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DEVELOPMENT OF SELF–LEARNING MONTE CARLO TECHNIQUE FOR MORE EFFICIENT MODELING OF NUCLEAR LOGGING MEASUREMENTS

JAN M. ZAZULA

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DEVELOPMENT OF SELF-LEARNING MONTE CARLO TECHNIQUE FOR MORE EFFICIENT MODELING OF NUCLEAR LOGGING MEASUREMENTS

OPRACOWANIE ALGORYTMU SAMOUCZACEGO DLA BARDZIEJ EFEKTYWNEGO MODELOWANIA WSKAZAŃ ODWIERTOWYCH SOND NEUTRONOWYCH METODA MONTE CARLO

РОЗРОБОТКА САМОУЧАЩЕЙСЯ МЕТОДЫ МОНТЕ КАРЛО ДЛЯ БОЛЕЕ ЭФФЕКТИВНОГО МОДЕЛИРОВАНИЯ ПРОБЛЕМОВ НЕЙТРОННОГО КАРОТАЖА

Jan M. Zazula

Institute of Nuclear Physics
ul. Radzikowskiego 152
PL-31-342 Krakow, Poland

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Academy of Mining and Metallurgy, Kraków

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INSTYTUTU FIZYKI JĄDROWEJ W KRAKOWIE
UL. RADZIKOWSKIEGO 152
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Abstract

The self-learning Monte Carlo technique has been implemented to the commonly used general purpose neutron transport code MORSE, in order to enhance sampling of the particle histories that contribute to a detector response. The parameters of all the biasing techniques available in MORSE, i.e. of splitting, Russian roulette, source and collision outgoing energy importance sampling, path length transformation, and additional biasing of the source angular distribution are optimized. The learning process is iteratively performed after each batch of particles, by retrieving the data concerning the subset of histories that passed the detector region and energy range in the previous batches. This procedure has been tested on two sample problems in nuclear geophysics, where an unoptimized Monte Carlo calculation is particularly inefficient. The results are encouraging, although the presented method does not directly minimize the variance and the convergence of our algorithm is restricted by the statistics of successful histories from previous random walk. Further applications for modeling of the nuclear logging measurements seem to be promising.

Streszczenie

Autor opracował algorytm samouczący, który został zastosowany w uniwersalnym programie komputerowym Monte Carlo MORSE (otrzymanym wraz z bibliotekami przekrojów czynnych z Radiation Shielding Information Center, USA) dla symulacji transportu neutronów i kwantów gamma w materii. Podejście to ma wzbogacić próbę statyatyczną tych cząstek, które wnoszą wkład do zliczanej odpowiedzi detektora. Wzbogacanie jest osiągane poprzez optymalizację parametrów dla wszystkich technik redukcji wariancji, dostępnych w kodzie MORSE, na podstawie analizy historii poprzednio symulowanych cząstek. Procedura ta została przetestowana na dwóch przykładach dotyczących modelowania pola neutronów termicznych w skale oraz wskazań odwiertowej sondy neutronowej, dla których niezoptymalizowane obliczenia Monte Carlo są szczególnie nieefektywne.

Резюме

В роботе был розроботан саноучающийся алгоритм Монте Карло, которой был исползован в американском програмне MORSE, вычисливающим задачи переноса нейтронов с глубоким проникновением вещества. Обогащение стохастической пробы частиш падающих в детектор есть полученные через оптимизацию метолов моделирования по ценности. Как тестовые задачи были розрешенные два проблемы из ядерной гиеофизики, получая в первом случае улучшение точности, и во втором случае излучшение эффективности вычислений.

1. *Introduction*

Multidimensional particle transport calculational techniques on the nuclear logging problems have been actively pursued[1] in recent years. Despite progress in the deterministic solutions to the neutron transport equation, use of the Monte Carlo (MC) codes, however consuming large computational efforts, is continually recommended for detailed three-dimensional models of neutron logging tools, and this approach has provided convincing results when compared with borehole measurements.

The geometrical configuration and the particle transport physics in a typical log-borehole-rock system imply severe requirements for the calculational model, such as:

(a) The wide neutron energy range from several MeV to a few hundredths of eV should be taken into account, including the neutron cross section data, the source energy spectrum and the detector response function. Usually, the thermal neutrons are of particular significance for log count rates and they cannot be cut off, which can result in prohibitively long computing times.

(b) Both the deep penetration of neutrons into a rock and the small scale transport effects in a logging tool and in a borehole should be modelled, including three-dimensional details such as eccentric log configuration or dipped beds of a rock matrix.

