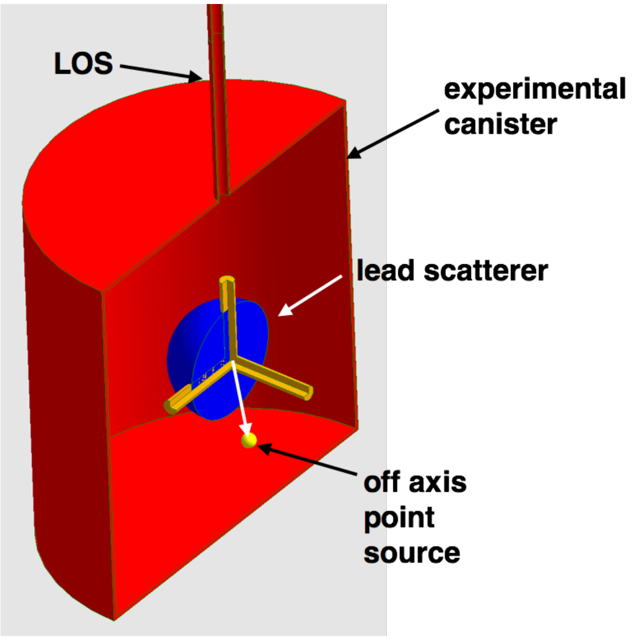

Fig. 1. The experimental platform consists of an off-axis point source, an 8 cm radius on-axis lead scattering sphere, an evacuated experimental canister (25 cm radius and 50 cm height), and a 1 cm radius evacuated LOS. The off-axis point source is located -12.5 cm in X and -12.5 cm in Y relative to the center of the lead scatterer. Fiducial XYZ axes, each with a length of 12.5 cm, run through the lead scatterer.

The PRT has a parabolic response: its peak raw sensitivity is 10^{-19} C/neutron at 3.5 MeV, and goes to zero at 3 and 4 MeV. This detector is located at 150 cm up the LOS, with a radius of 1 cm, aligned along the LOS.

Intermediate sources are constructed from particle tallies collected on 4 cm disks at 75 cm, 87.5 cm, and 100 cm up the LOS. These three disks are large enough in area to fully encompass those neutrons and gammas that would have either directly, or through their descendants, produced particles that scored at the 1 cm radius detectors. Fig. (2) shows a 100 cm LOS disk. Transport particles with energies less than 2 MeV are killed, in order to limit the calculation of particles that are vanishingly unlikely in eventually producing neutrons that would score at the detectors. For verification, enough MC transport particles from the physical source are run in order to get good statistics in a single stage calculation to the 150 cm detector. In this report, phase 1 calculations refer to a transport calculation that uses the physical point source off axis from the LOS. Phase 2 calculations refer to transport from a source constructed from the 4 cm disks up the LOS.

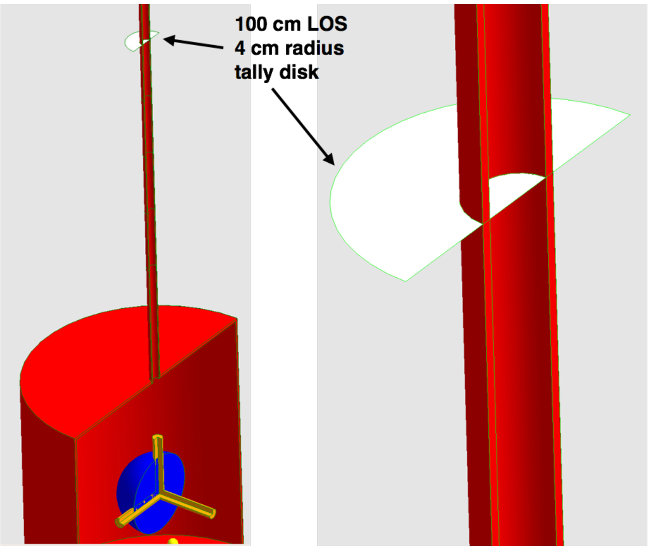

Fig. 2. A tally disk, from which an intermediate source is constructed from particles tallied on this surface, located 100 cm up the LOS.

The source, transport neutron and gamma particles, and tallies used to construct and characterize intermediate sources and model the PRTs are generated using `Mercury` [5]. `Mercury` is a general-purpose Monte Carlo radiation transport code developed at LLNL. It currently tracks neutrons, gammas, and charged particles. I generate the experiment geometry using `PMESH` [6], a tool originally developed to develop geometric meshes for arbitrary Langrangian-Eulerian physics codes but enhanced with the ability to construct arbitrary three dimensional constructive solid geometries.

