Investigation of Chord Length Sampling in Finite 1-D Binary Stochastic Media

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INTRODUCTION

Much work has been done to establish chord length sampling (CLS) method as an acceptable modeling technique over the past two decades since it was first proposed by Zimmerman and Adams [1]. Brantley [2] followed and extended Zimmerman and Adams' original work to calculate average flux distribution in 1-D geometry. Murata et al. [3,4] applied empirical nearest neighbor distribution functions (NNDs) to sample chord length to next TRISO particles in high temperature gas cooled reactor analysis and excellent results were obtained in criticality calculations. Donovan et al. [5,6] systemically investigated the application of CLS to 2D/3D geometry for fixed source problems and proposed an empirical method to determine the mean chord length of CLS. Ji and Martin [7,8] used a theoretical chord length distribution function to validate CLS application in a general 3D geometry and developed a self-consistent correction algorithm to obtain an effective volume packing fraction used in CLS to analyze Very High Temperature Reactor (VHTR) unit cells.

Although CLS was originally proposed in sampling material interface in both binary stochastic mixtures [1], in practice, CLS is used only in background material to sample the next inclusion material while regular Monte Carlo is used in inclusion material, such as disks in 2D and spheres in 3D [3-8]. In these applications, the system is finite and mono-size inclusions are uniformly distributed in the background materials. When CLS is applied to analyze neutronic behavior in such geometry, some complications exist to cause inaccurate solutions compared to benchmark results. Most appreciable factors for inaccuracy are rooted from CLS procedure itself. When neutron leaves an inclusion and scatters back, should a new inclusion be sampled or the old one be remembered? This is the memory effect in CLS. The other effect is boundary effect. When sampled inclusion is overlapped with external boundary, it is rejected and a re-sampling is performed. This would result in non-uniform distribution of inclusions in background material and affect neutron spatial distributions. How these two effects affect the CLS accuracy is not yet thoroughly investigated.

In current work, by applying CLS to radiation transport in finite 1D random media with uniformly distributed inclusions for fixed-source and eigenvalue problems, we have studied memory and boundary effects

in calculating reflection rate, multiplication factor and flux distribution. To authors' knowledge, these calculations and investigations have not yet been performed before.
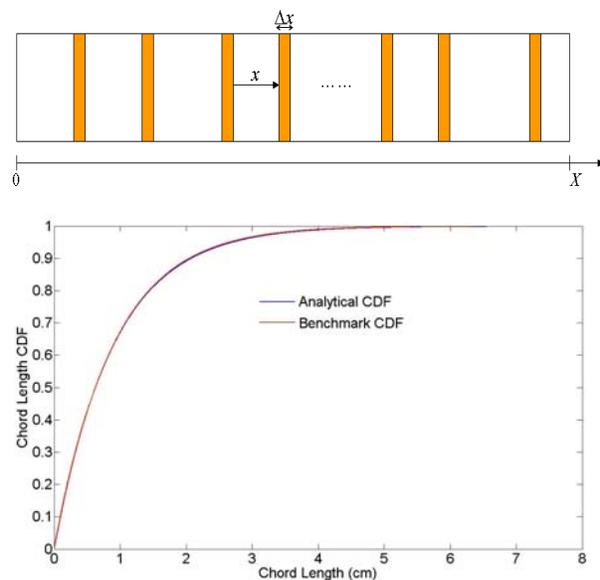
RADIATION TRANSPORT PROBLEMS

Fig. 1. System configuration and chord length distribution function

A finite 1D binary stochastic geometry is configured as benchmark system shown in Figure 1: inclusions with fixed thickness Δx are uniformly distributed in background material and are constrained to reside completely within the range $(0, X)$, i.e. partial inclusions at the boundaries are not permitted. In fixed-source problem, a beam of neutron enters system from left to right. In eigenvalue problems, a uniformly distributed source is assumed at the beginning. Only inclusions have fissile materials. When CLS is applied to solving both radiation transport problems, the chord length probability density function (PDF) between two inclusions is assumed exponential based on [9]:

$$f(x) = \frac{1}{\Delta x} \cdot \frac{frac}{1 - frac} \cdot e^{\frac{-x}{\Delta x} \frac{frac}{1 - frac}} \qquad (1)$$

where *frac* is the volume packing fraction. To verify the

accuracy of the PDF, empirical PDF was calculated by simulating 10^9 realizations of the stochastic geometry with *frac*=10%. The cumulative density functions of both analytical and empirical results are also shown in Figure 1 and excellent agreement is obtained.