(c) A small detector volume when compared to the whole phase space of the system results in a poor detector output statistics for reasonable numbers of particle histories simulated.

Thus the Monte Carlo approach to the logging problems would never give practical and accurate results without numerous variance reduction techniques[2] that enhance sampling of those neutron histories which are scored in a detector. The parameters of the variance reduction schemes are usually guessed from physical recognition of a problem or by a trial and error procedure, or they are derived from approximate solutions of the

adjoint transport equation in a configuration simplified relative to the original problem (e.g. using the discrete ordinates codes).

In the current decade new adaptive methods have been proposed[2-6] as an attempt for automatization of the trial and error process. The basic idea of these techniques, further called self-learning Monte Carlo (SLMC), is:

(a) to collect information (from the physical[2-5] or from the random number[6] spaces) concerning the "successful" particle histories (i.e. contributing to the response),

(b) to process this information through adjusting the biasing parameters (as the weight thresholds, the optimal free flight paths or the desirable secondary neutron energy and angular distributions to be sampled, etc.)

(c) to iteratively use such obtained experience about a problem for guiding the trajectories of the next simulated particles towards a detector.

In the course of the current work we applied this technique to implement the SLMC algorithms for optimizing all the variance reduction methods available in the multigroup Monte Carlo code MORSE[8], i.e. source and collision outgoing energy importance sampling (section 2.1), splitting and Russian roulette (section 2.2) and path length transformation (section 2.3). Then we have tested the accuracy and the efficiency of this approach on two sample problems taken from the nuclear geophysics area (section 3). The first relatively simple problem was considered to obtain a comparison with the deterministic, discrete ordinates solution to the neutron transport equation. The second problem involved a more realistic borehole and probe layout with the stratified rock medium. However, for this case only poor results from MC calculations with not optimized variance reduction techniques have been available for comparison.

2. *Description of the self-learning algorithm*

2.1 Estimation of the importance function

The essential feature of the biased Monte Carlo simulation is the use of a relevant importance function $I(p)$, which accounts for a potential contribution to the detector response of a particle occurring at a phase space point $p=(\vec{r},E,\vec{\Omega})$ (the particle position, energy and direction). It has been shown[3] that the adjoint flux ϕ^+, which is the transport theory equivalent of the best importance function, can be estimated during the forward Monte Carlo calculation.

This idea has been incorporated by us to the MORSE code in the following manner. Let the particle "i" leave the source or the collision "k" in the volume region "r" and the energy group "g", with the weight w_{rg}^{ik}. For K such collisions their mean contribution to the total particle weight leaving phase space bin "rg" is recorded as :

$$w_{rg}^{i} = \left(\prod_{k=1}^{K} w_{rg}^{ik} \right)^{1/K} \qquad (1)$$

since the geometrical averaging account for the multiplicative weight character in successive collisions. If the particle "i" reaches the detector, its contribution to the response f^i is added as f_{rg}^{i} to the total detector count versus bin rg, for all those bins rg which it passed during its history, and all its weight contributions w_{rg}^{i} are added to the total weight leaving bin rg. If the history of particle "i" is terminated (escape, slowing down below an energy or a weight cutoff), all its weight contributions w_{rg}^{i} from its emission from the source or from its last escape from the detector region (for the volume tracklength response estimation) are neglected. After completing a batch, we can estimate the mean value of the adjoint flux in region r and in group g from the following formula (it can be derived in the same way as in Cramer's[3] paper):

$$\left\langle \phi^{+}_{rg} \right\rangle = \sum_{i=1}^{N} f^{i}_{rg} \Big/ \sum_{i=1}^{N} w^{i}_{rg} \equiv \frac{\langle f_{rg} \rangle}{\langle w_{rg} \rangle} \qquad (2)$$

where averaging relates to N successful histories in a batch.

This circumstantial description of the adjoint flux estimation exhibits the stochastic character of the learning process. Estimating could as well be performed after each single particle history[5], but that would not guarantee statistically significant results. The problem is that for the importance sampling purpose (to bias the subsequent random walk) knowledge of the adjoint solution in the whole phase space is required. It can happen, however, that for a finite sample of the machine particles tracked, numerous bins (energy groups and regions) are not represented within the subset of successive histories. The open question was what to assume as the importance value for the bins that were not represented : the zero value (somewhat pessimistic), the minimum, or the average of the values encountered in other bins? Our way to solve this problem was to combine automatically the neighboring energy groups into wider intervals (coarse energy group structure) until the statistics gathered together was sufficiently large. Sometimes this bin redefinition led to the situation where in order to distinguish differences in the adjoint flux, instead of the fine group mesh, only a division into two broad energy ranges, e.g. the fast and the slow neutrons, could be acceptable. This procedure correspond to the clusterization process, described in the machine learning theory[7].