RESULTS

The **Application** subsection discusses how a KDE is constructed and used to resample a source. The **Justification** subsection, motivates the use of KDEs to represent the intermediate source in a full transport calculation. The **Main Results** subsection summarizes the most important results. A single phase 1 calculation, and three phase 2 calculations, are run using intermediate sources from disks at 75 cm, 87.5 cm, and 100 cm up the LOS. The phase 1 calculation runs with 4.32×10^{10} MC source neutrons, and the phase 2 calculations run with 5×10^{9} MC source neutrons each.

Application of the KDE

A KDE representation of a tally on the disk can then be converted into a random variable that can sample a source with arbitrary many particles. One is not limited to resample down to the relatively few (10^5 to 10^6) MC particles used to construct the KDE, but may sample arbitrarily many (such as 10^9 or more) MC particles. For the purposes of this work, a python implementation of a Gaussian KDE[7], `scipy.stats.gaussian_kde`, is used inline in `Mercury`. Bandwidths for the KDE are chosen so that they match the smallest significant scale in phase space within the disk tally. Fig. (3) demonstrates the basic criterion for bandwidth, in this case on the energy spectrum through the tally disk.

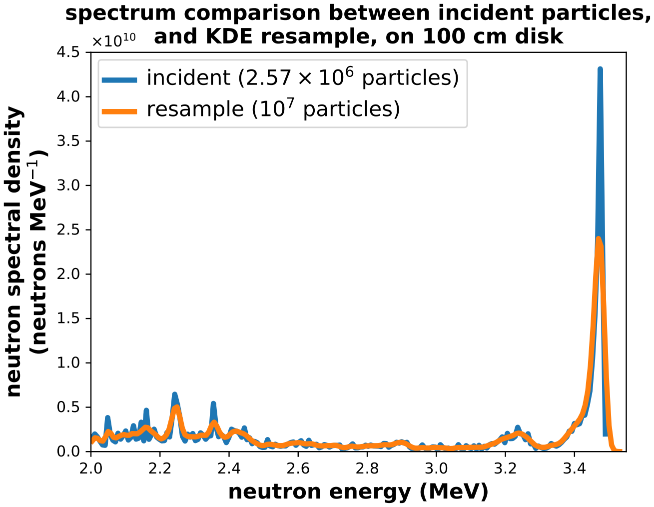

Fig. 3. The spectrum from the KDE resampled source, constructed from particles incident on the 100 cm inspection disk, matches fairly well with the incident neutron spectrum. By construction, this source has the same number of physical particles as the total number of incident particles on the disk.

Justification

The necessity of staged transport, when performing full transport, is demonstrated. KDE sources are also shown to provide a more efficient representation of an intermediate source than what a gridded source needs.

Full transport is required, but it may easily become impractical to perform full transport from the physical source up to realistic detectors. Tab. (I) demonstrates the Monte Carlo transmission efficiency – the number of MC particles through the disk versus the number launched from the source, divided by the disk area – for the three intermediate disks from which sources are constructed, and additional 4 cm radius inspection disks at 125 cm and 150 cm. From this table, one can estimate that full transport will not even produce good enough statistics to get a scalar metric, such as charge or total number of physical particles, at ~ 450 cm up the LOS. This threshold height is estimated where 1000 or fewer MC particles go through the

TABLE I. MC efficiency to tally particles onto 4 cm disks along the LOS, using 4.32×10^{10} source particles

tally disk	number of MC particles	areal efficiency (cm^{-2})
75 cm	4.44×10^6	2.05×10^{-6}
87.5 cm	3.82×10^6	1.76×10^{-6}
100 cm	2.58×10^6	1.19×10^{-6}
125 cm	1.47×10^6	6.77×10^{-7}
150 cm	9.31×10^5	4.29×10^{-7}

inspection disk.

Finally, from Tab. (I) and results in the **Main Results** subsection, 10^6 MC particles at a tally disk is sufficient to represent an intermediate source that may be resampled to accurately and precisely transport particles up to the detectors. Six dimensions – for instance, time, neutron energy, polar angle direction, azimuthal angle direction, radial coordinate on disk, and azimuthal coordinate on disk – are needed to represent the source. Reductions of tallies along the six dimensions require the following space for a gridded source:

- 100 ns in time with 1 ns resolution (100 bins).
- 5 MeV in energy with 0.1 MeV resolution (50 bins).
- 30 degrees in polar angle with 1 degree resolution (30 bins).
- 4 cm in radius with 0.12 cm resolution (∼ 30 bins).
- 360 degrees in both azimuthal angle and directions, with 18 degree resolution (20 bins each).