Memory effect is investigated by calculating radiation reflection probabilities in the fixed source problem and comparisons are made with benchmark results. In benchmark calculation, traditional Monte Carlo (MC) procedure is performed over a total of 10^8 physical realizations. In each realization, one neutron history is tracked and the ensemble-averaged solutions are obtained over 10^8 neutrons. In CLS, when neutron leaves an inclusion, if the inclusion is not removed from memory until the neutron enters another inclusion, it is called CLS w/ memory. Otherwise, it is CLS w/o memory. With memory, neutron may enter the same inclusion multiple times by backscattering events in background material. Both cases are examined and results are compared. A total of 10^8 neutron particles are tracked in CLS calculation.

Eigenvalue problem is also implemented to verify the effectiveness of CLS. Path-length estimator and non-analog variance reduction methods are used to calculate the multiplication factor and neutron flux distribution. In benchmark, the ensemble-averaged solutions are obtained over 60 realizations. In each realization, the simulation is terminated until the convergence criterion, defined as the difference of the batch-averaged flux of consecutive batches reaches 1e-6, and 100 inactive batches are performed with 10^5 initial neutron sources in each batch. For CLS, the same parameters and convergence criteria are used.

Finally, boundary effect is addressed quantitatively by analyzing CLS in a vacuum stochastic system.

RESULTS AND ANALYSIS

From Table I, CLS w/o memory of last inclusion shows better agreement with benchmark than the CLS w/ memory. This phenomenon systemically exists under different thickness ratio $\Delta x/X$ (X is fixed at 1000 cm) and packing fraction. This can be explained by contrasting Zimmerman and Adams' "Algorithm B and C" [1,2], where retaining memory improves the accuracy. In Zimmerman's work, both media have random thickness and follow exponential distributions, i.e. only the distance from interface to interface can be sampled exactly from exponential functions in CLS. If a scattering happens inside one material, the distance from the scattering spot to the interface will not follow exponential distribution, and cannot be sampled from exponential functions in CLS. That is why the material interfaces should be remembered to improve accuracy. In current work, only the background material thickness is random and it closely approximates exponential distribution. What's more, the distance from any point inside background to

the interface of fixed-thickness inclusions also closely follows the exponential distribution [10]. This means that even if a back-scattering happens in background, the distance from the scattering spot to the interface still follows exponential distribution, and thus, should be sampled from exponential functions in CLS. Remembering last inclusion will cause non-exponential distribution. This is why CLS w/o memory shows better accuracy in current work.

In eigenvalue problems, CLS w/o memory is chosen to calculate K_{eff} and neutron flux distribution. The system geometry data are set at *frac*=10% and $\Delta x/X$=1e-4; cross sections for background material are $\Sigma_{t,1}$=0.1cm^{-1}, $\Sigma_{a,1}$=0cm^{-1}, $\Sigma_{s,1}$=0.1cm^{-1}; inclusion material $\Sigma_{t,2}$=0.1cm^{-1}, $\Sigma_{f,2}$=0.02cm^{-1}, $\Sigma_{s,2}$=0.05cm^{-1}.
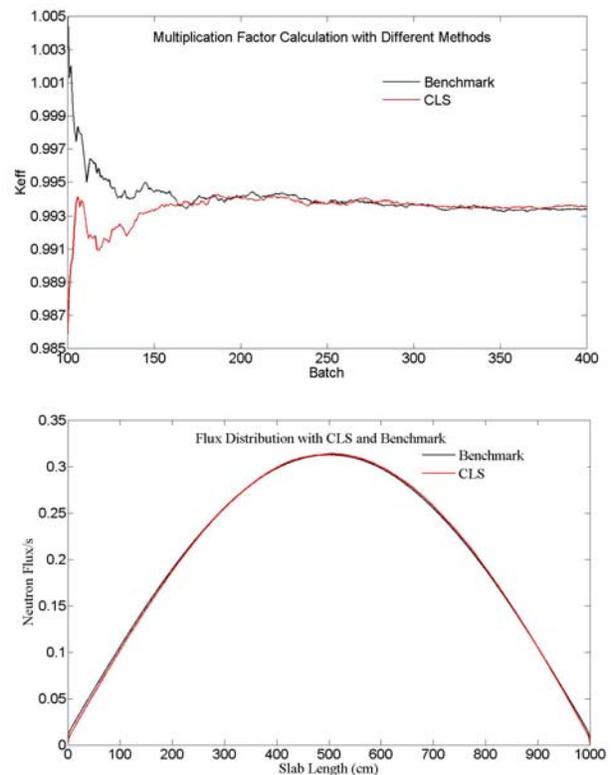

Fig. 2. Multiplication factor and neutron flux simulation with different methods

The comparison of K_{eff} and neutron flux distribution between CLS and benchmark are shown in Figure 2. It can be seen that K_{eff}'s calculated in CLS and benchmark converge to the same value rapidly. This is partly due to the mass conservation of fissile material (equivalent to the total packing fraction of inclusions) in CLS. Calculations have shown that the expected number of inclusions in the slab system in CLS is very close to the benchmark (~10^{-3} in relative error). Flux distribution with CLS shows only slight difference from benchmark, especially in the edge regions of the system. It is believed

TABLE I. Comparison between CLS (w/ and w/o memory) and benchmark for fixed source problem.