The use of the adjoint flux, estimated in this way, in the MORSE code is straightforward, as the importance of the secondary neutron energy outgoing from a collision, versus group and region (EPROB(IR,IG) in MORSE). When considering the source region, the same importance function can also be regarded as the source energy group importance (BFS(IG)). Thus after each batch we are able to obtain new biased distributions of the energy emitted from the source or from the collisions, to be sampled in the next batch.

Some small modification of the source routine has to be done to extend this procedure to the estimation of the source angular bin importances, i.e. of the adjoint flux $\phi^{+}(\mu)$, $\mu_m \leq \mu \leq \mu_{m+1}$, versus interval m of the cosine μ of the polar angle of tha source emission (relative to the "z" axis). The advantage of this modification is that it saves a computer time by sampling a source direction from the biased distribution peaked forward to the region surrounding the detector, instead of from the isotropic distribution. Obviously this algorithm also includes the particle weight renormalization factor, which is given by the ratio of the biased and the original angular distribution, to preserve the total yield from the source.

2.2 Weight window control

The next item in biased Monte Carlo calculation is the particle weight control. This procedure consists in keeping the statistical weight of particles within a reasonable interval [WTH,WTL] about the average value WTAV, all three parameters depending on the energy group and region. In the MORSE code the particle weight is controlled after each collision, the upper value by splitting of the particles with weight WT>WTH into two independent histories and the lower value by the Russian roulette, i.e. by setting the weight of particlea with WT<WTL to WT'=WTAV with the probability WT/WTAV, or by killing them with the probability 1-WT/WTAV.

The desirable mean weight of particles WTAV(IR,IG) is computed by us directly, by averaging weigbta of the particles passing region r in energy group g among those histories which finally contributed to the detector response. Since in the optimal calculation the particle weights are inversely proportional to the adjoint flux, the upper and lower weight thresholds WTH(IR,IG) and WTL(IR,IG) are determined by the lowest and the largest values of the adjoint flux in tha cluster "rg", following to the formulas:

$$WTH = \frac{\langle f_{rg} \rangle}{\min_i |\phi^{+i}_{rg}|} \quad (3A) \qquad WTL = \frac{\langle f_{rg} \rangle}{\max_i |\phi^{+i}_{rg}|} \quad (3B)$$

where ϕ^{+i}_{rg} was estimated separately for each particle i passing the cluster "rg" as f^i_{rg}/w^i_{rg}. Because of large oscillations in the denominators of eq. (3A,B) we have additionally required the limitations for the weight window width:

$$0.01*WTAV \le WTL \le 0.9*WTAV \quad (4A)$$

$$1.1*WTAV \le WTH \le 100*WTAV \quad (4B)$$

This evaluation of the weight window width is one of many possible.

2.3 Path length optimization

The exponential transformation of a path length is accomplished in MORSE by sampling the number η of mean free paths to the next collision of the particle from the formula:

$$\eta = BIAS * \xi \quad (5)$$

where ξ is a random number taken from the exponential generator. The average path length BIAS(IR,IG) due to the biased distribution , versus the region and energy group, is determined by the parameter PATH(IR,IG):

$$BIAS = 1 / (1 - PATH*DIREC) \quad (6)$$

where DIREC is the cosine between the current particle flight direction and the user-provided preferable direction (towards the detector). For PATH>0 the particle path length η is stretched for DIREC>0 and shortened for DIREC<0. Note that the appropriate weight modification is included in the path transformation procedure.

Assuming some starting value of the parameter PATH, we perform random walk of a batch, recalculating all current path lengths η to the equivalent path lengths η', which correspond to the directions towards the detector (DIREC=1), from the formula:

$$\eta' = \eta * (1 - PATH*DIREC) / (1 - PATH) \qquad (7)$$

Averaging the η' values in each cluster "rg" among those histories only, which have contributed to the detector, we obtain from eq. 6 the new estimate:

$$PATH'(IR,IG) = (\langle\eta'(IR,IG)\rangle - 1) / \langle\eta'(IR,IG)\rangle \qquad (7)$$

As is to be seen, when retrieving the average path length of the successful histories $\langle\eta'\rangle$ greater than one mean free path, the algorithm learns the optimizad value of PATH>1.