If one multiplies all these together, one needs a gridded source with $\sim 1.8 \times 10^9$ total bins to represent all necessary correlations at sufficient resolution in the six-dimensional domain. Approximately 1% of the hypervolume in this domain lies within 1% or more of the maximum density of this source. If one requires at least 10 particles within those bins, then $\gtrsim 10^8$ MC particles are needed to represent a gridded source sufficiently well. Given the efficiency at this disk, we would then need at least 10^{13} MC particles launched from the source. Instead, the KDE source requires on the order of 10^6 points to represent a source that can then be resampled for an arbitrarily large number of particles.

Main Results

The KDE source method is shown to be numerically robust. A single phase 1 calculation is run with 4.32×10^{10} source MC particles. This phase 1 calculation also generates particle tallies, used to construct KDE sources, for the phase 2 calculations. Three phase 2 calculations with 5×10^9 source Monte Carlo particles are run, from disks at 75 cm, 87.5 cm, and 100 cm, up the LOS. Some results of these phase 1 and 2 calculations are in the **Justifications** subsection.

Fig. (4) compares the forward modeled 150 cm detector signals from the phase 1 and phase 2 calculations. Tab. (II) summarizes integral measures of 150 cm detector response for the phase 1 and phase 2 calculations. This table uses results from a convolution of forward modeled signals, by a 5 ns symmetric tophat response[1], to construct signals smooth enough to estimate peak signal and time. Both Fig. (4) and Tab. (II) demonstrate numerical robustness of the KDE source, and a match to the forward model from a phase 1 calculation. Numerical robustness means that the forward models, from given phase 2 sources constructed consistently from a single phase 1 source, are similar to within Monte Carlo error.

TABLE II. Summary of forward model signals through 150 cm detector.

calc	number MC particles ×10^6	charge (nC)	peak time (ns)	peak current (× 0.1A)
phase1	0.931	6.51	75.9	2.01
phase2 75 cm	0.575	6.06	80.9	1.92
phase2 87.5 cm	3.60	6.08	79.3	1.93
phase2 100 cm	21.5	6.08	79.3	1.92

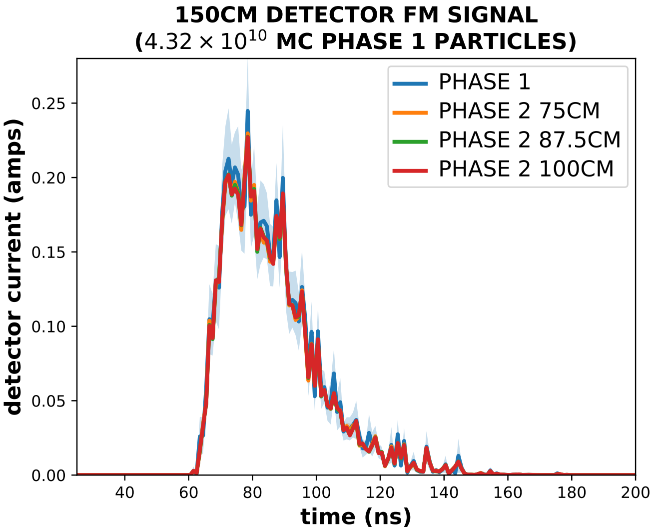

Fig. 4. Forward model of 150 cm detector from phase 1 and phase 2 calculations. Bands denote one standard deviation variation about the mean signal.

SUMMARY AND FURTHER WORK

This proceeding demonstrates that the KDE representation in phase 2 calculations provide a promising avenue to forward model the detector responses due to an off-LOS source: they are numerically robust, where possible they match phase 1 calculations, and they are space efficient both in their representation and in the nature of the number of MC particles that need to be launched from a phase 1 calculation.

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[1] This response only smooths the forward model signal. The response is symmetric about zero time, so that it does not introduce a time offset.

A relatively cursory validation on the goodness of a KDE source compares its 1D reductions (in time, energy, and other domain variables) of the KDE to the 1D reduction from an input particle tally in a phase 1 calculation (see Fig. [3]). However, one should *cross-validate* to determine how or whether a KDE or any other PDF representation is a good fit. A necessary element in cross validation is to determine how well a KDE constructed from a collection of training points (usually a majority subset of input samples) can accurately predict a sampling of holdout points (those input samples not included in the training set).

Finally, the KDE representation is not a unique method of sampling a distribution in order to construct a source or tally. In the context of Monte Carlo neutron transport, others have successfully appled functional expansion tallies (FET)[8, 9] and hybrid FET and KDE[10] approaches. FETs are similarly space-conserving, robust representations of underlying distributions, and either FETs or hybrid constructions may also find use in this unique application.

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