Solution Method	Reflection Probability	Relative Error %	Reflection Probability	Relative Error %	Reflection Probability	Relative Error %
(Background) $\Sigma_{t,1}$=0.1cm^{-1}, $\Sigma_{a,1}$=0cm^{-1}, $\Sigma_{s,1}$=0.1cm^{-1}; (Inclusion) $\Sigma_{t,2}$=0.1cm^{-1}, $\Sigma_{a,2}$=0.05cm^{-1}, $\Sigma_{s,2}$=0.05cm^{-1}						
frac=5%	$\Delta x/X$=1e-5		$\Delta x/X$=1e-4		$\Delta x/X$=1e-3	
Benchmark	0.6413		0.6447		0.6731	
CLS(w/o)	0.6415	**0.031**	0.6421	**-0.400**	0.6517	**-3.180**
CLS(w/)	0.6388	**-0.390**	0.6270	**-2.750**	0.6067	**-9.860**
frac=10%	$\Delta x/X$=1e-5		$\Delta x/X$=1e-4		$\Delta x/X$=1e-3	
Benchmark	0.5357		0.5399		0.5674	
CLS(w/o)	0.5366	**0.170**	0.5360	**-0.720**	0.5452	**-3.910**
CLS(w/)	0.5344	**-0.240**	0.5256	**-2.650**	0.5155	**-9.150**
frac=15%	$\Delta x/X$=1e-5		$\Delta x/X$=1e-4		$\Delta x/X$=1e-3	
Benchmark	0.4668		0.4709		0.4960	
CLS(w/o)	0.4675	**0.150**	0.4676	**-0.700**	0.4761	**-4.010**
CLS(w/)	0.4656	**-0.260**	0.4616	**-1.970**	0.4553	**-8.210**

that the difference is caused by the boundary effect of CLS. In CLS, when the sampled inclusion is overlapped with the system boundary, re-sampling is performed. This manipulation seems physically realistic, but, it also causes complications, e.g. boundary effect, because it changes the packing fraction distribution of inclusions in the system.
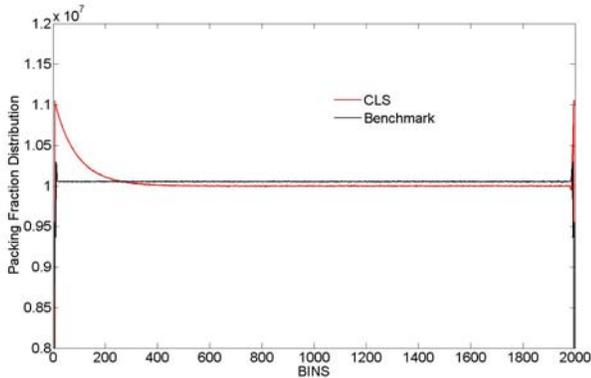

Fig. 3. Comparison of packing fraction distributions.

In order to investigate the boundary effect, a simulation of packing fraction distribution of inclusions was performed using CLS. Assuming that 10^9 neutrons enter a vacuum system (inclusions are also vacuum) of 20cm length, and that CLS is performed during neutron transport, and then the packing fraction of inclusions is tallied as a function of space. The result compared to benchmark is shown in Figure 3. It can be seen that packing fraction distribution from CLS is not uniform, especially near the boundary of system.

Olson et al [11] have also mentioned boundary effects while investigating chord length distribution in 2D/3D systems. In the CLS procedure, this effect becomes more complicated due to re-sampling, i.e. the packing fraction becomes spatial dependent in the boundary region. It is expected that such an effect can also be observed in 2D/3D geometries, including VHTR configuration, when applying CLS to analyzing neutronic behavior. This feature inevitably changes the neutron transport behavior in the system. Future research will focus on this investigation.

CONCLUSIONS

Two typical radiation transport problems, fixed-source and eigenvalue problems are investigated in 1D binary stochastic system of uniformly distributed inclusions.

It is concluded from the results in both problems that CLS is an effective and accurate method to be applied in obtaining ensemble-averaged solutions. The resultant accuracy is improved by taking into account two characteristics of CLS, i.e. memory and boundary effects. Based on the simulation, it is suggestive that neutron transport through a stochastic mixture is a complete composite Markovian process. And due to the boundary effect, packing fraction of inclusion in CLS procedure becomes a spatial dependent quantity. Corresponding

amendments to CLS are needed before application into pragmatic simulation.

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