3. Results of the test problems

The SLMC algorithm described above was tested on two sample problems taken from the nuclear geophysics area. The cross sections for the two problems were taken from the DLC-31[9] multigroup library, containing data for 37 neutron groups from 19.5 MeV to the thermal range, assumed below 0.4 eV. All the calculations were performed on the CDC-6600/CYBER-73 computer. In the source version of the MORSE -CG[8] code the BANKR subroutine has been modified as the control routine for the learning process, and 5 new subroutines, INROLB (initializes data arrays), RETREVP (retrieves event parameters), AFXEST (estimates adjoint flux), ADAPTBP (reevaluates biasing parameters) and FWRLBP (writes them in the MORSE input format for further runs) have been called from BANKR.

The first model (shown in Fig. 1) consisted of a homogeneous sandstone sphere (the elemental compositions have been taken from Woolson and Gritzner[11]) of radius 100 cm with 19% volume fraction of H_2O. There was a point monoenergetic isotropic source of 2.5

MeV neutrons in the center. For the scoring and the importance sampling purposes, the system was divided into 10 spherical shell regions 10 cm thick each, and the thermal neutron field was analyzed in these regions. The thermal flux results from the ANISN[10] code with P_3 order cross section expansion, S_8 angular quadrature and 50 radial intervals were obtained for comparison. Both the MORSE-CG and ANISN results have been averaged over the region volumes.

The results of the first sample problem are given in Tab. 1. The first column of the table contains limits of the detection regions (3,5,7 and 9). The next columns contain the thermal neutron flux in [$n*cm^{-2}*s^{-1}$] per unit source neutron, calculated by ANISN (column 2) and by MORSE (columns 3-5). The results in column 3 were obtained from the original version of MORSE, without implementation of the SLMC algorithm, and with a very crude guess of the biasing parameters: WTH=100.0, WTL=0.05, WTAV=0.2 PATH=0.2 and EPROB=1.0 for all the energy groups, for all the volume regions and for all the detector positions. All the MORSE results in columns 2-4 concern the program runs with similar computing times (about 7 minutes) and for each response in parenthesis we have included the corresponding fractional standard deviation.

The results in column 3 were obtained using the self-learning procedure described above. Note that the calculations for each of the four detector positions were performed in separate program runs, since the optimal set of biasing parameters, forcing the particle histories to contribute to the response, should ultimately depend on the detector location. The biasing parameters were adjusted after each batch. However, one can argue that in such conditions, when the biasing parameters are not stable between the successive batches, the usual interpretation of the statistical errors is no more valid[4]. Therefore we recorded the final values of the biasing parameters after a number of batches and then we transferred them as the input for the next run based on the fixed values of the parameters. The results obtained are given in the last column of Tab. 1. For the large volume detectors discussed here the SLMC procedure has not

significantly reduced the error limits. Still, much better agreement with the discrete ordinates data has been achieved. Additionally, Tab. 3 presents an example set of the biasing parameters evaluated for the case with the response scored at the distance of 60-70 cm from the source, after 18 batches of 50 particles.

The second test model (Fig. 2) included a borehole of 15 cm diameter, filled up with the borehole fluid, surrounded by two rock media up to 50 cm from the borehole axis, the lower layer made of sandstone and the upper layer made of black shale, both containing 14% volume fraction of the formation fluid. There was an active neutron probe on the borehole axis, containing three cylindrical segments: the first void capsule containing the Am-Be neutron source, then the 15 cm iron filter, and above the ^{3}He neutron counter of 10 cm diameter and 25 cm height. The corresponding response function was the ^{3}He(n,p) reaction cross section in the detector volume. The reaction rate was scored in MORSE using volume-tracklength estimation.

The results of the second test problem are included in Tab. 2. The successive columns of the table provide the value of detector signal, in [^{3}He(n,p) reactions / 1 g ^{3}He / 1 source neutron], the fractional standard deviation σ, the computing time T in c.p.s (central processor second), the number N of histories simulated, the number NEST of estimates made (which is equivalent to the number of particle tracks in the volume of the counter). Since all the results were obtained from the program runs with different numbers of particles simulated and different computing times, the σ^2T products, which are inversely proportional to the computing efficiency , are also included in the last column of the table. The first row of the table shows the results for the first unoptimized run with the biasing parameters fixed on the same values for all regions and energy groups. Then we made trials of the self-learning algorithm switching on the successive variance reduction methods available. One can observe that activating more of the biasing techniques has improved the results, and the last run with all the parameters optimized seems to be the best one, increasing the efficiency by more than a

factor 100. The optimization progress, better than for the first problem, can be explained in this case by the small detector volume. However, the benefit factor could be strongly dependent on the particular problem analyzed and it unfortunately cannot be generalized for further possible applications of the SLMC.

4. Discussion

In the course of this work the self-learning technique has been implemented to the sophisticated Monte Carlo code MORSE and numerical experiments on the well-logging test problems have been made. This seemed to be a promising way to automatically reach a better performance of the particle transport simulation, without the coupling of more computer codes into a complicated system.

For the first test problem, the SLMC results have given a better accuracy than unoptimized MC calculation, when being compared with the responses calculated by ANISN. Unfortunately, progress in the calculational efficiency has still been discouraging. For the second test problem, which is a more realistic model of a borehole measurement, the independent, exact estimate of the calculated signal has not been available for comparison, but the efficiency has significantly been increased. Thus, if further developed and tested, applications of the artificial intelligence techniques can be taken into account as a useful way to improve the MC modeling of nuclear logging tools.

Many theoretical and practical programming problems have been encountered. The basic, statistical limit of the learning process is the lack of information from the phase space regions which had not been passed by successful particle histories during the previous random walk. This problem has been approached by the clusterization procedure, described in section 2.1. The second problem was how to retrieve and process the data necessary to reevaluate the biasing parameters: after each single contribution to the response, after each batch separately, or by gathering all the previous statistics of the relevant event data from the start of run (this way has got the best results for our test). One can

also ask whether to modify all the biasing parameters simultaneously (as we have done), or whether to learn each of them in sequence, temporarily leaving other parameters constant. The open question is how a physical problem layout and a user-dependent region arrangement could affect the benefit factors from the SLMC application. Unfortunately, the experience gained from the individual cases does not permit a general answer.

We have also observed the convergence of the optimization procedure and we have searched for convergence criterion. We have found that only a few first iterations of the biasing parameters rapidly improve the variance reduction scheme. The next batches, however, do not significantly influence the mean number of contributions to the detector per one source neutron and they do not favor decreasing of the variance. Also in the similar study by Cramer[3] serious convergence and stability problems have been encountered, and the code generated biasing parameters have been found to be sensitive to the empirically set initial values. Note that the quoted article had still not been available to the author of this report while performing this work, and Cramer's observations could not be taken into account here.

Let us emphasize that the technique introduced here is directly oriented towards enhancing the particle sampling in the detector region, but it does not necessarily warrant the variance reduction. To achieve this goal, one should try to maintain the particle weight constant or even to make it inversely proportional to the response function when reaching the detector region. Sampling from the biased distributions, to force the occurrence of random walk events in the desired phase space region, should be followed by uncontrolled weight modifications. This undesirable weight oscillations can cause divergence of the statistical errors. All the problems mentioned above are left to be examined during further work on the SLMC.

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Tab. 1

Results of the first test problem (2.5 MeV point isotropic source, sandstone 19% porosity, spherical shell detectors)

Distance R [cm]	Thermal neutron flux [$n*cm^{-2}*s^{-1}$] / 1 source neutron			
	ANISN	MORSE[a]	MORSE[b]	MORSE[c]
20. - 30.	5.17-4*	4.85-4(.17)**	4.94-4(.04)	5.05-4(.07)
40. - 50.	9.33-5	8.66-5(.10)	7.91-5(.12)	9.11-5(.13)
60. - 70.	1.25-5	7.87-6(.38)	1.42-5(.40)	9.16-6(.40)
80. - 90.	1.46-6	5.05-7(.55)	2.75-7(.63)	8.89-7(.35)

(a) without the self-learning algorithm

(b) using the self-learning algorithm on-line

(c) using the optimized and then fixed biasing parameters

(*) read as $5.17*10^{-4}$

(**) the fractional standard deviation 0.17 was obtained, for the 7 minutes computation time (similar for all cases)

Tab. 2

Results of the second test problem (Am-Be source, ^{3}He counter, 15 cm diameter borehole, stratified sandstone/black shale rock)

Biasing techniques optimized	Detector counts $^{3}He(n,p)$ F	Fractional standard deviation σ	Computing time [s] T	Number of histories NSOUR	Number of estimates NEST	Inverse of efficiency $\sigma^2 T$
-	2.44	0.91	649	500	30	189.
RSI	1.96	0.66	184	180	7	91.3
ERSI	3.69	0.63	118	200	4	48.2
EARS	4.20	0.35	190	150	45	23.3
EARSI	2.36	0.24	207	150	31	11.9
EARSIP	1.67	0.08	191	100	19	1.2

R - Russian roulette
A - source angular biasing
P - path length transformation
S - splitting
E - source energy biasing
I - post-collision energy importance sampling

Tab. 3

Example set of learned biasing parameters from the first test problem (thermal flux response at 65 cm from the 2.5 MeV source), after 18 batches of 50 particles

IR	IG	NEST	RESP	EPROB	WTH	WTL	WTA	XNU
1	1 - 37	142	94.3	51.9	182.	.216	1.82	.494
2	1 - 18	65	78.9	38.1	206.	.180	2.07	.391
2	19 - 37	334	81.8	51.0	160.	.116	1.60	-.143
3	1 - 18	50	88.4	29.7	231.	.202	2.98	.214
3	10 - 37	502	81.6	32.6	250.	.135	2.50	-.261
4	1 - 18	29	109.	24.9	284.	.260	4.37	.632
4	19 - 37	389	94.8	41.3	230.	.235	2.30	.045
5	1 - 18	28	108.	26.0	284.	.260	4.17	.544
5	19 - 20	3	311.	76.4	7.10	1.11	4.07	.391
5	21 - 23	11	177.	20.9	100.	2.77	8.47	.276
5	24	4	4.26	3.87	37.5	.505	1.10	.359
5	25 - 37	357	82.0	48.3	170.	.118	1.70	-.014
6	1 - 18	24	111.	38.0	47.3	1.52	2.92	.382
6	19	5	73.0	45.6	32.1	.755	1.60	.382
6	20	2	180.	68.2	5.50	1.73	3.63	.306
6	21	3	3.08	1.67	3.17	1.31	1.85	.727
6	22	13	18.2	20.8	12.6	.354	.873	.360
6	23	10	23.1	26.0	9.19	.499	.887	.153
6	24	15	74.1	47.2	29.9	.684	1.57	.497
6	25 - 26	4	43.0	33.9	5.83	.589	1.27	.182
6	27	13	84.4	66.6	31.9	.726	1.27	.371
6	28 - 29	12	104.	84.0	2.71	.902	1.24	.596
6	30	8	75.1	63.6	33.3	.599	1.18	.382
6	31	21	102.	77.8	63.4	.620	1.31	.342
6	32	20	94.8	46.0	16.3	1.13	2.06	.723
6	33	12	35.7	20.2	17.9	.294	1.77	.293
6	34	30	50.0	41.6	28.1	.258	1.20	.413
6	35	31	50.2	31.0	23.2	.263	1.62	-.041
6	36	6	23.8	13.1	4.54	.621	1.82	-.166
6	37	175	149.	77.9	192.	.399	1.92	.388

IR, IG - the volume region and the energy group range

NEST, RESP - the number of estimates and the response contributed

WTH, WTL, WTA - the upper, lower and mean weight standards

EPROB - the downscattered group importance

XNU - parameter of the path length transformation

Starting values : WTH=100., WTL=0.05, WTAV=0.2, XNU=0.2, EPROB=1.0

Fig. 1

Geometrical model of the test problem 1.

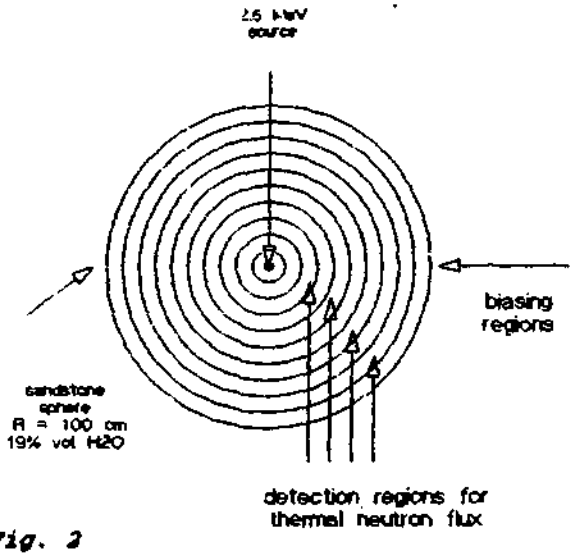

Fig. 2

Geometrical model of the test problem 2.